

# User Documentation for KINSOL v6.6.2

SUNDIALS v6.6.2

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# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Historical Background . . . . .	1
1.2	Changes from previous versions . . . . .	2
1.3	Reading this User Guide . . . . .	22
1.4	SUNDIALS License and Notices . . . . .	23
1.5	Acknowledgments . . . . .	24
<b>2</b>	<b>Mathematical Considerations</b>	<b>25</b>
2.1	Basic Newton iteration . . . . .	25
2.2	Newton method variants . . . . .	26
2.3	Jacobian information update strategy . . . . .	26
2.4	Scaling . . . . .	27
2.5	Globalization strategy . . . . .	27
2.6	Nonlinear iteration stopping criteria . . . . .	28
2.7	Additional constraints . . . . .	28
2.8	Residual monitoring for Modified Newton method . . . . .	28
2.9	Stopping criteria for iterative linear solvers . . . . .	29
2.10	Difference quotient Jacobian approximations . . . . .	29
2.11	Basic Fixed Point iteration . . . . .	30
2.12	Anderson Acceleration . . . . .	30
2.13	Anderson Acceleration QR Factorization . . . . .	31
2.14	Fixed-point - Anderson Acceleration Stopping Criterion . . . . .	32
2.15	Picard - Anderson Acceleration Stopping Criterion . . . . .	32
<b>3</b>	<b>Code Organization</b>	<b>33</b>
3.1	KINSOL organization . . . . .	33
<b>4</b>	<b>Using SUNDIALS</b>	<b>37</b>
4.1	The SUNContext Type . . . . .	37
4.2	SUNDIALS Status Logging . . . . .	42
4.3	Performance Profiling . . . . .	46
4.4	SUNDIALS Version Information . . . . .	49
4.5	SUNDIALS Fortran Interface . . . . .	50
4.6	Features for GPU Accelerated Computing . . . . .	58
<b>5</b>	<b>Using KINSOL for the Solution of Nonlinear Systems</b>	<b>61</b>
5.1	Access to library and header files . . . . .	61
5.2	Data Types . . . . .	62
5.3	Header files . . . . .	64
5.4	A skeleton of the user's main program . . . . .	64
5.5	User-callable functions . . . . .	66
5.6	User-supplied functions . . . . .	93
5.7	A parallel band-block-diagonal preconditioner module . . . . .	98

5.8	Alternative to KINSOL for difficult systems . . . . .	102
<b>6</b>	<b>Vector Data Structures</b>	<b>103</b>
6.1	Description of the NVECTOR Modules . . . . .	103
6.2	Description of the NVECTOR operations . . . . .	109
6.3	NVECTOR functions used by KINSOL . . . . .	121
6.4	The NVECTOR_SERIAL Module . . . . .	123
6.5	The NVECTOR_PARALLEL Module . . . . .	126
6.6	The NVECTOR_OPENMP Module . . . . .	130
6.7	The NVECTOR_PTHREADS Module . . . . .	133
6.8	The NVECTOR_PARHYP Module . . . . .	137
6.9	The NVECTOR_PETSC Module . . . . .	139
6.10	The NVECTOR_CUDA Module . . . . .	141
6.11	The NVECTOR_HIP Module . . . . .	147
6.12	The NVECTOR_SYCL Module . . . . .	152
6.13	The NVECTOR_RAJA Module . . . . .	157
6.14	The NVECTOR_KOKKOS Module . . . . .	160
6.15	The NVECTOR_OPENMPDEV Module . . . . .	162
6.16	The NVECTOR_TRILINOS Module . . . . .	166
6.17	The NVECTOR_MANYVECTOR Module . . . . .	167
6.18	The NVECTOR_MPIMANYVECTOR Module . . . . .	170
6.19	The NVECTOR_MPIPLUSX Module . . . . .	174
6.20	NVECTOR Examples . . . . .	175
<b>7</b>	<b>Matrix Data Structures</b>	<b>179</b>
7.1	Description of the SUNMATRIX Modules . . . . .	179
7.2	Description of the SUNMATRIX operations . . . . .	181
7.3	The SUNMATRIX_DENSE Module . . . . .	183
7.4	The SUNMATRIX_MAGMADENSE Module . . . . .	186
7.5	The SUNMATRIX_ONEMKLDENSE Module . . . . .	191
7.6	The SUNMATRIX_BAND Module . . . . .	195
7.7	The SUNMATRIX_CUSPARSE Module . . . . .	201
7.8	The SUNMATRIX_SPARSE Module . . . . .	204
7.9	The SUNMATRIX_SLUNRLOC Module . . . . .	210
7.10	The SUNMATRIX_KOKKOSDENSE Module . . . . .	212
7.11	SUNMATRIX Examples . . . . .	215
7.12	SUNMatrix functions used by KINSOL . . . . .	215
<b>8</b>	<b>Linear Algebraic Solvers</b>	<b>217</b>
8.1	The SUNLinearSolver API . . . . .	218
8.2	KINSOL SUNLinearSolver interface . . . . .	230
8.3	The SUNLinSol_Band Module . . . . .	232
8.4	The SUNLinSol_Dense Module . . . . .	234
8.5	The SUNLinSol_KLU Module . . . . .	235
8.6	The SUNLinSol_LapackBand Module . . . . .	239
8.7	The SUNLinSol_LapackDense Module . . . . .	241
8.8	The SUNLinSol_MagmaDense Module . . . . .	242
8.9	The SUNLinSol_OneMklDense Module . . . . .	244
8.10	The SUNLinSol_PCG Module . . . . .	245
8.11	The SUNLinSol_SPBCGS Module . . . . .	250
8.12	The SUNLinSol_SPGMR Module . . . . .	255
8.13	The SUNLinSol_SPGMR Module . . . . .	260
8.14	The SUNLinSol_SPTFQMR Module . . . . .	265
8.15	The SUNLinSol_SuperLUDIST Module . . . . .	270

8.16	The SUNLinSol_SuperLUMT Module . . . . .	273
8.17	The SUNLinSol_cuSolverSp_batchQR Module . . . . .	276
8.18	The SUNLINEARSOLVER_GINKGO Module . . . . .	277
8.19	The SUNLINEARSOLVER_KOKKOSDENSE Module . . . . .	280
8.20	SUNLinearSolver Examples . . . . .	282
<b>9</b>	<b>Tools for Memory Management</b>	<b>283</b>
9.1	The SUNMemoryHelper API . . . . .	283
9.2	The SUNMemoryHelper_Cuda Implementation . . . . .	288
9.3	The SUNMemoryHelper_Hip Implementation . . . . .	290
9.4	The SUNMemoryHelper_Sycl Implementation . . . . .	292
<b>10</b>	<b>SUNDIALS Installation Procedure</b>	<b>295</b>
10.1	CMake-based installation . . . . .	296
10.2	Installed libraries and exported header files . . . . .	318
<b>11</b>	<b>KINSOL Constants</b>	<b>323</b>
11.1	KINSOL input constants . . . . .	323
11.2	KINSOL output constants . . . . .	324
<b>12</b>	<b>Appendix: SUNDIALS Release History</b>	<b>325</b>
	<b>Bibliography</b>	<b>327</b>
	<b>Index</b>	<b>331</b>





# Chapter 1

## Introduction

KINSOL is part of a software family called SUNDIALS: SUite of Nonlinear and Differential/ALgebraic equation Solvers [31]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities.

KINSOL is a general-purpose nonlinear system solver based on Newton-Krylov solver technology. A fixed point iteration is also included with the release of KINSOL v.2.8.0 and higher.

### 1.1 Historical Background

The first nonlinear solver packages based on Newton-Krylov methods were written in Fortran. In particular, the NKSOL package, written at LLNL, was the first Newton-Krylov solver package written for solution of systems arising in the solution of partial differential equations [16]. This Fortran code made use of Newton's method to solve the discrete nonlinear systems and applied a preconditioned Krylov linear solver for solution of the Jacobian system at each nonlinear iteration. The key to the Newton-Krylov method was that the matrix-vector multiplies required by the Krylov method could effectively be approximated by a finite difference of the nonlinear system-defining function, avoiding a requirement for the formation of the actual Jacobian matrix. Significantly less memory was required for the solver as a result.

In the late 1990's, there was a push at LLNL to rewrite the nonlinear solver in C and port it to distributed memory parallel machines. Both Newton and Krylov methods are easily implemented in parallel, and this effort gave rise to the KINSOL package. KINSOL is similar to NKSOL in functionality, except that it provides for more options in the choice of linear system methods and tolerances, and has a more modular design to provide flexibility for future enhancements.

At present, KINSOL may utilize a variety of Krylov methods provided in SUNDIALS. These methods include the GMRES (Generalized Minimal RESidual) [41], FGMRES (Flexible Generalized Minimum RESidual) [40], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [45], TFQMR (Transpose-Free Quasi-Minimal Residual) [27], and PCG (Preconditioned Conjugate Gradient) [30] linear iterative methods. As Krylov methods, these require little matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner, and, for most problems, preconditioning is essential for an efficient solution. For very large nonlinear algebraic 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.

For the sake of completeness in functionality, direct linear system solvers are included in KINSOL. These include methods for both dense and banded linear systems, with Jacobians that are either user-supplied or generated internally by difference quotients. KINSOL also includes interfaces to sparse direct solvers, including KLU [3, 19] and the threaded sparse direct solver, SuperLU\_MT [8, 21, 35], among others (see Chapter §8 for further details).

In the process of translating NKSOL into C, the overall KINSOL organization has been changed considerably. One key feature of the KINSOL organization is that a separate module devoted to vector operations was created. This module facilitated extension to multiprocessor environments with minimal impact on the rest of the solver. The vector module design is shared across the SUNDIALS suite. This `N_Vector` module is written in terms of abstract vector operations with the actual routines attached by a particular implementation (such as serial or parallel) of `N_Vector`. This abstraction 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 KINSOL) is supplied with serial, MPI-parallel, OpenMP and Pthreads thread-parallel `N_Vector` implementations, as well as multiple `N_Vector` implementations designed to leverage GPU architectures (see Chapter §6 for further details).

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

## 1.2 Changes from previous versions

### 1.2.1 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.

### 1.2.2 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.

### 1.2.3 Changes in v6.6.0

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

### 1.2.4 Changes in v6.5.1

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.

### 1.2.5 Changes in v6.5.0

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 the functions `KINGetJac()` and `KINGetJacNumIters()` to assist in debugging simulations utilizing a matrix-based linear solver.

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

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 `FSUNSparseMatrix_IndexPointers` functions. Compiling and running code that uses the SUNDIALS Fortran interfaces with bounds checking will now work.

### 1.2.6 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.

### 1.2.7 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 `SUNMatrix.Ginkgo` and §8.18.

Added new `N_Vector`, dense `SUNMatrix`, and dense `SUNLinearSolver` implementations utilizing the `Kokkos Ecosystem` for performance portability, see sections §6.14, §7.10, 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.

## 1.2.8 Changes in v6.3.0

Added the function `KINGetUserData()` to retrieve the user data pointer provided to `KINSetUserData()`.

Fixed the unituitive 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'.

## 1.2.9 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 `KINSetInfoFile()`, `KINSetDebugFile()`, `SUNNonlinSolSetPrintLevel_Newton()`, `SUNNonlinSolSetInfoFile_Newton()`, `SUNNonlinSolSetPrintLevel_FixedPoint()`, `SUNNonlinSolSetInfoFile_FixedPoint()`, `SUNLinSolSetInfoFile_PCG()`, `SUNLinSolSetPrintLevel_PCG()`, `SUNLinSolSetInfoFile_SPGMR()`, `SUNLinSolSetPrintLevel_SPGMR()`, `SUNLinSolSetInfoFile_SPGFMR()`, `SUNLinSolSetPrintLevel_SPGFMR()`, `SUNLinSolSetInfoFile_SPTFQM()`, `SUNLinSolSetPrintLevel_SPTFQM()`, `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  $\geq 3$ .

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

Added the function `KINPrintAllStats()` to output all of the 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.

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_mpmmanyvector.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`.

## 1.2.10 Changes in v6.1.1

Fixed exported `SUNDIALSConfig.cmake`.

### 1.2.11 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.

### 1.2.12 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 release 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 `SUNMemoryHelper_Copy()` have been updated to accept an opaque handle as the last input. At a minimum, user-defined `SUNMemoryHelper` 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, *hypr*, 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_VSetKernelExecPolicy_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	<code>SUNLinSol_Band()</code>
SUNDenseLinearSolver	<code>SUNLinSol_Dense()</code>
SUNKLU	<code>SUNLinSol_KLU()</code>
SUNKLUReInit	<code>SUNLinSol_KLUReInit()</code>
SUNKLUSetOrdering	<code>SUNLinSol_KLUSetOrdering()</code>
SUNLapackBand	<code>SUNLinSol_LapackBand()</code>
SUNLapackDense	<code>SUNLinSol_LapackDense()</code>
SUNPCG	<code>SUNLinSol_PCG()</code>
SUNPCGSetPrecType	<code>SUNLinSol_PCGSetPrecType()</code>
SUNPCGSetMaxl	<code>SUNLinSol_PCGSetMaxl()</code>
SUNSPBCGS	<code>SUNLinSol_SPBCGS()</code>
SUNSPBCGSSetPrecType	<code>SUNLinSol_SPBCGSSetPrecType()</code>
SUNSPBCGSSetMaxl	<code>SUNLinSol_SPBCGSSetMaxl()</code>
SUNSPFGMR	<code>SUNLinSol_SPFGMR()</code>
SUNSPFGMRSetPrecType	<code>SUNLinSol_SPFGMRSetPrecType()</code>
SUNSPFGMRSetGType	<code>SUNLinSol_SPFGMRSetGType()</code>
SUNSPFGMRSetMaxRestarts	<code>SUNLinSol_SPFGMRSetMaxRestarts()</code>
SUNSPGMR	<code>SUNLinSol_SPGMR()</code>
SUNSPGMRSetPrecType	<code>SUNLinSol_SPGMRSetPrecType()</code>
SUNSPGMRSetGType	<code>SUNLinSol_SPGMRSetGType()</code>
SUNSPGMRSetMaxRestarts	<code>SUNLinSol_SPGMRSetMaxRestarts()</code>
SUNSPTFQMR	<code>SUNLinSol_SPTFQMR()</code>
SUNSPTFQMRSetPrecType	<code>SUNLinSol_SPTFQMRSetPrecType()</code>
SUNSPTFQMRSetMaxl	<code>SUNLinSol_SPTFQMRSetMaxl()</code>
SUNSuperLUMT	<code>SUNLinSol_SuperLUMT()</code>
SUNSuperLUMTSetOrdering	<code>SUNLinSol_SuperLUMTSetOrdering()</code>

## KINSOL

New orthogonalization methods were added for use within the KINSOL Anderson acceleration routine. See §2.13 and `KINSetOrthAA()` for more details.

The KINSOL 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
KINDlsSetLinearSolver	KINSetLinearSolver
KINDlsSetJacFn	KINSetJacFn
KINDlsGetWorkSpace	KINGetLinWorkSpace
KINDlsGetNumJacEvals	KINGetNumJacEvals
KINDlsGetNumFuncEvals	KINGetNumLinFuncEvals
KINDlsGetLastFlag	KINGetLastLinFlag
KINDlsGetReturnFlagName	KINGetLinReturnFlagName
KINSpilsSetLinearSolver	KINSetLinearSolver
KINSpilsSetPreconditioner	KINSetPreconditioner
KINSpilsSetJacTimesVecFn	KINSetJacTimesVecFn
KINSpilsGetWorkSpace	KINGetLinWorkSpace
KINSpilsGetNumPrecEvals	KINGetNumPrecEvals
KINSpilsGetNumPrecSolves	KINGetNumPrecSolves
KINSpilsGetNumLinIters	KINGetNumLinIters
KINSpilsGetNumConvFails	KINGetNumLinConvFails

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Table 1.1 – continued from previous page

Deprecated Name	New Name
KINSpilsGetNumJtimesEvals	KINGetNumJtimesEvals
KINSpilsGetNumFuncEvals	KINGetNumLinFuncEvals
KINSpilsGetLastFlag	KINGetLastLinFlag
KINSpilsGetReturnFlagName	KINGetLinReturnFlagName
DenseGETRF	SUNDlsMat_DenseGETRF
DenseGETRS	SUNDlsMat_DenseGETRS
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

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Table 1.1 – continued from previous page

Deprecated Name	New Name
<code>newBandMat</code>	<code>SUNDlsMat_newBandMat</code>
<code>destroyMat</code>	<code>SUNDlsMat_destroyMat</code>
<code>newIntArray</code>	<code>SUNDlsMat_newIntArray</code>
<code>newIndexArray</code>	<code>SUNDlsMat_newIndexArray</code>
<code>newRealArray</code>	<code>SUNDlsMat_newRealArray</code>
<code>destroyArray</code>	<code>SUNDlsMat_destroyArray</code>

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.

### 1.2.13 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.

A new `SUNMatrix` and `SUNLinearSolver` implementation 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.

New KINSOL options have been added to apply a constant damping in the fixed point and Picard iterations (see `KINSetDamping`), to delay the start of Anderson acceleration with the fixed point and Picard iterations (see `KINSetDelayAA`), and to return the newest solution with the fixed point iteration (see `KINSetReturnNewest`).

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.

A bug was fixed in the Picard iteration where the value of `KINSetMaxSetupCalls` would be ignored.

### 1.2.14 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.

A new `SUNMatrix` and `SUNLinearSolver` implementation 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.

### 1.2.15 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.

### 1.2.16 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.

### 1.2.17 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.

### 1.2.18 Changes in v5.4.0

A new API, `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 §4.6.1, §6.10, §6.13, and §9 for more information.

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

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

Added support for CUDA v11.

### 1.2.19 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 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 `NVECTOR_CUDA` 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 performance 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 CMake option `SUNDIALS_BUILD_WITH_MONITORING` to use these capabilities.

Added the optional function `KINSetJacTimesVecSysFn` to specify an alternative system function for computing Jacobian-vector products with the internal difference quotient approximation.

### 1.2.20 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`, `xl f2003`, or `xl f2003_r`.

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

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

### 1.2.21 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 when using Anderson acceleration. See §2 and the description of the `KINSetDampingAA` function for more details.

## 1.2.22 Changes in v5.0.0

### 1.2.22.1 Build system changes

- Increased the minimum required CMake version to 3.5 for most SUNDIALS configurations, and 3.10 when CUDA or OpenMP with device offloading are enabled.
- The CMake option `BLAS_ENABLE` and the variable `BLAS_LIBRARIES` have been removed to simplify builds as SUNDIALS packages do not use BLAS directly. For third party libraries that require linking to BLAS, the path to the BLAS library should be included in the `_LIBRARIES` variable for the third party library *e.g.*, `SUPERLUDIST_LIBRARIES` when enabling `SuperLU_DIST`.
- Fixed a bug in the build system that prevented the `NVECTOR_PTHREADS` module from being built.

### 1.2.22.2 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(w, v)` has been added to copy the operation function pointers between vector objects. When used in clone routines for custom vector objects these functions also will ease the introduction of any new optional operations to the `N_Vector` API by ensuring all operations are copied when cloning objects. See §6.1.1 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, `N_VGetLength`, returns the global length of an `N_Vector`. The optional operations have been added to support the new `NVECTOR_MPIMANYVECTOR` implementation. The operation `N_VGetCommunicator` must be implemented by subvectors that are combined to create an `NVECTOR_MPIMANYVECTOR`, but is not used outside of this context. The remaining nine operations are optional local reduction operations intended to eliminate unnecessary latency when performing vector reduction operations (norms, etc.) on distributed memory systems. The optional local reduction vector operations are `N_VDotProdLocal`, `N_VMaxNormLocal`, `N_VMinLocal`, `N_VL1NormLocal`, `N_VWSqrSumLocal`, `N_VWSqrSumMaskLocal`, `N_VInvTestLocal`, `N_VConstrMaskLocal`, and `N_VMinQuotientLocal`. If an `N_Vector` implementation defines any of the local operations as `NULL`, then the `NVECTOR_MPIMANYVECTOR` will call standard `N_Vector` operations to complete the computation. See §6.2.4 for more details.
- 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 `*_MPICuda` and `*_MPIRaja` functions have been removed from the `NVECTOR_CUDA` and `NVECTOR_RAJA` implementations respectively. Accordingly, the `nvector_mpicuda.h`, `nvector_mpiraja.h`, `libsundials_nvecmpicuda.lib`, and `libsundials_nvecmpicudaraja.lib` files have been removed. Users should use the `NVECTOR_MPIPLUSX` module coupled in conjunction with the `NVECTOR_CUDA` or `NVECTOR_RAJA` modules to replace the functionality. The necessary changes are minimal and should require few code modifications. See the programs in `examples/ida/mpicuda` and `examples/ida/mpiraja` for examples of how to use the `NVECTOR_MPIPLUSX` module with the `NVECTOR_CUDA` and `NVECTOR_RAJA` modules respectively.
- Fixed a memory leak in the `NVECTOR_PETSC` module clone function.

- Made performance improvements to the `NVECTOR_CUDA` module. Users who utilize a non-default stream should no longer see default stream synchronizations after memory transfers.
- Added a new constructor to the `NVECTOR_CUDA` module that allows a user to provide custom allocate and free functions for the vector data array and internal reduction buffer. See §6.10.1 for more details.
- Added new Fortran 2003 interfaces for most `N_Vector` modules. See Chapter §6 for more details on how to use the interfaces.
- Added three new `N_Vector` utility functions, `FN_VGetVecAtIndexVectorArray`, `FN_VSetVecAtIndexVectorArray`, and `FN_VNewVectorArray`, for working with `N_Vector` arrays when using the Fortran 2003 interfaces. See §6.1.1 for more details.

### 1.2.22.3 SUNMatrix module changes

- Two new functions were added to aid in creating custom `SUNMatrix` objects. The constructor `SUNMatNewEmpty` allocates an “empty” generic `SUNMatrix` with the object’s content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the `SUNMatrix` API by ensuring only required operations need to be set. Additionally, the function `SUNMatCopyOps(A, B)` has been added to copy the operation function pointers between matrix objects. When used in clone routines for custom matrix objects these functions also will ease the introduction of any new optional operations to the `SUNMatrix` API by ensuring all operations are copied when cloning objects. See §7.1 for more details.
- A new operation, `SUNMatMatvecSetup`, was added to the `SUNMatrix` API to perform any setup necessary for computing a matrix-vector product. This operation is useful for `SUNMatrix` implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product. Users who have implemented custom `SUNMatrix` modules will need to at least update their code to set the corresponding ops structure member, `matvecsetup`, to `NULL`. See §7.2 for more details.
- The generic `SUNMatrix` API now defines error codes to be returned by `SUNMatrix` operations. Operations which return an integer flag indicating success/failure may return different values than previously. See §7.2.1 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 Chapter §7 for more details on how to use the interfaces.

### 1.2.22.4 SUNLinearSolver module changes

- A new function was added to aid in creating custom `SUNLinearSolver` objects. The constructor `SUNLinSolNewEmpty` allocates an “empty” generic `SUNLinearSolver` 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 `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 `SUNLinSolLastFlag` has changed from `long int` to `sunindextype` to be consistent with the type used to store row indices in dense and banded linear solver modules.
- Added a new optional operation to the `SUNLinearSolver` API, `SUNLinSolGetID`, that returns a `SUNLinearSolver_ID` 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_batchQR`, which leverages the NVIDIA cuSOLVER sparse batched QR method for efficiently solving block diagonal linear systems on NVIDIA GPUs. See §8.17 for more details.
- Added three new accessor functions to the `SUNLINSOL_KLU` module, `SUNLinSol_KLUGetSymbolic`, `SUNLinSol_KLUGetNumeric`, and `SUNLinSol_KLUGetCommon`, to provide user access to the underlying KLU solver structures. See §8.5.1 for more details.
- Added new Fortran 2003 interfaces for most `SUNLinearSolver` modules. See Chapter §8 for more details on how to use the interfaces.

#### 1.2.22.5 KINSOL changes

- Fixed a bug in the KINSOL linear solver interface where the auxiliary scalar `sJpnorm` was not computed when necessary with the Picard iteration and the auxiliary scalar `sFdotJp` was unnecessarily computed in some cases.
- The KINLS 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`.
- Added a Fortran 2003 interface to KINSOL. See §4.5 for more details.

#### 1.2.23 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.

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

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

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

#### 1.2.24 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 KINSOL library, `libsundials_kinsol`.

#### 1.2.25 Changes in v4.0.1

No changes were made in this release.



### 1.2.26 Changes in v4.0.0

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

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

The names of all constructor routines for SUNDIALS-provided `SUNLinearSolver` implementations have been updated to follow the naming convention `SUNLinSol_*` where `*` is the name of the linear solver. The new names are `SUNLinSol_Band`, `SUNLinSol_Dense`, `SUNLinSol_KLU`, `SUNLinSol_LapackBand`, `SUNLinSol_LapackDense`, `SUNLinSol_PCG`, `SUNLinSol_SPBCGS`, `SUNLinSol_SPGMR`, `SUNLinSol_SPTFQMR`, and `SUNLinSol_SuperLUMT`. Solver-specific "set" routine names have been similarly standardized. To minimize challenges in user migration to the new names, the previous routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon. All KINSOL example programs and the standalone linear solver examples have been updated to use the new naming convention.

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

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 Chapter §6 for more details). The new operations are intended to increase data reuse in vector operations, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. The fused operations are `N_VLinearCombination`, `N_VScaleAddMulti`, and `N_VDotProdMulti` and the vector array operations are `N_VLinearCombinationVectorArray`, `N_VScaleVectorArray`, `N_VConstVectorArray`, `N_VWrmsNormVectorArray`, `N_VWrmsNormMaskVectorArray`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. If an `N_Vector` implementation defines any of these operations as `NULL`, then standard `N_Vector` operations will automatically be called as necessary to complete the computation. Multiple updates to `NVECTOR_CUDA` were made:

- Changed `N_VGetLength_Cuda` to return the global vector length instead of the local vector length.
- Added `N_VGetLocalLength_Cuda` to return the local vector length.
- Added `N_VGetMPIComm_Cuda` to return the MPI communicator used.
- Removed the accessor functions in the namespace `suncudavec`.
- Changed the `N_VMake_Cuda` function to take a host data pointer and a device data pointer instead of an `N_VectorContent_Cuda` object.
- Added the ability to set the `cudaStream_t` used for execution of the `NVECTOR_CUDA` kernels. See the function `N_VSetCudaStreams_Cuda`.
- Added `N_VNewManaged_Cuda`, `N_VMakeManaged_Cuda`, and `N_VIsManagedMemory_Cuda` functions to accommodate using managed memory with the `NVECTOR_CUDA`.

Multiple changes to `NVECTOR_RAJA` were made:

- Changed `N_VGetLength_Raja` to return the global vector length instead of the local vector length.
- Added `N_VGetLocalLength_Raja` to return the local vector length.
- Added `N_VGetMPIComm_Raja` to return the MPI communicator used.

- Removed the accessor functions in the namespace `suncudavec`.

A new `N_Vector` implementation for leveraging OpenMP 4.5+ device offloading has been added, `NVECTOR_OPENMPDEV`. See §6.15 for more details.

### 1.2.27 Changes in v3.2.1

The changes in this minor release include the following:

- Fixed a bug in the CUDA `N_Vector` where the `N_VInvTest` operation could write beyond the allocated vector data.
- Fixed library installation path for multiarch systems. This fix changes the default library installation path to `CMAKE_INSTALL_PREFIX/CMAKE_INSTALL_LIBDIR` from `CMAKE_INSTALL_PREFIX/lib`. `CMAKE_INSTALL_LIBDIR` is automatically set, but is available as a CMake option that can be modified.

### 1.2.28 Changes in v3.2.0

Fixed a problem with setting `sunindextype` which would occur with some compilers (e.g. `armclang`) that did not define `__STDC_VERSION__`. Added hybrid MPI/CUDA and MPI/RAJA vectors to allow use of more than one MPI rank when using a GPU system. The vectors assume one GPU device per MPI rank. Changed the name of the RAJA `N_Vector` library to `libsundials_nveccudaraja.lib` from `libsundials_nvecraja.lib` to better reflect that we only support CUDA as a backend for RAJA currently. Several changes were made to the build system:

- CMake 3.1.3 is now the minimum required CMake version.
- Deprecate the behavior of the `SUNDIALS_INDEX_TYPE` CMake option and added the `SUNDIALS_INDEX_SIZE` CMake option to select the `sunindextype` integer size.
- The native CMake FindMPI module is now used to locate an MPI installation.
- If MPI is enabled and MPI compiler wrappers are not set, the build system will check if `CMAKE_  
<language>-COMPILE` can compile MPI programs before trying to locate and use an MPI installation.
- The previous options for setting MPI compiler wrappers and the executable for running MPI programs have been deprecated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPI_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.
- When a Fortran name-mangling scheme is needed (e.g., `ENABLE_LAPACK` is ON) the build system will infer the scheme from the Fortran compiler. If a Fortran compiler is not available or the inferred or default scheme needs to be overridden, the advanced options `SUNDIALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` can be used to manually set the name-mangling scheme and bypass trying to infer the scheme.
- Parts of the main `CMakeLists.txt` file were moved to new files in the `src` and `example` directories to make the CMake configuration file structure more modular.

### 1.2.29 Changes in v3.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using `rpath` by default to locate shared libraries on OSX.
- Fixed Windows specific problem where `sunindextype` was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows `sunindextype` is now defined as the MSVC basic type `__int64`.
- Added sparse SUNMatrix “Reallocate” routine to allow specification of the nonzero storage.



- Updated the KLU SUNLinearSolver module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.
- Updated the “ScaleAdd” and “ScaleAddI” implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum  $I + \gamma J$  manually (with zero entries if needed).
- Changed the LICENSE install path to `instdir/include/sundials`.

### 1.2.30 Changes in v3.1.1

The changes in this minor release include the following:

- Fixed a potential memory leak in the SPGMR and SPFGMR linear solvers: if “Initialize” was called multiple times then the solver memory was reallocated (without being freed).
- Updated KLU SUNLinearSolver module to use a `typedef` for the precision-specific solve function to be used (to avoid compiler warnings).
- Added missing typecasts for some `(void*)` pointers (again, to avoid compiler warnings).
- Bugfix in `sunmatrix_sparse.c` where we had used `int` instead of `sunindextype` in one location.
- Fixed a minor bug in `KINPrintInfo` where a case was missing for `KIN_REPTD_SYSFUNC_ERR` leading to an undefined info message.
- Added missing `#include <stdio.h>` in `N_Vector` and `SUNMatrix` header files.
- Fixed an indexing bug in the CUDA `N_Vector` implementation of `N_VWrmsNormMask` 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 `SUNLinearSolver` module (e.g., iterative linear solvers or fixed pointer solver).

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

### 1.2.31 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 `make` and installing with `make install` respectively.

### 1.2.32 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 the interfacing of 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 DIs and SIs 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: SUNDIALS native dense, SUNDIALS native banded, LAPACK dense, LAPACK band, KLU, SuperLU\_MT, SPGMR, SPBCGS, SPT-FQMR, SPFGMR, and 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 (DIs) 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 DIs/Spils interfaces and `SUNLINEARSOLVER/SUNMATRIX` modules. The exception is CVDIAG, a diagonal approximate Jacobian solver available to CVODE and CVODES.
- Converted all SUNDIALS example problems to utilize new generic `SUNMATRIX` and `SUNLINEARSOLVER` objects, along with updated DIs 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 the web site, <https://software.llnl.gov/RAJA/>. These additions are accompanied by additions to various interface functions and to user documentation.

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

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

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

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

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>.

Added functions `SUNDIALSGetVersion` and `SUNDIALSGetVersionNumber` to get SUNDIALS release version information at runtime.

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 done to correct the `fcmix` name translation for `FKIN_SPFGMR`.

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

### 1.2.33 Changes in v2.9.0

Two additional `N_Vector` implementations were added – one for Hypre (parallel) 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.

The Picard iteration return was changed to always return the newest iterate upon success. A minor bug in the line search was fixed to prevent an infinite loop when the beta condition fails and lambda is below the minimum size.

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

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.

Corrections were made to three Fortran interface functions. The Anderson acceleration scheme was enhanced by use of QR updating.

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.

The functions `FKINCREATE` and `FKININIT` were added to split the `FKINMALLOC` routine into two pieces. `FKINMALLOC` remains for backward compatibility, but documentation for it has been removed.

A new examples was added for use of the OpenMP vector.

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

### 1.2.34 Changes in v2.8.0

Two major additions were made to the globalization strategy options (KINSOL argument `strategy`). One is fixed-point iteration, and the other is Picard iteration. Both can be accelerated by use of the Anderson acceleration method. See the relevant paragraphs in Chapter §2.

Three additions were made to the linear system solvers that are available for use with the KINSOL 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 KINSOL. Finally, a variation of GMRES called Flexible GMRES was added.

Otherwise, only relatively minor modifications were made to KINSOL:

In function `KINStop`, two return values were corrected to make the values of `uu` and `fval` consistent.

A bug involving initialization of `mxnewstep` was fixed. The error affects the case of repeated user calls to `KINSol` with no intervening call to `KINSetMaxNewtonStep`.

A bug in the increments for difference quotient Jacobian approximations was fixed in function `kinDlsBandDQJac`.

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

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

In the `FKINSOL` module, an incorrect return value `ier` in `FKINfunc` was fixed.

In the `FKINSOL` optional input routines `FKINSETIIN`, `FKINSETRIN`, and `FKINSETVIN`, the optional fourth argument `key_length` was removed, with hardcoded key string lengths passed to all `strncmp` tests.

In all `FKINSOL` 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.

### 1.2.35 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 errors have been fixed. Three major logic bugs were fixed – involving updating the solution vector, updating the `linesearch` parameter, and a missing error return. Three minor errors were fixed – involving setting `etachoice` in the Matlab/KINSOL interface, a missing error case in `KINPrintInfo`, and avoiding an exponential overflow in the evaluation of  $\omega$ . In each linear solver interface function, the linear solver memory is freed on an error return, and the `**Free` function now includes a line setting to `NULL` the main memory pointer to the linear solver memory. In the 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.

### 1.2.36 Changes in v2.6.0

This release introduces a new linear solver module, based on BLAS and LAPACK for both dense and banded matrices.

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 already present family of scaled preconditioned iterative linear solvers, the direct solvers, including the new LAPACK-based ones, were also organized into a *direct* family); (b) maintaining a single pointer to user data, optionally specified through a `Set`-type function; (c) a general streamlining of the band-block-diagonal preconditioner module distributed with the solver.

### 1.2.37 Changes in v2.5.0

The main changes in this release involve a rearrangement of the entire SUNDIALS source tree (see §3). 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 <cnode/cnode.h>`). Additional changes were made to the build system: all exported header files are now installed in separate subdirectories of the installation *include* directory.

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

### 1.2.38 Changes in v2.4.0

KINSPBCG, KINSPTFQMR, KINDENSE, and KINBAND modules have been added to interface with the Scaled Preconditioned Bi-CGStab (SPBCG), Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR), DENSE, and BAND linear solver modules, respectively. (For details see Chapter :numref:KINSOL.Usage.CC.) Corresponding additions were made to the Fortran interface module FKINSOL. 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.

Regarding the Fortran interface module FKINSOL, optional inputs are now set using `FKINSETIIN` (integer inputs), `FKINSETRIN` (real inputs), and `FKINSETVIN` (vector inputs). Optional outputs are still obtained from the `IOUT` and `ROUT` arrays which are owned by the user and passed as arguments to `FKINMALLOC`.

The KINDENSE and KINBAND linear solver modules include support for nonlinear residual monitoring which can be used to control Jacobian updating.

To reduce the possibility of conflicts, the names of all header files have been changed by adding unique prefixes (`kinsol_` and `sundials_`). When using the default installation procedure, the header files are exported under various subdirectories of the target `include` directory. For more details see Appendix §10.

### 1.2.39 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. Additionally, to resolve potential variable scope issues, all SUNDIALS solvers release user data right after its use. The build system has been further improved to make it more robust.

### 1.2.40 Changes in v2.2.1

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

### 1.2.41 Changes in v2.2.0

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

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

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

## 1.3 Reading this User Guide

This user guide is a combination of general usage instructions and specific examples. 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 KINSOL. The most casual user, with a small nonlinear system, can get by with reading all of Chapter §2, then Chapter :numref:KINSOL.Usage.CC through §5 only, and looking at examples in [18]. In a different direction, a more expert user with a nonlinear system may want to (a) use a package preconditioner (§5.7), (b) supply his/her own Jacobian or preconditioner routines (§5.6), (c) supply a new `N_Vector` module (Chapter §6), or even (d) supply a different linear solver module (§5.5.2 and Chapter §8).

The structure of this document is as follows:

- In Chapter §2, we provide short descriptions of the numerical methods implemented by KINSOL for the solution of nonlinear systems.
- The following chapter describes the structure of the SUNDIALS suite of solvers (§3) and the software organization of the KINSOL solver (§3.1).
- Chapter :numref:KINSOL.Usage.CC is the main usage document for KINSOL for C applications. It includes a complete description of the user interface for the solution of nonlinear algebraic systems.
- Chapter §6 gives a brief overview of the generic `N_Vector` module shared among the various components of SUNDIALS, and details on the four `N_Vector` implementations provided with SUNDIALS.
- Chapter §7 gives a brief overview of the generic `SUNMatrix` module shared among the various components of SUNDIALS, and details on the `SUNMatrix` implementations provided with SUNDIALS.
- Chapter §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.
- Finally, in the appendices, we provide detailed instructions for the installation of KINSOL, within the structure of SUNDIALS (Appendix §10), as well as a list of all the constants used for input to and output from KINSOL functions (Appendix §11).

Finally, the reader should be aware of the following notational conventions in this user guide: program listings and identifiers (such as `KINInit`) within textual explanations appear in typewriter type style; fields in C structures (such as *content*) appear in italics; and packages or modules are written in all capitals. Usage and

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**Note:** If you are using SUNDIALS with any third party libraries linked in (e.g., LAPACK, KLU, SuperLU\_MT, PETSc, or *hypre*), be sure to review the respective license of the package as that license may have more restrictive terms than the SUNDIALS license. For example, if someone builds SUNDIALS with a statically linked KLU, the build is subject to terms of the more-restrictive LGPL license (which is what KLU is released with) and *not* the SUNDIALS BSD license anymore.

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### **1.4.3 SUNDIALS Release Numbers**

LLNL-CODE-667205 (ARKODE)

UCRL-CODE-155951 (CVODE)

UCRL-CODE-155950 (CVODES)

UCRL-CODE-155952 (IDA)

UCRL-CODE-237203 (IDAS)

LLNL-CODE-665877 (KINSOL)

## **1.5 Acknowledgments**

We wish to acknowledge the contributions to previous versions of the KINSOL code and user guide by Allan G. Taylor.



## Chapter 2

# Mathematical Considerations

KINSOL solves nonlinear algebraic systems in real  $N$ -space.

Using Newton's method, or the Picard iteration, one can solve

$$F(u) = 0, \quad F : \mathbb{R}^N \rightarrow \mathbb{R}^N, \quad (2.1)$$

given an initial guess  $u_0$ . Using a fixed-point iteration, the convergence of which can be improved with Anderson acceleration, one can solve

$$G(u) = u, \quad G : \mathbb{R}^N \rightarrow \mathbb{R}^N, \quad (2.2)$$

given an initial guess  $u_0$ .

### 2.1 Basic Newton iteration

Depending on the linear solver used, KINSOL can employ either an Inexact Newton method [14, 16, 20, 22, 34], or a Modified Newton method. At the highest level, KINSOL implements the following iteration scheme:

1. Set  $u_0$  = an initial guess
2. For  $n = 0, 1, 2, \dots$  until convergence do:
  - a. Solve  $J(u_n)\delta_n = -F(u_n)$
  - b. Set  $u_{n+1} = u_n + \lambda\delta_n, 0 < \lambda \leq 1$
  - c. Test for convergence

Here,  $u_n$  is the  $n$ th iterate to  $u$ , and  $J(u) = F'(u)$  is the system Jacobian. At each stage in the iteration process, a scalar multiple of the step  $\delta_n$ , is added to  $u_n$  to produce a new iterate,  $u_{n+1}$ . A test for convergence is made before the iteration continues.

## 2.2 Newton method variants

For solving the linear system given in step (2a), KINSOL provides several choices, including the option of a user-supplied linear solver module. The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- band direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- sparse direct solver interfaces to various libraries, including KLU [3, 19], SuperLU\_MT [8, 21, 35], SuperLU\_Dist [7, 28, 36, 37], and cuSPARSE [6] [Note that users will need to download and install the relevant external packages independent of KINSOL],
- 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.

When using a direct linear solver, the linear system in 2a is solved exactly, thus resulting in a Modified Newton method (the Jacobian matrix is normally out of date; see below). Note that KINSOL allows the user to enforce a Jacobian evaluation at each iteration thus allowing for an Exact Newton iteration. Note that each direct linear solver is only compatible with a subset of vector representations (see §8.1.7 for details).

When using an iterative linear solver, the linear system in (2a) is solved only approximately, thus resulting in an Inexact Newton method. Here right preconditioning is available by way of the preconditioning setup and solve routines supplied by the user, in which case the iterative method is applied to the linear systems  $(JP^{-1})(P\delta) = -F$ , where  $P$  denotes the right preconditioning matrix.

Additionally, it is possible for users to supply a matrix-based iterative linear solver to KINSOL, resulting in a Modified Inexact Newton method. As with the direct linear solvers, the Jacobian matrix is updated infrequently; similarly as with iterative linear solvers the linear system is solved only approximately.

## 2.3 Jacobian information update strategy

In general, unless specified otherwise by the user, KINSOL strives to update Jacobian information (the actual system Jacobian  $J$  in the case of matrix-based linear solvers, and the preconditioner matrix  $P$  in the case of iterative linear solvers) as infrequently as possible to balance the high costs of matrix operations against other costs. Specifically, these updates occur when:

- the problem is initialized,
- $\|\lambda\delta_{n-1}\|_{D_u,\infty} > 1.5$  (Inexact Newton only),
- `mbset` = 10 nonlinear iterations have passed since the last update,
- the linear solver failed recoverably with outdated Jacobian information,
- the global strategy failed with outdated Jacobian information, or
- $\|\lambda\delta_n\|_{D_u,\infty} < \text{septol}$  with outdated Jacobian or preconditioner information,

where the norm  $\|\cdot\|_{D_u, \infty}$  is defined below in (2.3).

KINSOL allows, through optional solver inputs, changes to the above strategy. Indeed, the user can disable the initial Jacobian information evaluation or change the default value of `mbset`, the number of nonlinear iterations after which a Jacobian information update is enforced.

## 2.4 Scaling

To address the case of ill-conditioned nonlinear systems, KINSOL allows users to prescribe scaling factors both for the solution vector and for the residual vector. For scaling to be used, the user should supply values  $D_u$ , which are diagonal elements of the scaling matrix such that  $D_u u_n$  has all components roughly the same magnitude when  $u_n$  is close to a solution, and  $D_F$ , which are diagonal scaling matrix elements such that  $D_F F$  has all components roughly the same magnitude when  $u_n$  is not too close to a solution. Based on these scaling matrices, we define the following scaled norms:

$$\|z\|_{D_u} = \|D_u z\|_2, \quad \|z\|_{D_F} = \|D_F z\|_2, \quad \|z\|_{D_u, \infty} = \|D_u z\|_\infty, \quad \text{and} \quad \|z\|_{D_F, \infty} = \|D_F z\|_\infty \quad (2.3)$$

where  $\|\cdot\|_\infty$  is the max norm. When scaling values are provided for the solution vector, these values are automatically incorporated into the calculation of the perturbations used for the default difference quotient approximations for Jacobian information; see (2.6) and (2.8) below.

## 2.5 Globalization strategy

Two methods of applying a computed step  $\delta_n$  to the previously computed solution vector are implemented. The first and simplest is the standard Newton strategy which applies step 2(b) as above with  $\lambda$  always set to 1. The other method is a global strategy, which attempts to use the direction implied by  $\delta_n$  in the most efficient way for furthering convergence of the nonlinear problem. This technique is implemented in the second strategy, called Linesearch. This option employs both the  $\alpha$  and  $\beta$  conditions of the Goldstein-Armijo linesearch given in [22] for step 2(b), where  $\lambda$  is chosen to guarantee a sufficient decrease in  $F$  relative to the step length as well as a minimum step length relative to the initial rate of decrease of  $F$ . One property of the algorithm is that the full Newton step tends to be taken close to the solution.

KINSOL implements a backtracking algorithm to first find a value  $\lambda$  such that  $u_n + \lambda \delta_n$  satisfies the sufficient decrease condition (or  $\alpha$ -condition)

$$F(u_n + \lambda \delta_n) \leq F(u_n) + \alpha \nabla F(u_n)^T \lambda \delta_n,$$

where  $\alpha = 10^{-4}$ . Although backtracking in itself guarantees that the step is not too small, KINSOL secondly relaxes  $\lambda$  to satisfy the so-called  $\beta$ -condition (equivalent to Wolfe's curvature condition):

$$F(u_n + \lambda \delta_n) \geq F(u_n) + \beta \nabla F(u_n)^T \lambda \delta_n,$$

where  $\beta = 0.9$ . During this second phase,  $\lambda$  is allowed to vary in the interval  $[\lambda_{min}, \lambda_{max}]$  where

$$\lambda_{min} = \frac{steptol}{\|\bar{\delta}_n\|_\infty}, \quad \bar{\delta}_n^j = \frac{\delta_n^j}{1/D_u^j + |u^j|},$$

and  $\lambda_{max}$  corresponds to the maximum feasible step size at the current iteration (typically  $\lambda_{max} = stepmax / \|\delta_n\|_{D_u}$ ). In the above expressions,  $v^j$  denotes the  $j$ th component of a vector  $v$ .

For more details, the reader is referred to [22].

## 2.6 Nonlinear iteration stopping criteria

Stopping criteria for the Newton method are applied to both of the nonlinear residual and the step length. For the former, the Newton iteration must pass a stopping test

$$\|F(u_n)\|_{D_F, \infty} < \text{ftol} ,$$

where  $\text{ftol}$  is an input scalar tolerance with a default value of  $U^{1/3}$ . Here  $U$  is the machine unit roundoff. For the latter, the Newton method will terminate when the maximum scaled step is below a given tolerance

$$\|\lambda \delta_n\|_{D_u, \infty} < \text{steptol} ,$$

where  $\text{steptol}$  is an input scalar tolerance with a default value of  $U^{2/3}$ . Only the first condition (small residual) is considered a successful completion of KINSOL. The second condition (small step) may indicate that the iteration is stalled near a point for which the residual is still unacceptable.

## 2.7 Additional constraints

As a user option, KINSOL permits the application of inequality constraints,  $u^i > 0$  and  $u^i < 0$ , as well as  $u^i \geq 0$  and  $u^i \leq 0$ , where  $u^i$  is the  $i$ th component of  $u$ . Any such constraint, or no constraint, may be imposed on each component. KINSOL will reduce step lengths in order to ensure that no constraint is violated. Specifically, if a new Newton iterate will violate a constraint, the maximum step length along the Newton direction that will satisfy all constraints is found, and  $\delta_n$  in Step 2(b) is scaled to take a step of that length.

## 2.8 Residual monitoring for Modified Newton method

When using a matrix-based linear solver, in addition to the strategy described above for the update of the Jacobian matrix, KINSOL also provides an optional nonlinear residual monitoring scheme to control when the system Jacobian is updated. Specifically, a Jacobian update will also occur when `mbsetsub=5` nonlinear iterations have passed since the last update and

$$\|F(u_n)\|_{D_F} > \omega \|F(u_m)\|_{D_F} ,$$

where  $u_n$  is the current iterate and  $u_m$  is the iterate at the last Jacobian update. The scalar  $\omega$  is given by

$$\omega = \min \left( \omega_{min} e^{\max(0, \rho-1)}, \omega_{max} \right) , \quad (2.4)$$

with  $\rho$  defined as

$$\rho = \frac{\|F(u_n)\|_{D_F}}{\text{ftol}} ,$$

where  $\text{ftol}$  is the input scalar tolerance discussed before. Optionally, a constant value  $\omega_{const}$  can be used for the parameter  $\omega$ .

The constants controlling the nonlinear residual monitoring algorithm can be changed from their default values through optional inputs to KINSOL. These include the parameters  $\omega_{min}$  and  $\omega_{max}$ , the constant value  $\omega_{const}$ , and the threshold `mbsetsub`.

## 2.9 Stopping criteria for iterative linear solvers

When using an Inexact Newton method (i.e. when an iterative linear solver is used), the convergence of the overall nonlinear solver is intimately coupled with the accuracy with which the linear solver in 2(a) above is solved. KINSOL provides three options for stopping criteria for the linear system solver, including the two algorithms of Eisenstat and Walker [25]. More precisely, the Krylov iteration must pass a stopping test

$$\|J\delta_n + F\|_{D_F} < (\eta_n + U)\|F\|_{D_F},$$

where  $\eta_n$  is one of:

### Eisenstat and Walker Choice 1

$$\eta_n = \frac{|\|F(u_n)\|_{D_F} - \|F(u_{n-1}) + J(u_{n-1})\delta_n\|_{D_F}|}{\|F(u_{n-1})\|_{D_F}},$$

### Eisenstat and Walker Choice 2

$$\eta_n = \gamma \left( \frac{\|F(u_n)\|_{D_F}}{\|F(u_{n-1})\|_{D_F}} \right)^\alpha,$$

where default values of  $\gamma$  and  $\alpha$  are 0.9 and 2, respectively.

### Constant $\eta$

$$\eta_n = \text{constant},$$

with 0.1 as the default.

The default strategy is “Eisenstat and Walker Choice 1”. For both options 1 and 2, appropriate safeguards are incorporated to ensure that  $\eta$  does not decrease too quickly [25].

## 2.10 Difference quotient Jacobian approximations

With the `SUNMATRIX_DENSE` and `SUNMATRIX_BAND` matrix modules, 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

$$J^{ij} = [F^i(u + \sigma_j e^j) - F^i(u)]/\sigma_j. \quad (2.5)$$

The increments  $\sigma_j$  are given by

$$\sigma_j = \sqrt{U} \max \{|u^j|, 1/D_u^j\}. \quad (2.6)$$

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. The parameter  $U$  above can (optionally) be replaced by a user-specified value, `relfunc`.

We note that with sparse and user-supplied matrix-based linear solvers, the Jacobian *must* be supplied by a user routine, i.e. it is not approximated internally within KINSOL.

In the case of a matrix-free iterative linear solver, Jacobian information is needed only as matrix-vector products  $Jv$ . If a routine for  $Jv$  is not supplied, these products are approximated by directional difference quotients as

$$J(u)v \approx [F(u + \sigma v) - F(u)]/\sigma, \quad (2.7)$$

where  $u$  is the current approximation to a root of (2.1), and  $\sigma$  is a scalar. The choice of  $\sigma$  is taken from [16] and is given by

$$\sigma = \frac{\max\{|u^T v|, u_{typ}^T |v|\}}{\|v\|_2^2} \text{sign}(u^T v) \sqrt{U}, \quad (2.8)$$

where  $u_{typ}$  is a vector of typical values for the absolute values of the solution (and can be taken to be inverses of the scale factors given for  $u$  as described below). This formula is suitable for *scaled* vectors  $u$  and  $v$ , and so is applied to  $D_u u$  and  $D_u v$ . The parameter  $U$  above can (optionally) be replaced by a user-specified value, `relfunc`. Convergence of the Newton method is maintained as long as the value of  $\sigma$  remains appropriately small, as shown in [14].

## 2.11 Basic Fixed Point iteration

The basic fixed-point iteration scheme implemented in KINSOL is given by:

1. Set  $u_0$  = an initial guess
2. For  $n = 0, 1, 2, \dots$  until convergence do:
  - Set  $u_{n+1} = (1 - \beta)u_n + \beta G(u_n)$ .
  - Test for convergence.

Here,  $u_n$  is the  $n$ -th iterate to  $u$ . At each stage in the iteration process, the function  $G$  is applied to the current iterate with the damping parameter  $\beta$  to produce a new iterate,  $u_{n+1}$ . A test for convergence is made before the iteration continues.

For Picard iteration, as implemented in KINSOL, we consider a special form of the nonlinear function  $F$ , such that  $F(u) = Lu - N(u)$ , where  $L$  is a constant nonsingular matrix and  $N$  is (in general) nonlinear. Then the fixed-point function  $G$  is defined as  $G(u) = u - L^{-1}F(u)$ . The Picard iteration is given by:

1. Set  $u_0$  = an initial guess
2. For  $n = 0, 1, 2, \dots$  until convergence do:
  - Set  $u_{n+1} = (1 - \beta)u_n + \beta G(u_n)$  where  $G(u_n) \equiv u_n - L^{-1}F(u_n)$ .
  - Test  $F(u_{n+1})$  for convergence.

Here,  $u_n$  is the  $n$ -th iterate to  $u$ . Within each iteration, the Picard step is computed then added to  $u_n$  with the damping parameter  $\beta$  to produce the new iterate. Next, the nonlinear residual function is evaluated at the new iterate, and convergence is checked. Noting that  $L^{-1}N(u) = u - L^{-1}F(u)$ , the above iteration can be written in the same form as a Newton iteration except that here,  $L$  is in the role of the Jacobian. Within KINSOL, however, we leave this in a fixed-point form as above. For more information, see page 182 of [39].

## 2.12 Anderson Acceleration

The Picard and fixed point methods can be significantly accelerated using Anderson's method [10, 26, 38, 46]. Anderson acceleration can be formulated as follows:

1. Set  $u_0$  = an initial guess and  $m \geq 1$
2. Set  $u_1 = G(u_0)$
3. For  $n = 1, 2, \dots$  until convergence do:
  - a. Set  $m_n = \min\{m, n\}$
  - b. Set  $F_n = (f_{n-m_n}, \dots, f_n)$ , where  $f_i = G(u_i) - u_i$

- c. Determine  $\alpha^{(n)} = (\alpha_0^{(n)}, \dots, \alpha_{m_n}^{(n)})$  that solves  $\min_{\alpha} \|F_n \alpha^T\|_2$  such that  $\sum_{i=0}^{m_n} \alpha_i = 1$
- d. Set  $u_{n+1} = \beta \sum_{i=0}^{m_n} \alpha_i^{(n)} G(u_{n-m_n+i}) + (1 - \beta) \sum_{i=0}^{m_n} \alpha_i^{(n)} u_{n-m_n+i}$
- e. Test for convergence

It has been implemented in KINSOL by turning the constrained linear least-squares problem in step 3c into an unconstrained one leading to the algorithm given below:

1. Set  $u_0 =$  an initial guess and  $m \geq 1$
2. Set  $u_1 = G(u_0)$
3. For  $n = 1, 2, \dots$  until convergence do:
  - a. Set  $m_n = \min\{m, n\}$
  - b. Set  $\Delta F_n = (\Delta f_{n-m_n}, \dots, \Delta f_{n-1})$ , where  $\Delta f_i = f_{i+1} - f_i$  and  $f_i = G(u_i) - u_i$
  - c. Determine  $\gamma^{(n)} = (\gamma_0^{(n)}, \dots, \gamma_{m_n-1}^{(n)})$  that solves  $\min_{\gamma} \|f_n - \Delta F_n \gamma^T\|_2$
  - d. Set  $u_{n+1} = G(u_n) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} - (1 - \beta)(f(u_n) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta f_{n-m_n+i})$  with  $\Delta g_i = G(u_{i+1}) - G(u_i)$
  - e. Test for convergence

The least-squares problem in 3c is solved by applying a QR factorization to  $\Delta F_n = Q_n R_n$  and solving  $R_n \gamma = Q_n^T f_n$ . By default the damping is disabled i.e.,  $\beta = 1.0$ .

The Anderson acceleration implementation includes an option to delay the start of acceleration until after a given number of initial fixed-point or Picard iterations have been completed. This delay can be beneficial when the underlying method has strong global convergence properties as the initial iterations may help bring the iterates closer to a solution before starting the acceleration.

## 2.13 Anderson Acceleration QR Factorization

The default QR factorization routine used in Anderson acceleration is Modified Gram-Schmidt, a stable orthogonalization routine that requires an increasing number of synchronizations per iteration dependent upon the number of vectors being orthogonalized against. While practical use of Anderson acceleration only requires a small number of vectors to be used in the QR factorization, this linearly scaling number of synchronizations per iteration can yield poor performance when Anderson acceleration is performed in a parallel setting. To combat this poor performance, low synchronization QR routines are available to the user, in particular: Inverse Compact WY Modified Gram-Schmidt [9], along with variants of Classical Gram-Schmidt with Reorthogonalization [29]. While all of these QR factorization routines are mathematically equivalent, they do not exhibit the same stability when performed with floating point arithmetic or in a parallel setting.

Inverse Compact WY Modified Gram-Schmidt, which is based on triangular solve variants of Gram-Schmidt that were developed within the context of GMRES, is an option that only requires two synchronizations per iteration. Additionally, it adds a lower triangular solve at every iteration, but this generally does not affect performance due to the system solve being small i.e., the number of vectors being orthogonalized against.

The remaining orthogonalization options are based on and include Classical Gram-Schmidt with Reorthogonalization (CGS-2). CGS-2 only requires three synchronizations per iteration, but does not exhibit the same stability as Modified Gram-Schmidt. Classical Gram-Schmidt with Delayed Reorthogonalization has the same stability as CGS-2, but it reduces the number of synchronizations per iteration to two.

## 2.14 Fixed-point - Anderson Acceleration Stopping Criterion

The default stopping criterion is

$$\|u_{n+1} - u_n\|_{D_F, \infty} < \text{gtol},$$

where  $D_F$  is a user-defined diagonal matrix that can be the identity or a scaling matrix chosen so that the components of  $D_F(G(u) - u)$  have roughly the same order of magnitude. Note that when using Anderson acceleration, convergence is checked after the acceleration is applied.

## 2.15 Picard - Anderson Acceleration Stopping Criterion

The default stopping criterion is

$$\|F(u_{n+1})\|_{D_F, \infty} < \text{ftol},$$

where  $D_F$  is a user-defined diagonal matrix that can be the identity or a scaling matrix chosen so that the components of  $D_F F(u)$  have roughly the same order of magnitude. Note that when using Anderson acceleration, convergence is checked after the acceleration is applied.



## 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 KINSOL organization

The KINSOL 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 KINSOL package is shown in [Fig. 3.3](#). KINSOL utilizes generic linear solvers defined by the `SUNLinearSolver` (see §8). As such, KINSOL has no knowledge of the method being used to solve the linear and nonlinear systems that arise. For any given user problem, there exists a single nonlinear solver interface and, if necessary, one of the linear system solver interfaces is specified, and invoked as needed during the integration.

KINSOL has a single unified linear solver interface, `KINSOLLS`, supporting both direct and iterative linear solvers built using the generic `SUNLinearSolver` interface (see §8). These solvers may utilize a `SUNMatrix` object (see §7) for storing Jacobian information, or they may be matrix-free. Since KINSOL can operate on any valid `SUNLinearSolver`,

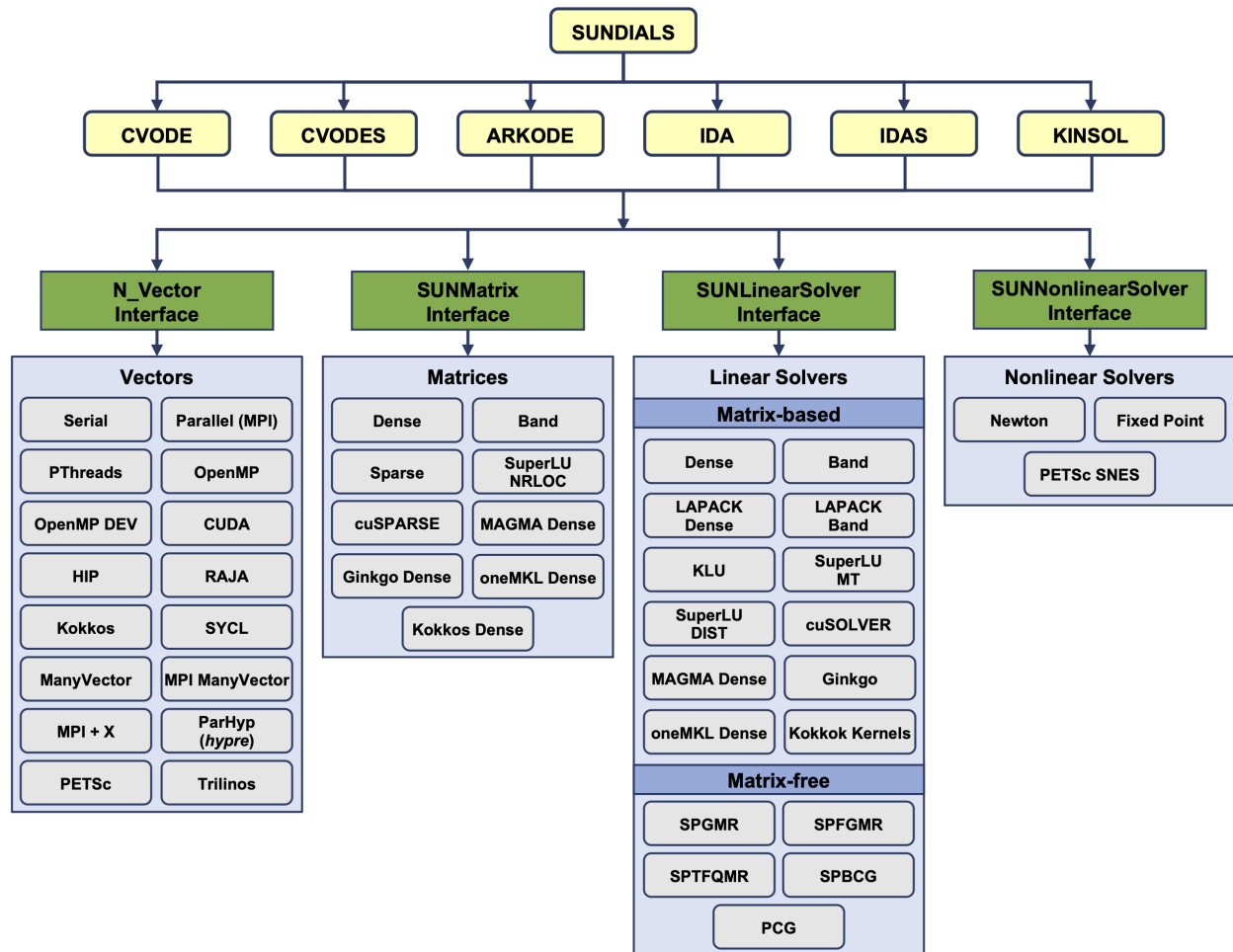


Fig. 3.1: High-level diagram of the SUNDIALS suite.

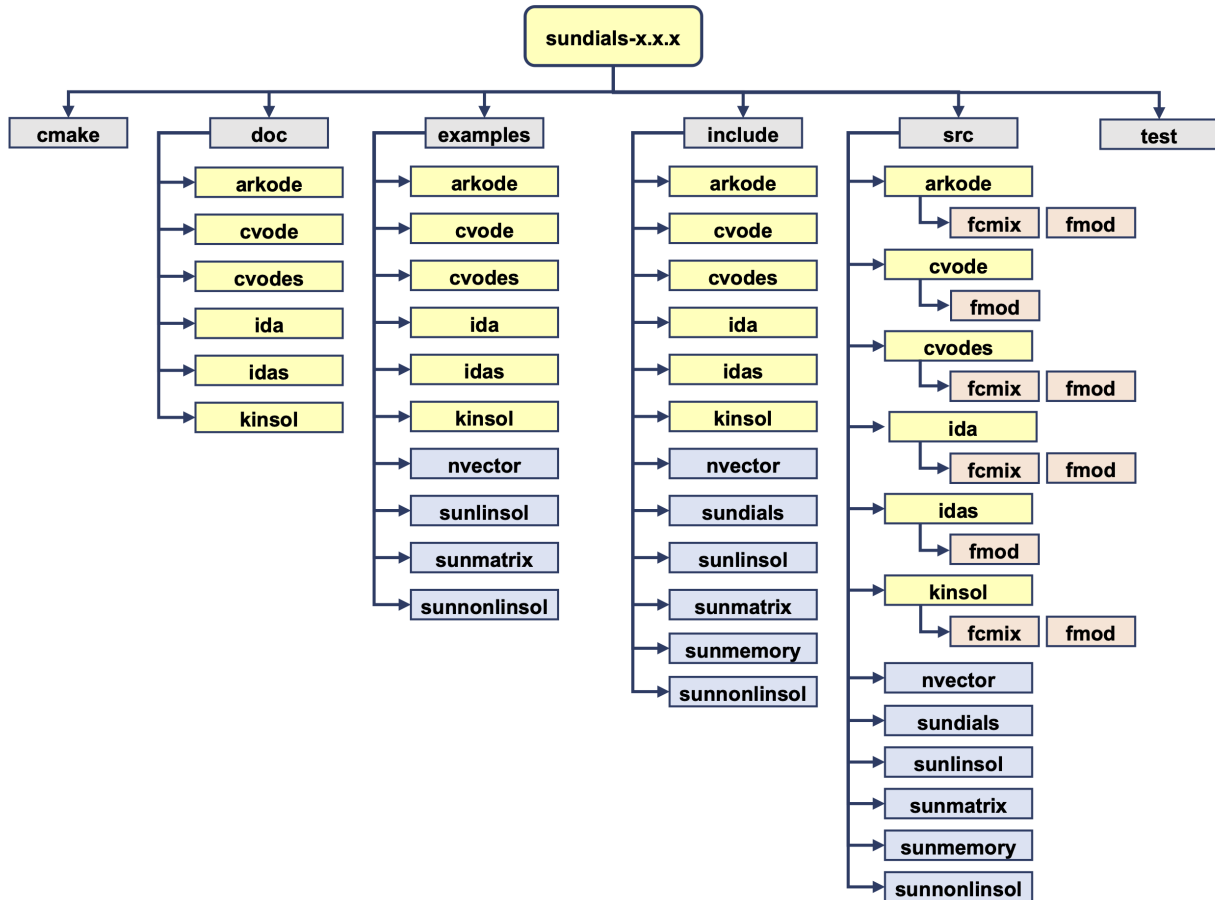


Fig. 3.2: Directory structure of the SUNDIALS source tree.

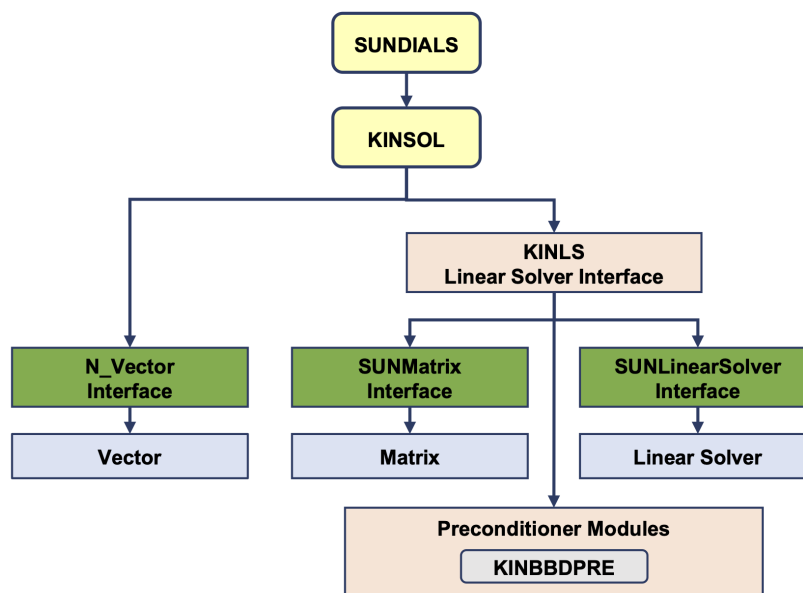


Fig. 3.3: Overall structure diagram of the KINSOL package. Components specific to KINSOL begin with “KINSOL” (KINLS and KINSOLBBDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver interfaces.

the set of linear solver modules available to KINSOL will expand as new `SUNLinearSolver` implementations are developed.

For users employing `SUNMATRIX_DENSE` or `SUNMATRIX_BAND` Jacobian matrices, KINSOL 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, KINSOL includes an algorithm for the approximation by difference quotients of the product  $Jv$ . 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 KINSOL, offer considerable assistance in building preconditioners.

KINSOL'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. The call list within the central KINSOL module to each of the four associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

KINSOL also provides a preconditioner module, for use with any of the Krylov iterative linear solvers. It works in conjunction with the `NVECTOR_PARALLEL` and generates a preconditioner that is a block-diagonal matrix with each block being a banded matrix.

All state information used by KINSOL to solve a given problem is stored in `N_Vector` instances. There is no global data in the KINSOL package, and so, in this respect, it is reentrant. State information specific to the linear and nonlinear solver are saved in the `SUNLinearSolver` and `SUNNonlinearSolver` instances respectively. The reentrancy of KINSOL enables the setting where two or more problems are solved by intermixed or parallel calls to different instances of 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 suncctx;  
void* package_mem;  
N_Vector x;  
  
SUNContext_Create(NULL, &suncctx);
```

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```
package_mem = CNodeCreate(..., 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 ccode_initialized[num_threads];
void* ccode_mem[num_threads];

// Create
for (int i = 0; i < num_threads; i++) {
    sunctxs[i] = SUNContext_Create(...);
    ccode_mem[i] = CCodeCreate(..., sunctxs[i]);
    ccode_initialized[i] = 0; // not yet initialized
    // set optional ccode inputs...
}

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

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```
int tid = omp_get_thread_num();
if (!ccode_initialized[tid]) {
    retval = CCodeInit(ccode_mem[tid], ...);
    ccode_initialized[tid] = 1;
} else {
    retval = CCodeReInit(ccode_mem[tid], ...);
}
CCode(ccode_mem[i], ...);
}

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

Since each thread has its own unique CCODE 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* ccode_mem;
    SUNContext sunctx;

    sunctx = SUNContext_Create(...);
    ccode_mem = CCodeCreate(..., sunctx);
    retval = CCodeInit(ccode_mem, ...);

    // set optional ccode inputs...

    CCode(ccode_mem, ...);

    // get optional ccode outputs...

    CCodeFree(&ccode_mem);
    SUNContext_Free(&sunctx);
}
```

So long as the overhead of creating/destroying the CCODE 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 CCODE create/free routines.



### 4.1.2 Convenience class for C++ Users

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

```
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 `SUNDIALS_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 §10.

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 debug-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 [13] 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 §10.

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 *SUNPROFILER\_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.

**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\_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");
```

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```

umax = N_VMaxNorm(u);
PrintHeader(reltol, abstol, umax);
for(iout=1, tout=T1; iout <= NOUT; iout++, tout += DTOUT) {
    retval = CCode(cvode_mem, tout, u, &t, CV_NORMAL);
    umax = N_VMaxNorm(u);
    retval = CCodeGetNumSteps(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`, and `SUNLinearSolver`) 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`, and `SUNLinearSolver` classes is given alongside the C documentation (§6, §7, and §8, respectively). For details on where the Fortran 2003 module (`.mod`) files and libraries are installed see §10.

The Fortran 2003 interface modules were generated with SWIG Fortran [33], 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	<code>farkode_mod</code>
ARKODE::ARKSTEP	<code>farkode_arkstep_mod</code>

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Table 4.1 – continued from previous page

<b>Class/Module</b>	<b>Fortran 2003 Module Name</b>
ARKODE::ERKSTEP	farkode_erkstep_mod
ARKODE::MRISTEP	farkode_mrimestep_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
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_spgmrs_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 `real` type 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	<code>real(c_double)</code>
int	in, inout, out, return	<code>integer(c_int)</code>
long	in, inout, out, return	<code>integer(c_long)</code>
booleantype	in, inout, out, return	<code>integer(c_int)</code>
realtype	in, inout, out, return	<code>real(c_double)</code>
sunindextype	in, inout, out, return	<code>integer(c_long)</code>
double*	in, inout, out	<code>real(c_double), dimension(*)</code>
double*	return	<code>real(c_double), pointer, dimension(:)</code>
int*	in, inout, out	<code>real(c_int), dimension(*)</code>
int*	return	<code>real(c_int), pointer, dimension(:)</code>
long*	in, inout, out	<code>real(c_long), dimension(*)</code>
long*	return	<code>real(c_long), pointer, dimension(:)</code>
realtype*	in, inout, out	<code>real(c_double), dimension(*)</code>
realtype*	return	<code>real(c_double), pointer, dimension(:)</code>
sunindextype*	in, inout, out	<code>real(c_long), dimension(*)</code>
sunindextype*	return	<code>real(c_long), pointer, dimension(:)</code>
realtype[]	in, inout, out	<code>real(c_double), dimension(*)</code>
sunindextype[]	in, inout, out	<code>integer(c_long), dimension(*)</code>
N_Vector	in, inout, out	<code>type(N_Vector)</code>
N_Vector	return	<code>type(N_Vector), pointer</code>
SUNMatrix	in, inout, out	<code>type(SUNMatrix)</code>
SUNMatrix	return	<code>type(SUNMatrix), pointer</code>
SUNLinearSolver	in, inout, out	<code>type(SUNLinearSolver)</code>
SUNLinearSolver	return	<code>type(SUNLinearSolver), pointer</code>
SUNNonlinearSolver	in, inout, out	<code>type(SUNNonlinearSolver)</code>
SUNNonlinearSolver	return	<code>type(SUNNonlinearSolver), pointer</code>
FILE*	in, inout, out, return	<code>type(c_ptr)</code>
void*	in, inout, out, return	<code>type(c_ptr)</code>
T**	in, inout, out, return	<code>type(c_ptr)</code>
T***	in, inout, out, return	<code>type(c_ptr)</code>
T****	in, inout, out, return	<code>type(c_ptr)</code>

## 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 *ccode_mem;

ierr = CCodeSetUserData(ccode_mem, udata);
```

Fortran code:

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

ierr = FARKStepSetUserData(arkcode_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

! Dissociate 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 dissociated 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);

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

Fortran code:

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

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

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```
! 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:

```

1  integer(c_int) function ff(t, yvec, ydotvec, user_data) &
2      result(ierr) bind(C)
3
4      use, intrinsic :: iso_c_binding
5      use fsundials_nvector_mod
6      implicit none
7
8      real(c_double) :: t ! <===== Missing value attribute
9      type(N_Vector) :: yvec
10     type(N_Vector) :: ydotvec
11     type(c_ptr)     :: user_data
12
13     real(c_double) :: e
14     real(c_double) :: u, v
15     real(c_double) :: tmp1, tmp2
16     real(c_double), pointer :: yarr(:)
17     real(c_double), pointer :: ydotarr(:)
18
19     ! get N_Vector data arrays
20     yarr => FN_VGetArrayPointer(yvec)
21     ydotarr => FN_VGetArrayPointer(ydotvec) ! <===== SEGFAULTS HERE
22
23     ! extract variables
24     u = yarr(1)
25     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

```

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```

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, and §8) 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 [12], 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 4.5 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`, or `SUNLinearSolver` implementation, and the capabilities will be leveraged since SUNDIALS operates on data through these APIs.

In addition, SUNDIALS provides a memory management helper module (see §9) 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
<i>NVECTOR_CUDA</i>	X			X	X
<i>NVECTOR_HIP</i>	X	X		X	X
<i>NVECTOR_SYCL</i>	X <sup>3</sup>	X <sup>3</sup>	X	X	X
<i>NVECTOR_RAJA</i>	X	X	X	X	X
<i>NVECTOR_KOKKOS</i>	X	X	X	X	X
<i>NVECTOR_OPENMPDEV</i>	X	X <sup>2</sup>	X <sup>2</sup>	X	

Table 4.4: List of SUNDIALS GPU-enabled SUNMatrix Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
<i>SUNMATRIX_CUSPARSE</i>	X			X	X
<i>SUNMATRIX_ONEMKLDENSE</i>	X <sup>3</sup>	X <sup>3</sup>	X	X	X
<i>SUNMATRIX_MAGMADENSE</i>	X	X		X	X
<i>SUNMATRIX_GINKGO</i>	X	X		X	X
<i>SUNMATRIX_KOKKOSDENSE</i>	X	X		X	X

Table 4.5: List of SUNDIALS GPU-enabled SUNLinearSolver Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
<i>SUNLINSOL_CUSOLVERSP</i>	X			X	X
<i>SUNLINSOL_ONEMKLDENSE</i>	X <sup>3</sup>	X <sup>3</sup>	X	X	X
<i>SUNLINSOL_MAGMADENSE</i>	X			X	X
<i>SUNLINSOL_GINKGO</i>	X	X		X	X
<i>SUNLINSOL_KOKKOSDENSE</i>	X	X		X	X
<i>SUNLINSOL_SPGMR</i>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>
<i>SUNLINSOL_SPFGMR</i>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>
<i>SUNLINSOL_SPTFQMR</i>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>
<i>SUNLINSOL_SPBCGS</i>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>
<i>SUNLINSOL_PCG</i>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>	X <sup>1</sup>

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 evaluation function, or the preconditioner evaluation 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 KINSOL for the Solution of Nonlinear Systems

This section is concerned with the use of KINSOL for the solution of nonlinear systems.

The following sections treat the header files and the layout of the user's main program, and provide descriptions of the KINSOL user-callable functions and user-supplied functions. The sample programs described in the companion document [18] 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 KINSOL package.

KINSOL uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in §11.

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

### 5.1 Access to library and header files

At this point, it is assumed that the installation of KINSOL, following the procedure described in §10, 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 KINSOL. The relevant library files are

```
<libdir>/libsundials_kinsol.<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>/kinsol  
<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` or `<instdir>/lib64` and `<instdir>/include`, respectively, where `instdir` is the directory where SUNDIALS was installed (see §10).

## 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 §10.1.2).

## 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 §10.1.2).

## 5.2.3 Boolean type

### type `boolean_type`

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

The advantage of using the name `boolean_type` (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 `boolean_type` 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:

- `kinsol/kinsol.h` the main header file for kinsol, which defines the types and various constants, and includes function prototypes. This includes the header file for KINLS, `kinsol/kinsol_ls.h`.

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

The calling program must also include an `N_Vector` implementation header file, of the form `nvector/nvector_*.h` (see §6 for more information). This file in turn includes the header file `sundials_nvector.h` which defines the abstract vector data type.

If using a Newton or Picard nonlinear solver that requires the solution of a linear system, then a linear solver module header file will be required. If the linear solver is matrix-based, the linear solver header will also include a header file of the form `sunmatrix/sunmatrix_*.h` where `*` is the name of the matrix implementation compatible with the linear solver. The matrix header file provides access to the relevant matrix functions/macros and in turn includes the header file `sundials_matrix.h` which defines the abstract matrix data type.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the example `kinFood-Web_kry_p` (see [18]), preconditioning is done with a block-diagonal matrix. For this, even though the `SUNLINSOL-SPGMR` linear solver is used, the header `sundials/sundials_dense.h` is included for access to the underlying generic dense matrix arithmetic routines.

## 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 solution of a nonlinear system problem.. Most of the steps are independent of the `N_Vector`, `SUNMatrix`, and `SUNLinearSolver` implementations used. For the steps that are not, refer to §6, §7, and §8 for the specific name of the function to be called or macro to be referenced.

1. **Initialize parallel or multi-threaded environment** (*if appropriate*)

For example, call `MPI_Init` to initialize MPI if used.

2. **Create the SUNDIALS context object**

Call `SUNContext_Create()` to allocate the `SUNContext` object.

3. **Set the problem dimensions etc.**

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

4. **Create the vector with the initial guess**

Construct an `N_Vector` of initial guess values using the appropriate functions defined by the particular `N_Vector` implementation (see §6 for details).

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)`. Here, `***` is the name of the vector implementation.

For `hypre`, PETSc, and Trilinos 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`, PETSc, or Trilinos vector. Note that calls like `N_VNew_***(...)` and `N_VGetArrayPointer(...)` are not available for these vector wrappers.



**5. Create matrix object** *(if appropriate)*

If a linear solver is required (e.g., when using the default Newton solver) and the linear solver will be a matrix-based linear solver, then a template Jacobian matrix must be created by calling the appropriate constructor 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).

**6. Create linear solver object** *(if appropriate)*

If a linear solver is required (e.g., when using the default Newton solver), then the desired linear solver object must be created by calling the appropriate constructor defined by the particular `SUNLinearSolver` implementation.

For any of the native SUNDIALS `SUNLinearSolver` implementations, the linear solver object may be created using a call of the form `SUNLinearSolver LS = SUNLinSol_***(...)`; where `***` is the name of the linear solver (see §8 for details).

**7. Create KINSOL object**

Call `KINCreate()` to create the KINSOL solver object.

**8. Initialize KINSOL solver**

Call `KINInit()` to allocate internal memory.

**9. Attach the linear solver** *(if appropriate)*

If a linear solver was created above, initialize the KINLS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with `KINSetLinearSolver()`.

**10. Set linear solver optional inputs** *(if appropriate)*

See Table 5.1 for KINLS optional inputs and Chapter §8 for linear solver specific optional inputs.

**11. Set optional inputs**

Call `KINSet***` functions to change any optional inputs that control the behavior of KINSOL from their default values. See §5.5.4 for details.

**12. Solve problem**

Call `ier = KINSol(...)` to solve the nonlinear problem for a given initial guess.

See `KINSol()` for details.

**13. Get optional outputs**

Call `KINGet***` functions to obtain optional output. See §5.5.5 for details.

**14. Deallocate memory**

Upon completion of the integration call the following, as necessary, to free any objects or memory allocated above:

- Call `N_VDestroy()` to free vector objects.
- Call `SUNMatDestroy()` to free matrix objects.
- Call `SUNLinSolFree()` to free linear solvers objects.
- Call `SUNNonlinSolFree()` to free nonlinear solvers objects.
- Call `KINFree()` to free the memory allocated by KINSOL.
- Call `SUNContext_Free()` to free the `SUNContext` object

### 15. Finalize MPI, if used

Call `MPI_Finalize` to terminate MPI.

## 5.5 User-callable functions

This section describes the KINSOL functions that are called by the user to setup and then solve an IVP. Some of these are required. However, starting with §5.5.4, the functions listed involve optional inputs/outputs or restarting, and those paragraphs may be skipped for a casual use of KINSOL. 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 §5.5.4).

### 5.5.1 KINSOL initialization and deallocation functions

void **KINCreate**(*SUNContext* sunctx)

The function `KINCreate()` instantiates a KINSOL solver object.

**Arguments:**

- `sunctx` – the *SUNContext* object (see §4.1)

**Return value:**

- void

int **KINInit**(void \*kin\_mem, *KINSysFn* func, *N\_Vector* tmpl)

The function `KINInit()` specifies the problem-defining function, allocates internal memory, and initializes KINSOL.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block returned by `KINCreate()`.
- `func` – is the CC function which computes the system function  $F(u)$  (or  $G(u)$  for fixed-point iteration) in the nonlinear problem. This function has the form `func(u, fval, user_data)`. (For full details see §5.6.1).
- `tmpl` – is any *N\_Vector* (e.g. the initial guess vector `u`) which is used as a template to create (by cloning) necessary vectors in `kin_mem`.

**Return value:**

- `KIN_SUCCESS` – The call to `KINInit()` was successful.
- `KIN_MEM_NULL` – The KINSOL memory block was not initialized through a previous call to `KINCreate()`.
- `KIN_MEM_FAIL` – A memory allocation request has failed.
- `KIN_ILL_INPUT` – An input argument to `KINInit()` has an illegal value.

**Notes:**

If an error occurred, `KINInit()` sends an error message to the error handler function.

void **KINFree**(void \*\*kin\_mem)

The function `KINFree()` frees the pointer allocated by a previous call to `KINCreate()`.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.

**Return value:**

- `void`

### 5.5.2 Linear solver specification functions

As previously explained, Newton and Picard iterations require the solution of linear systems of the form  $J\delta = -F$ . Solution of these linear systems is handled using the KINLS linear solver interface. This interface supports all valid `SUNLinearSolver` modules. Here, matrix-based `SUNLinearSolver` modules utilize `SUNMatrix` objects to store the Jacobian matrix  $J = F'(u)$  and factorizations used throughout the solution process. Conversely, matrix-free `SUNLinearSolver` modules instead use iterative methods to solve the linear systems of equations, and only require the *action* of the Jacobian on a vector,  $Jv$ .

With most iterative linear solvers, preconditioning can be done on the left only, on the right only, on both the left and the right, or not at all. However, only right preconditioning is supported within KINLS. If preconditioning is done, user-supplied functions define the linear operator corresponding to a right preconditioner matrix  $P$ , which should approximate the system Jacobian matrix  $J$ . For the specification of a preconditioner, see the iterative linear solver sections in §5.5.4 and §5.6. A preconditioner matrix  $P$  must approximate the Jacobian  $J$ , at least crudely.

To specify a generic linear solver to KINSOL, after the call to `KINCreate()` but before any calls to `KINSol()`, the user's program must create the appropriate `SUNLinearSolver` object and call the function `KINSetLinearSolver()`, 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_*(...);
```

For a current list of such constructor routines see §8.

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 Chapters §7 and §8.

Once this solver object has been constructed, the user should attach it to KINSOL via a call to `KINSetLinearSolver()`. The first argument passed to this function is the KINSOL memory pointer returned by `KINCreate()`; the second argument is the desired `SUNLinearSolver` object to use for solving Newton or Picard 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 KINLS linear solver interface, linking it to the main KINSOL solver, and allows the user to specify additional parameters and routines pertinent to their choice of linear solver.

```
int KINSetLinearSolver(void *kin_mem, SUNLinearSolver LS, SUNMatrix J)
```

The function `KINSetLinearSolver()` attaches a generic `SUNLinSol` object `LS` and corresponding template Jacobian `SUNMatrix` object `J` (if applicable) to KINSOL, initializing the KINLS linear solver interface.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `LS` – `SUNLinearSolver` object to use for solving Newton linear systems.
- `J` – `SUNMATRIX` object for used as a template for the Jacobian (or `NULL` if not applicable).

**Return value:**

- `KINLS_SUCCESS` – The KINLS initialization was successful.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is `NULL`.

- KINLS\_ILL\_INPUT – The KINLS interface is not compatible with the LS or J input objects or is incompatible with the current NVECTOR module.
- KINLS\_SUNLS\_FAIL – A call to the LS object failed.
- KINLS\_MEM\_FAIL – A memory allocation request failed.

**Notes:**

If LS is a matrix-based linear solver, then the template Jacobian matrix J will be used in the solve process, so if additional storage is required within the SUNMatrix object (e.g. for factorization of a banded matrix), ensure that the input object is allocated with sufficient size (see the documentation of the particular SUNMatrix type in Chapter §7 for further information).

The previous routines KINdlsSetLinearSolver() and KINspilsSetLinearSolver() 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.

### 5.5.3 KINSOL solver function

This is the central step in the solution process, the call to solve the nonlinear algebraic system.

int **KINSo1**(void \*kin\_mem, *N\_Vector* u, int strategy, *N\_Vector* u\_scale, *N\_Vector* f\_scale)

The function **KINSo1()** computes an approximate solution to the nonlinear system.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- u – vector set to initial guess by user before calling **KINSo1()**, but which upon return contains an approximate solution of the nonlinear system  $F(u) = 0$ .
- strategy – strategy used to solve the nonlinear system. It must be of the following:
  - KIN\_NONE basic Newton iteration
  - KIN\_LINESEARCH Newton with globalization
  - KIN\_FP fixed-point iteration with Anderson Acceleration (no linear solver needed)
  - KIN\_PICARD Picard iteration with Anderson Acceleration (uses a linear solver)
- u\_scale – vector containing diagonal elements of scaling matrix  $D_u$  for vector u chosen so that the components of  $D_u u$  (as a matrix multiplication) all have roughly the same magnitude when u is close to a root of  $F(u)$ .
- f\_scale – vector containing diagonal elements of scaling matrix  $D_F$  for  $F(u)$  chosen so that the components of  $D_F F(u)$  (as a matrix multiplication) all have roughly the same magnitude when u is not too near a root of  $F(u)$ . In the case of a fixed-point iteration, consider  $F(u) = G(u) - u$ .

**Return value:**

- KIN\_SUCCESS – **KINSo1()** succeeded; the scaled norm of  $F(u)$  is less than `fnormtol`.
- KIN\_INITIAL\_GUESS\_OK – The guess  $u = u_0$  satisfied the system  $F(u) = 0$  within the tolerances specified (the scaled norm of  $F(u_0)$  is less than  $0.01 * \text{fnormtol}$ ).
- KIN\_STEP\_LT\_STPTOL – KINSOL stopped based on scaled step length. This means that the current iterate may be an approximate solution of the given nonlinear system, but it is also quite possible that the algorithm is “stalled” (making insufficient progress) near an invalid solution, or that the scalar `scsteptol` is too large (see **KINSetScaledStepTol()** in §5.5.4 to change `scsteptol` from its default value).
- KIN\_MEM\_NULL – The KINSOL memory block pointer was NULL.

- `KIN_ILL_INPUT` – An input parameter was invalid.
- `KIN_NO_MALLOC` – The KINSOL memory was not allocated by a call to `KINCreate()`.
- `KIN_MEM_FAIL` – A memory allocation failed.
- `KIN_LINESEARCH_NONCONV` – The line search algorithm was unable to find an iterate sufficiently distinct from the current iterate, or could not find an iterate satisfying the sufficient decrease condition. Failure to satisfy the sufficient decrease condition could mean the current iterate is “close” to an approximate solution of the given nonlinear system, the difference approximation of the matrix-vector product  $J(u)v$  is inaccurate, or the real scalar `scstoptol` is too large.
- `KIN_MAXITER_REACHED` – The maximum number of nonlinear iterations has been reached.
- `KIN_MXNEWT_5X_EXCEEDED` – Five consecutive steps have been taken that satisfy the inequality  $\|D_u p\|_{L_2} > 0.99 \text{ mxnewtstep}$ , where  $p$  denotes the current step and `mxnewtstep` is a scalar upper bound on the scaled step length. Such a failure may mean that  $\|D_F F(u)\|_{L_2}$  asymptotes from above to a positive value, or the real scalar `mxnewtstep` is too small.
- `KIN_LINESEARCH_BCFAIL` – The line search algorithm was unable to satisfy the “beta-condition” for `MXNBCF+1` nonlinear iterations (not necessarily consecutive), which may indicate the algorithm is making poor progress.
- `KIN_LINSOLV_NO_RECOVERY` – The user-supplied routine `psolve` encountered a recoverable error, but the preconditioner is already current.
- `KIN_LINIT_FAIL` – The KINLS initialization routine (`linit`) encountered an error.
- `KIN_LSETUP_FAIL` – The KINLS setup routine (`lsetup`) encountered an error; e.g., the user-supplied routine `pset` (used to set up the preconditioner data) encountered an unrecoverable error.
- `KIN_LSOLVE_FAIL` – The KINLS solve routine (`lsolve`) encountered an error; e.g., the user-supplied routine `psolve` (used to solve the preconditioned linear system) encountered an unrecoverable error.
- `KIN_SYSFUNC_FAIL` – The system function failed in an unrecoverable manner.
- `KIN_FIRST_SYSFUNC_ERR` – The system function failed recoverably at the first call.
- `KIN_REPTD_SYSFUNC_ERR` – The system function had repeated recoverable errors. No recovery is possible.

**Notes:**

The components of vectors `u_scale` and `f_scale` should be strictly positive. `KIN_SUCCESS=0`, `KIN_INITIAL_GUESS_OK=1`, and `KIN_STEP_LT_STPTOL=2`. All remaining return values are negative and therefore a test `flag < 0` will trap all `KINSol()` failures.

## 5.5.4 Optional input functions

There are numerous optional input parameters that control the behavior of the KINSOL solver. KINSOL provides functions that can be used to change these from their default values. Table 5.1 lists all optional input functions in KINSOL which are then described in detail in the remainder of this section, beginning with those for the main KINSOL solver and continuing with those for the KINLS linear solver interface.

We note that, on error return, all of these functions also send an error message to the error handler function. We also note that all error return values are negative, so a test `retval < 0` will catch any error.

Table 5.1: Optional inputs for KINSOL and KINLS

Optional input	Function name	Default
KINSOL main solver		

continues on next page

Table 5.1 – continued from previous page

Optional input	Function name	Default
Error handler function	<i>KINSetErrHandlerFn()</i>	internal fn.
Pointer to an error file	<i>KINSetErrFile()</i>	stderr
Info handler function	<i>KINSetInfoHandlerFn()</i>	internal fn.
Pointer to an info file	<i>KINSetInfoFile()</i>	stdout
Data for problem-defining function	<i>KINSetUserData()</i>	NULL
Verbosity level of output	<i>KINSetPrintLevel()</i>	0
Max. number of nonlinear iterations	<i>KINSetNumMaxIters()</i>	200
No initial matrix setup	<i>KINSetNoInitSetup()</i>	SUNFALSE
No residual monitoring	<i>KINSetNoResMon()</i>	SUNFALSE
Max. iterations without matrix setup	<i>KINSetMaxSetupCalls()</i>	10
Max. iterations without residual check	<i>KINSetMaxSubSetupCalls()</i>	5
Form of $\eta$ coefficient	<i>KINSetEtaForm()</i>	KIN_ETACHOICE1
Constant value of $\eta$	<i>KINSetEtaConstValue()</i>	0.1
Values of $\gamma$ and $\alpha$	<i>KINSetEtaParams()</i>	0.9 and 2.0
Values of $\omega_{min}$ and $\omega_{max}$	<i>KINSetResMonParams()</i>	0.00001 and 0.9
Constant value of $\omega$	<i>KINSetResMonConstValue()</i>	0.9
Lower bound on $\epsilon$	<i>KINSetNoMinEps()</i>	SUNFALSE
Max. scaled length of Newton step	<i>KINSetMaxNewtonStep()</i>	$1000 D_u u_0 _2$
Max. number of $\beta$ -condition failures	<i>KINSetMaxBetaFails()</i>	10
Rel. error for D.Q. $Jv$	<i>KINSetRelErrFunc()</i>	$\sqrt{\text{around}}$
Function-norm stopping tolerance	<i>KINSetFuncNormTol()</i>	$\text{around}^{1/3}$
Scaled-step stopping tolerance	<i>KINSetScaledStepTol()</i>	$\text{around}^{2/3}$
Inequality constraints on solution	<i>KINSetConstraints()</i>	NULL
Nonlinear system function	<i>KINSetSysFunc()</i>	none
Return the newest fixed point iteration	<i>KINSetReturnNewest()</i>	SUNFALSE
Fixed point/Picard damping parameter	<i>KINSetDamping()</i>	1.0
Anderson Acceleration subspace size	<i>KINSetMAA()</i>	0
Anderson Acceleration damping parameter	<i>KINSetDampingAA()</i>	1.0
Anderson Acceleration delay	<i>KINSetDelayAA()</i>	0
Anderson Acceleration orthogonalization routine	<i>KINSetOrthAA()</i>	KIN_ORTH_MGS
<b>KINLS linear solver interface</b>		
Jacobian function	<i>KINSetJacFn()</i>	DQ
Preconditioner functions and data	<i>KINSetPreconditioner()</i>	NULL, NULL, NULL
Jacobian-times-vector function and data	<i>KINSetJacTimesVecFn()</i>	internal DQ, NULL
Jacobian-times-vector system function	<i>KINSetJacTimesVecSysFn()</i>	NULL

int **KINSetErrFile**(void \*kin\_mem, FILE \*errfp)

The function *KINSetErrFile()* specifies the pointer to the file where all KINSOL messages should be directed when the default KINSOL error handler function is used.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL memory block.
- *errfp* – pointer to output file.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The *kin\_mem* pointer is NULL.

**Notes:**

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

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

**Warning:** If `KINSetErrFile()` 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 **KINSetErrorHandlerFn**(void \*kin\_mem, *KINErrorHandlerFn* ehfun, void \*eh\_data)

The function `KINSetErrorHandlerFn()` specifies the optional user-defined function to be used in handling error messages.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- ehfun – is the user's CC error handler function (see §5.6.2).
- eh\_data – pointer to user data passed to ehfun every time it is called.

**Return value:**

- KIN\_SUCCESS – The function ehfun and data pointer eh\_data have been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

**Notes:**

The default internal error handler function directs error messages to the file specified by the file pointer errfp (see `KINSetErrFile()` above).

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

int **KINSetInfoFile**(void \*kin\_mem, FILE \*infofp)

The function `KINSetInfoFile()` specifies the pointer to the file where all informative (non-error) messages should be directed.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- infofp – pointer to output file.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

**Notes:**

The default value for infofp is stdout.

Deprecated since version 6.2.0: Use `SUNLogger_SetInfoFilename()` instead.

int **KINSetInfoHandlerFn**(void \*kin\_mem, *KINInfoHandlerFn* ihfun, void \*ih\_data)

The function `KINSetInfoHandlerFn()` specifies the optional user-defined function to be used in handling informative (non-error) messages.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- ihfun – is the user's CC information handler function (see §5.6.3).
- ih\_data – pointer to user data passed to ihfun every time it is called.

**Return value:**



- KIN\_SUCCESS – The function `ihfun` and data pointer `ih_data` have been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.

**Notes:**

The default internal information handler function directs informative (non-error) messages to the file specified by the file pointer `infofp` (see [`KINSetInfoFile\(\)`](#) above).

int **KINSetPrintLevel**(void \*kin\_mem, int printf1)

The function [`KINSetPrintLevel\(\)`](#) specifies the level of verbosity of the output.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `printf1` – flag indicating the level of verbosity. Must be one of:
  - 0 – no information is displayed.
  - 1 – for each nonlinear iteration display the following information:
    - the scaled Euclidean  $\ell_2$  norm of the system function evaluated at the current iterate,
    - the scaled norm of the Newton step (only if using KIN\_NONE), and
    - the number of function evaluations performed so far.
  - 2 – display level 1 output and the following values for each iteration:
    - $\|F(u)\|_{D_F}$  (only for KIN\_NONE).
    - $\|F(u)\|_{D_F, \infty}$  (for KIN\_NONE and KIN\_LINESEARCH).
  - 3 – display level 2 output plus
    - additional values used by the global strategy (only if using KIN\_LINESEARCH), and
    - statistical information for iterative linear solver modules.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.
- KIN\_ILL\_INPUT – The argument `printf1` had an illegal value.

**Notes:**

The default value for `printf1` is 0.

int **KINSetUserData**(void \*kin\_mem, void \*user\_data)

The function [`KINSetUserData\(\)`](#) specifies the pointer to user-defined memory that is to be passed to all user-supplied functions.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `user_data` – pointer to the user-defined memory.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.



**Notes:**

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

**Warning:** If `user_data` is needed in user linear solver or preconditioner functions, the call to `KINSetUserData()` must be made before the call to specify the linear solver module.

int **KINSetNumMaxIters**(void \*kin\_mem, long int mxiter)

The function `KINSetNumMaxIters()` specifies the maximum number of nonlinear iterations allowed.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `mxiter` – maximum number of nonlinear iterations.

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – The maximum number of iterations was non-positive.

**Notes:**

The default value for `mxiter` is `MXITER_DEFAULT = 200`.

int **KINSetNoInitSetup**(void \*kin\_mem, *booleantype* noInitSetup)

The function `KINSetNoInitSetup()` specifies whether an initial call to the preconditioner or Jacobian setup function should be made or not.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `noInitSetup` – flag controlling whether an initial call to the preconditioner or Jacobian setup function is made (pass `SUNFALSE`) or not made (pass `SUNTRUE`).

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

**Notes:**

The default value for `noInitSetup` is `SUNFALSE`, meaning that an initial call to the preconditioner or Jacobian setup function will be made. A call to this function is useful when solving a sequence of problems, in which the final preconditioner or Jacobian value from one problem is to be used initially for the next problem.

int **KINSetNoResMon**(void \*kin\_mem, *booleantype* noNNIResMon)

The function `KINSetNoResMon()` specifies whether or not the nonlinear residual monitoring scheme is used to control Jacobian updating

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `noNNIResMon` – flag controlling whether residual monitoring is used (pass `SUNFALSE`) or not used (pass `SUNTRUE`).

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.

**Notes:**

When using a direct solver, the default value for `noNNIResMon` is `SUNFALSE`, meaning that the nonlinear residual will be monitored.

**Warning:** Residual monitoring is only available for use with matrix-based linear solver modules.

int **KINSetMaxSetupCalls**(void \*kin\_mem, long int msbset)

The function *KINSetMaxSetupCalls()* specifies the maximum number of nonlinear iterations that can be performed between calls to the preconditioner or Jacobian setup function.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `msbset` – maximum number of nonlinear iterations without a call to the preconditioner or Jacobian setup function. Pass 0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.
- KIN\_ILL\_INPUT – The argument `msbset` was negative.

**Notes:**

The default value for `msbset` is `MSBSET_DEFAULT=10`. The value of `msbset` should be a multiple of `msbsetsub` (see *KINSetMaxSubSetupCalls()*).

int **KINSetMaxSubSetupCalls**(void \*kin\_mem, long int msbsetsub)

The function *KINSetMaxSubSetupCalls()* specifies the maximum number of nonlinear iterations between checks by the residual monitoring algorithm.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `msbsetsub` – maximum number of nonlinear iterations without checking the nonlinear residual. Pass 0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.
- KIN\_ILL\_INPUT – The argument `msbsetsub` was negative.

**Notes:**

The default value for `msbsetsub` is `MSBSET_SUB_DEFAULT = 5`. The value of `msbset` (see *KINSetMaxSetupCalls()*) should be a multiple of `msbsetsub`.

**Warning:** Residual monitoring is only available for use with matrix-based linear solver modules.

int **KINSetEtaForm**(void \*kin\_mem, int etachoice)

The function *KINSetEtaForm()* specifies the method for computing the value of the  $\eta$  coefficient used in the calculation of the linear solver convergence tolerance.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL memory block.
- *etachoice* – flag indicating the method for computing  $\eta$ . The value must be one of KIN\_ETACHOICE1, KIN\_ETACHOICE2, or KIN\_ETACONSTANT (see Chapter §2 for details).

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The *kin\_mem* pointer is NULL.
- KIN\_ILL\_INPUT – The argument *etachoice* had an illegal value.

**Notes:**

The default value for *etachoice* is KIN\_ETACHOICE1. When using either KIN\_ETACHOICE1 or KIN\_ETACHOICE2 the safeguard

$$\eta_n = \max(\eta_n, \eta_{\text{safe}})$$

is applied when  $\eta_{\text{safe}} > 0.1$ . For KIN\_ETACHOICE1

$$\eta_{\text{safe}} = \eta_{n-1}^{\frac{1+\sqrt{5}}{2}}$$

and for KIN\_ETACHOICE2

$$\eta_{\text{safe}} = \gamma \eta_{n-1}^{\alpha}$$

where  $\gamma$  and  $\alpha$  can be set with *KINSetEtaParams()*.

The following safeguards are always applied when using either KIN\_ETACHOICE1 or KIN\_ETACHOICE2 so that  $\eta_{\min} \leq \eta_n \leq \eta_{\max}$ :

$$\eta_n = \max(\eta_n, \eta_{\min})$$

$$\eta_n = \min(\eta_n, \eta_{\max})$$

where  $\eta_{\min} = 10^{-4}$  and  $\eta_{\max} = 0.9$ .

int **KINSetEtaConstValue**(void \*kin\_mem, *realt* eta)

The function *KINSetEtaConstValue()* specifies the constant value for  $\eta$  in the case *etachoice* = KIN\_ETACONSTANT.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL memory block.
- *eta* – constant value for  $\eta$ . Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The *kin\_mem* pointer is NULL.
- KIN\_ILL\_INPUT – The argument *eta* had an illegal value

**Notes:**

The default value for *eta* is 0.1. The legal values are  $0.0 < \text{eta} \leq 1.0$ .

int **KINSetEtaParams**(void \*kin\_mem, *realtype* egamma, *realtype* ealpha)

The function *KINSetEtaParams()* specifies the parameters  $\gamma$  and  $\alpha$  in the formula for  $\eta$ , in the case `etachoice = KIN_ETACHOICE2`.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `egamma` – value of the  $\gamma$  parameter. Pass 0.0 to indicate the default.
- `ealpha` – value of the  $\alpha$  parameter. Pass 0.0 to indicate the default.

**Return value:**

- `KIN_SUCCESS` – The optional values have been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – One of the arguments `egamma` or `ealpha` had an illegal value.

**Notes:**

The default values for `egamma` and `ealpha` are 0.9 and 2.0, respectively. The legal values are  $0.0 < \text{egamma} \leq 1.0$  and  $1.0 < \text{ealpha} \leq 2.0$ .

int **KINSetResMonConstValue**(void \*kin\_mem, *realtype* omegaconst)

The function *KINSetResMonConstValue()* specifies the constant value for  $\omega$  when using residual monitoring.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `omegaconst` – constant value for  $\omega$ . Passing 0.0 results in using Eqn. (2.4).

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – The argument `omegaconst` had an illegal value

**Notes:**

The default value for `omegaconst` is 0.9. The legal values are  $0.0 < \text{omegaconst} < 1.0$ .

int **KINSetResMonParams**(void \*kin\_mem, *realtype* omegamin, *realtype* omegamax)

The function *KINSetResMonParams()* specifies the parameters  $\omega_{min}$  and  $\omega_{max}$  in the formula (2.4) for  $\omega$ .

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `omegamin` – value of the  $\omega_{min}$  parameter. Pass 0.0 to indicate the default.
- `omegamax` – value of the  $\omega_{max}$  parameter. Pass 0.0 to indicate the default.

**Return value:**

- `KIN_SUCCESS` – The optional values have been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – One of the arguments `omegamin` or `omegamax` had an illegal value.

**Notes:**

The default values for `omegamin` and `omegamax` are 0.00001 and 0.9, respectively. The legal values are  $0.0 < \text{omegamin} < \text{omegamax} < 1.0$ .

**Warning:** Residual monitoring is only available for use with matrix-based linear solver modules.

int **KINSetNoMinEps**(void \*kin\_mem, *booleantype* noMinEps)

The function *KINSetNoMinEps()* specifies a flag that controls whether or not the value of  $\epsilon$ , the scaled linear residual tolerance, is bounded from below.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- noMinEps – flag controlling the bound on  $\epsilon$ . If SUNFALSE is passed the value of  $\epsilon$  is constrained and if SUNTRUE is passed then  $\epsilon$  is not constrained.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

**Notes:**

The default value for noMinEps is SUNFALSE, meaning that a positive minimum value, equal to  $0.01' * "f_{normtol}'$ , is applied to  $\epsilon$  (see *KINSetFuncNormTol()* below).

int **KINSetMaxNewtonStep**(void \*kin\_mem, *realtype* mxnewstep)

The function *KINSetMaxNewtonStep()* specifies the maximum allowable scaled length of the Newton step.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- mxnewstep – maximum scaled step length ( $\geq 0.0$ ). Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The input value was negative.

**Notes:**

The default value of mxnewstep is  $1000 \|u_0\|_{D_u}$ , where  $u_0$  is the initial guess.

int **KINSetMaxBetaFails**(void \*kin\_mem, *realtype* mxnbcf)

The function *KINSetMaxBetaFails()* specifies the maximum number of  $\beta$ -condition failures in the linesearch algorithm.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- mxnbcf – maximum number of  $\beta$ -condition failures. Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – mxnbcf was negative.

**Notes:**

The default value of mxnbcf is MXNBCF\_DEFAULT = 10.

int **KINSetRelErrFunc**(void \*kin\_mem, *realtype* relfunc)

The function *KINSetRelErrFunc()* specifies the relative error in computing  $F(u)$ , which is used in the difference quotient approximation to the Jacobian matrix [see Eq. (2.6)] or the Jacobian-vector product [see Eq. (2.8)]. The value stored is  $\sqrt{\text{relfunc}}$ .

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- relfunc – relative error in  $F(u)$  ( $\text{relfunc} \geq 0.0$ ). Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The relative error was negative.

**Notes:**

The default value for relfunc is  $U = \text{unit roundoff}$ .

int **KINSetFuncNormTol**(void \*kin\_mem, *realtype* fnormtol)

The function *KINSetFuncNormTol()* specifies the scalar used as a stopping tolerance on the scaled maximum norm of the system function  $F(u)$ .

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- fnormtol – tolerance for stopping based on scaled function norm ( $\geq 0.0$ ). Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The tolerance was negative.

**Notes:**

The default value for fnormtol is  $(\text{unit roundoff})^{1/3}$ .

int **KINSetScaledStepTol**(void \*kin\_mem, *realtype* scsteptol)

The function *KINSetScaledStepTol()* specifies the scalar used as a stopping tolerance on the minimum scaled step length.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- scsteptol – tolerance for stopping based on scaled step length ( $\geq 0.0$ ). Pass 0.0 to indicate the default.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The tolerance was non-positive.

**Notes:**

The default value for scsteptol is  $(\text{unit roundoff})^{2/3}$ .

int **KINSetConstraints**(void \*kin\_mem, *N\_Vector* constraints)

The function *KINSetConstraints()* specifies a vector that defines inequality constraints for each component of the solution vector  $u$ .

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- constraints – vector of constraint flags. If constraints[i] is
  - 0.0 then no constraint is imposed on  $u_i$ .
  - 1.0 then  $u_i$  will be constrained to be  $u_i \geq 0.0$ .
  - -1.0 then  $u_i$  will be constrained to be  $u_i \leq 0.0$ .
  - 2.0 then  $u_i$  will be constrained to be  $u_i > 0.0$ .
  - -2.0 then  $u_i$  will be constrained to be  $u_i < 0.0$ .

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The constraint 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. If a NULL vector is supplied, constraint checking will be disabled. The function creates a private copy of the constraints vector. Consequently, the user-supplied vector can be freed after the function call, and the constraints can only be changed by calling this function.

int **KINSetSysFunc**(void \*kin\_mem, *KINSysFn* func)

The function *KINSetSysFunc()* specifies the user-provided function that evaluates the nonlinear system function  $F(u)$  or  $G(u)$ .

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- func – user-supplied function that evaluates  $F(u)$  (or  $G(u)$  for fixed-point iteration).

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The argument func was NULL.

**Notes:**

The nonlinear system function is initially specified through *KINInit()*. The option of changing the system function is provided for a user who wishes to solve several problems of the same size but with different functions.

int **KINSetReturnNewest**(void \*kin\_mem, *booleantype* ret\_newest)

The function *KINSetReturnNewest()* specifies if the fixed point iteration should return the newest iteration or the iteration consistent with the last function evaluation.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.

- `ret_newest` – `SUNTRUE` – return the newest iteration. `SUNFALSE` – return the iteration consistent with the last function evaluation.

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

**Notes:**

The default value of `ret_newest` is `SUNFALSE`.

int **KINSetDamping**(void \*kin\_mem, *realtype* beta)

The function *KINSetDamping()* specifies the value of the damping parameter in the fixed point or Picard iteration.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `beta` – the damping parameter value  $0 < \textit{beta} \leq 1.0$ .

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – The argument `beta` was zero or negative.

**Notes:**

This function sets the damping parameter value, which needs to be greater than zero and less than one if damping is to be used. A value  $\geq 1$  disables damping. The default value of `beta` is 1.0, indicating no damping. To set the damping parameter used in Anderson acceleration see *KINSetDampingAA()*. With the fixed point iteration the difference between successive iterations is used to determine convergence. As such, when damping is enabled, the tolerance used to stop the fixed point iteration is scaled by `beta` to account for the effects of damping. If `beta` is extremely small (close to zero), this can lead to an excessively tight tolerance.

int **KINSetMAA**(void \*kin\_mem, long int maa)

The function *KINSetMAA()* specifies the size of the subspace used with Anderson acceleration in conjunction with Picard or fixed-point iteration.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `maa` – subspace size for various methods. A value of 0 means no acceleration, while a positive value means acceleration will be done.

**Return value:**

- `KIN_SUCCESS` – The optional value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_ILL_INPUT` – The argument `maa` was negative.

**Notes:**

This function sets the subspace size, which needs to be  $> 0$  if Anderson Acceleration is to be used. It also allocates additional memory necessary for Anderson Acceleration. The default value of `maa` is 0, indicating no acceleration. The value of `maa` should always be less than `mxiter`. This function **MUST** be called before calling *KINInit()*. If the user calls the function *KINSetNumMaxIters*, that call should be made before the call to *KINSetMAA*, as the latter uses the value of `mxiter`.



int **KINSetDampingAA**(void \*kin\_mem, *realtype* beta)

The function *KINSetDampingAA()* specifies the value of the Anderson acceleration damping paramter.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- beta – the damping parameter value  $0 < \textit{beta} \leq 1.0$ .

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The argument beta was zero or negative.

**Notes:**

This function sets the damping parameter value, which needs to be greater than zero and less than one if damping is to be used. A value  $\geq 1$  disables damping. The default value of beta is 1.0, indicating no damping. When delaying the start of Anderson acceleration with *KINSetDelayAA()*, use *KINSetDamping()* to set the damping parameter in the fixed point or Picard iterations before Anderson acceleration begins. When using Anderson acceleration without delay, the value provided to *KINSetDampingAA()* is applied to all iterations and any value provided to *KINSetDamping()* is ignored.

int **KINSetDelayAA**(void \*kin\_mem, long int delay)

The function *KINSetDelayAA()* specifies the number of iterations to delay the start of Anderson acceleration.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- delay – the number of iterations to delay Anderson acceleration.

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.
- KIN\_ILL\_INPUT – The argument delay was less than zero.

**Notes:**

The default value of delay is 0, indicating no delay.

int **KINSetOrthAA**(void \*kin\_mem, int orthaa)

The function *KINSetOrthAA()* specifies the orthogonalization routine to be used in the QR factorization portion of Anderson acceleration.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- **orthaa – the orthogonalization routine parameter. Can be set to any of the following**
  - KIN\_ORTH\_MGS – Modified Gram Schmidt (default)
  - KIN\_ORTH\_ICWY – Inverse Compact WY Modified Gram Schmidt
  - KIN\_ORTH\_CGS2 – Classical Gram Schmidt with Reorthogonalization (CGS2)
  - KIN\_ORTH\_DCGS2 – Classical Gram Schmidt with Delayed Reorthogonlization

**Return value:**

- KIN\_SUCCESS – The optional value has been successfully set.

- KIN\_MEM\_NULL – The `kin_mem` pointer is NULL.
- KIN\_ILL\_INPUT – The argument `orthaa` was not one of the predefined orthogonalization routines defined in KINSOL.

---

**Note:** This function *must* be called before calling `KINInit()`.

An example of how to use this function can be found in `examples/kinsol/serial/kinAnalytic_fp.c`

---

#### 5.5.4.1 Linear solver interface optional input functions

For matrix-based linear solver modules, the KINLS solver interface needs a function to compute an approximation to the Jacobian matrix  $J(u)$ . This function must be of type `KINLSJacFn`. The user can supply a Jacobian function, or if using the `SUNMATRIX_DENSE` or `SUNMATRIX_BAND` modules for  $J$  can use the default internal difference quotient approximation that comes with the KINLS solver. To specify a user-supplied Jacobian function `jac`, KINLS provides the function `KINSetJacFn()`. The KINLS 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 `KINSetUserData()`.

int **KINSetJacFn**(void \*kin\_mem, `KINLSJacFn` jac)

The function `KINSetJacFn()` specifies the Jacobian approximation function to be used for a matrix-based solver within the KINLS interface.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `jac` – user-defined Jacobian approximation function. See `KINLSJacFn` for more details.

**Return value:**

- KINLS\_SUCCESS – The optional value has been successfully set.
- KINLS\_MEM\_NULL – The `kin_mem` pointer is NULL.
- KINLS\_LMEM\_NULL – The KINLS linear solver interface has not been initialized.

**Notes:**

This function must be called after the KINLS linear solver interface has been initialized through a call to `KINSetLinearSolver()`. By default, KINLS uses an internal difference quotient function for the `SUNMATRIX_DENSE` and `SUNMATRIX_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.

**Warning:** The previous routine `KINDlsSetJacFn()` 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 matrix-free linear solver modules, the KINLS linear solver interface requires a function to compute an approximation to the product between the Jacobian matrix  $J(u)$  and a vector  $v$ . The user can supply his/her own Jacobian-times-vector approximation function, or use the internal difference quotient approximation that comes with the KINLS solver interface.

A user-defined Jacobian-vector function must be of type `KINLSJacTimesVecFn` and can be specified through a call to `KINLSSetJacTimesVecFn()` (see §5.6.5 for specification details). The pointer `user_data` received through `KINSetUserData()` (or a pointer to NULL if `user_data` was not specified) is passed to the Jacobian-times-vector function

`jtimes` each time it is 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 KINSetJacTimesVecFn(void *kin_mem, KINLsJacTimesVecFn jtimes)
```

The function *KINSetJacTimesVecFn()* specifies the Jacobian-vector product function.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `jtimes` – user-defined Jacobian-vector product function.

**Return value:**

- `KINLS_SUCCESS` – The optional value has been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.
- `KINLS_SUNLS_FAIL` – An error occurred when setting up the system matrix-times-vector routines in the SUNLINSOL object used by the KINLS interface.

**Notes:**

The default is to use an internal difference quotient for `jtimes`. If NULL is passed as `jtimes`, this default is used. This function must be called after the KINLS linear solver interface has been initialized through a call to *KINSetLinearSolver()*. The function type *KINLsJacTimesVecFn* is described in §5.6.5. The previous routine *KINSpilsSetJacTimesVecFn()* 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 system function for use in the Jacobian-vector product approximation by calling *KINSetJacTimesVecSysFn()*. The alternative system function should compute a suitable (and differentiable) approximation of the system function provided to *KINInit()*. For example, as done in [23] when solving the nonlinear systems that arise in the implicit integration of ordinary differential equations, the alternative function may use lagged values when evaluating a nonlinearity to avoid differencing a potentially non-differentiable factor.

```
int KINSetJacTimesVecSysFn(void *kin_mem, KINSysFn jtimesSysFn)
```

The function *KINSetJacTimesVecSysFn()* specifies an alternative system function for use in the internal Jacobian-vector product difference quotient approximation.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `jtimesSysFn` – is the CC function which computes the alternative system function to use in Jacobian-vector product difference quotient approximations. This function has the form `func(u, fval, user_data)`. (For full details see §5.6.1.)

**Return value:**

- `KINLS_SUCCESS` – The optional value has been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.
- `KINLS_ILL_INPUT` – The internal difference quotient approximation is disabled.

**Notes:**

The default is to use the system function provided to *KINInit()* in the internal difference quotient. If the input system function is NULL, the default is used. This function must be called after the KINLS linear solver interface has been initialized through a call to *KINSetLinearSolver()*.

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 KINLS using the function `KINSetPreconditioner()`. 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`. Both of these functions are fully specified in §5.6. The user data pointer received through `KINSetUserData()` (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.

```
int KINSetPreconditioner(void *kin_mem, KINLsPrecSetupFn psetup, KINLsPrecSolveFn psolve)
```

The function `KINSetPreconditioner()` specifies the preconditioner setup and solve functions.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `psetup` – user-defined function to set up the preconditioner. See `KINLsPrecSetupFn` for more details. Pass `NULL` if no setup is necessary.
- `psolve` – user-defined preconditioner solve function. See `KINLsPrecSolveFn` for more details.

**Return value:**

- `KINLS_SUCCESS` – The optional values have been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is `NULL`.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.
- `KINLS_SUNLS_FAIL` – An error occurred when setting up preconditioning in the `SUNLinearSolver` object used by the KINLS interface.

**Notes:**

The default is `NULL` for both arguments (i.e., no preconditioning). This function must be called after the KINLS linear solver interface has been initialized through a call to `KINSetLinearSolver()`.

**Warning:** The previous routine `KINSpilsSetPreconditioner()` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be removed in future releases, so we recommend that users transition to the new routine name soon.

### 5.5.5 Optional output functions

KINSOL provides an extensive list of functions that can be used to obtain solver performance information. Table 5.2 lists all optional output functions in KINSOL, which are then described in detail in the remainder of this section, beginning with those for the main KINSOL solver and continuing with those for the KINLS linear solver interface. Where the name of an output from a linear solver module would otherwise conflict with the name of an optional output from the main solver, a suffix `LS` (for Linear Solver) has been added here (e.g., `lenrwLS`).

Table 5.2: Optional outputs from KINSOL and KINLS

Optional output	Function name
<b>KINSOL main solver</b>	
Size of KINSOL real and integer workspaces	<a href="#"><i>KINGetWorkSpace()</i></a>
Number of function evaluations	<a href="#"><i>KINGetNumFuncEvals()</i></a>
Number of nonlinear iterations	<a href="#"><i>KINGetNumNonlinSolvIters()</i></a>
Number of $\beta$ -condition failures	<a href="#"><i>KINGetNumBetaCondFails()</i></a>
Number of backtrack operations	<a href="#"><i>KINGetNumBacktrackOps()</i></a>
Scaled norm of $F$	<a href="#"><i>KINGetFuncNorm()</i></a>
Scaled norm of the step	<a href="#"><i>KINGetStepLength()</i></a>
User data pointer	<a href="#"><i>KINGetUserData()</i></a>
Print all statistics	<a href="#"><i>KINPrintAllStats()</i></a>
Name of constant associated with a return flag	<a href="#"><i>KINGetReturnFlagName()</i></a>
<b>KINLS linear solver interface</b>	
Stored Jacobian of the nonlinear system	<a href="#"><i>KINGetJac()</i></a>
Nonlinear iteration number at which the Jacobian was evaluated	<a href="#"><i>KINGetJacNumIters()</i></a>
Size of real and integer workspaces	<a href="#"><i>KINGetLinWorkSpace()</i></a>
No. of Jacobian evaluations	<a href="#"><i>KINGetNumJacEvals()</i></a>
No. of $F$ calls for D.Q. Jacobian[-vector] evals.	<a href="#"><i>KINGetNumLinFuncEvals()</i></a>
No. of linear iterations	<a href="#"><i>KINGetNumLinIters()</i></a>
No. of linear convergence failures	<a href="#"><i>KINGetNumLinConvFails()</i></a>
No. of preconditioner evaluations	<a href="#"><i>KINGetNumPrecEvals()</i></a>
No. of preconditioner solves	<a href="#"><i>KINGetNumPrecSolves()</i></a>
No. of Jacobian-vector product evaluations	<a href="#"><i>KINGetNumJtimesEvals()</i></a>
Last return from a KINLS function	<a href="#"><i>KINGetLastLinFlag()</i></a>
Name of constant associated with a return flag	<a href="#"><i>KINGetLinReturnFlagName()</i></a>

#### 5.5.5.1 Main solver optional output functions

KINSOL 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 and solver performance statistics. These optional output functions are described next.

int **KINGetWorkSpace**(void \*kin\_mem, long int lenrw, long int leniw)

The function [\*KINGetWorkSpace\(\)\*](#) returns the KINSOL integer and real workspace sizes.

##### Arguments:

- `kin_mem` – pointer to the KINSOL memory block.
- `lenrw` – the number of `realtype` values in the KINSOL workspace.
- `leniw` – the number of integer values in the KINSOL workspace.

##### Return value:

- `KIN_SUCCESS` – The optional output values have been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

##### Notes:

KINSOL solver In terms of the problem size  $N$ , the actual size of the real workspace is  $17 + 5N$  `realtype` words. The real workspace is increased by an additional  $N$  words if constraint checking is enabled (see [\*KINSetConstraints\(\)\*](#)).

The actual size of the integer workspace (without distinction between `int` and `long int`) is  $22 + 5N$  (increased by  $N$  if constraint checking is enabled).

int **KINGetNumFuncEvals**(void \*kin\_mem, long int nfevals)

The function *KINGetNumFuncEvals()* returns the number of evaluations of the system function.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `nfevals` – number of calls to the user-supplied function that evaluates  $F(u)$ .

**Return value:**

- `KIN_SUCCESS` – The optional output value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

int **KINGetNumNonlinSolvIters**(void \*kin\_mem, long int nniters)

The function *KINGetNumNonlinSolvIters()* returns the number of nonlinear iterations.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `nniters` – number of nonlinear iterations.

**Return value:**

- `KIN_SUCCESS` – The optional output value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

int **KINGetNumBetaCondFails**(void \*kin\_mem, long int nbcfails)

The function *KINGetNumBetaCondFails()* returns the number of  $\beta$ -condition failures.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `nbcfails` – number of  $\beta$ -condition failures.

**Return value:**

- `KIN_SUCCESS` – The optional output value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

int **KINGetNumBacktrackOps**(void \*kin\_mem, long int nbacktr)

The function *KINGetNumBacktrackOps()* returns the number of backtrack operations (step length adjustments) performed by the line search algorithm.

**Arguments:**

- `kin_mem` – pointer to the KINSOL memory block.
- `nbacktr` – number of backtrack operations.

**Return value:**

- `KIN_SUCCESS` – The optional output value has been successfully set.
- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.

int **KINGetFuncNorm**(void \*kin\_mem, *realtype* fnorm)

The function *KINGetFuncNorm()* returns the scaled Euclidean  $\ell_2$  norm of the nonlinear system function  $F(u)$  evaluated at the current iterate.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- fnorm – current scaled norm of  $F(u)$ .

**Return value:**

- KIN\_SUCCESS – The optional output value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

int **KINGetStepLength**(void \*kin\_mem, *realtype* steplength)

The function *KINGetStepLength()* returns the scaled Euclidean  $\ell_2$  norm of the step used during the previous iteration.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- steplength – scaled norm of the Newton step.

**Return value:**

- KIN\_SUCCESS – The optional output value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

int **KINGetUserData**(void \*kin\_mem, void \*\*user\_data)

The function *KINGetUserData()* returns the user data pointer provided to *KINSetUserData()*.

**Arguments:**

- kin\_mem – pointer to the KINSOL memory block.
- user\_data – memory reference to a user data pointer.

**Return value:**

- KIN\_SUCCESS – The optional output value has been successfully set.
- KIN\_MEM\_NULL – The kin\_mem pointer is NULL.

New in version 6.3.0.

int **KINPrintAllStats**(void \*cvsd\_mem, FILE \*outfile, *SUNOutputFormat* fmt)

The function *KINPrintAllStats()* outputs all of the nonlinear solver, linear solver, and other statistics.

**Arguments:**

- kin\_mem – pointer to the KINSOL 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:**

- KIN\_SUCCESS – The output was successfully.

- `KIN_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KIN_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 \***KINGetReturnFlagName**(int flag)

The function *KINGetReturnFlagName()* returns the name of the KINSOL constant corresponding to `flag`.

**Arguments:**

- `flag` – return flag from a KINSOL function.

**Return value:**

- A string containing the name of the corresponding constant

### 5.5.5.2 KINLS linear solver interface optional output functions

The following optional outputs are available from the KINLS modules:

int **KINGetJac**(void \*kin\_mem, *SUNMatrix* \*J)

Returns the internally stored copy of the Jacobian matrix of the nonlinear system function.

**Parameters**

- `kin_mem` – the KINSOL solver object
- `J` – the Jacobian matrix

**Return values**

- `KINLS_SUCCESS` – the output value has been successfully set
- `KINLS_MEM_NULL` – `kin_mem` was NULL
- `KINLS_LMEM_NULL` – the linear solver interface has not been initialized

**Warning:** With linear solvers that overwrite the input Jacobian matrix as part of the linear solver setup (e.g., performing an in-place LU factorization) the matrix returned by *KINGetJac()* may differ from the matrix returned by the last Jacobian evaluation.

**Warning:** This function is provided for debugging purposes and the values in the returned matrix should not be altered.

int **KINGetJacNumIters**(void \*kin\_mem, sunrealtype \*nni\_J)

Returns the nonlinear iteration number at which the Jacobian was evaluated.

**Parameters**

- `kin_mem` – the KINSOL memory structure
- `nni_J` – the nonlinear iteration number



**Return values**

- **KINLS\_SUCCESS** – the output value has been successfully set
- **KINLS\_MEM\_NULL** – `kin_mem` was NULL
- **KINLS\_LMEM\_NULL** – the linear solver interface has not been initialized

int **KINGetLinWorkSpace**(void \*kin\_mem, long int \*lenrwLS, long int \*leniwLS)

The function *KINGetLinWorkSpace()* returns the sizes of the real and integer workspaces used by the KINLS linear solver interface.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `lenrwLS` – the number of real values in the KINLS workspace.
- `leniwLS` – the number of integer values in the KINLS workspace.

**Return value:**

- **KINLS\_SUCCESS** – The optional output value has been successfully set.
- **KINLS\_MEM\_NULL** – The `kin_mem` pointer is NULL.
- **KINLS\_LMEM\_NULL** – The KINLS 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 KINLS is not included in this report.

**Warning:** The previous routines `KINDlsGetWorkspace()` and `KINSpilsGetWorkspace()` are now deprecated.

int **KINGetNumJacEvals**(void \*kin\_mem, long int \*njevals)

The function *KINGetNumJacEvals()* returns the cumulative number of calls to the KINLS Jacobian approximation function.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `njevals` – the cumulative number of calls to the Jacobian function total so far.

**Return value:**

- **KINLS\_SUCCESS** – The optional output value has been successfully set.
- **KINLS\_MEM\_NULL** – The `kin_mem` pointer is NULL.
- **KINLS\_LMEM\_NULL** – The KINLS linear solver has not been initialized.

**Warning:** The previous routine `KINDlsGetNumJacEvals()` is now deprecated,

int **KINGetNumLinFuncEvals**(void \*kin\_mem, long int \*nrevalsLS)

The function `KINGetNumLinResEvals()` returns the cumulative number of calls to the user residual function due to the finite difference Jacobian approximation or finite difference Jacobian-vector product approximation.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `nrevalsLS` – the cumulative number of calls to the user residual function.

**Return value:**

- `KINLS_SUCCESS` – The optional output value has been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.

**Notes:**

The value `nrevalsLS` is incremented only if one of the default internal difference quotient functions is used.

**Warning:** The previous routines `KINDlsGetNumRhsEvals()` and `KINSpilsGetNumRhsEvals()` are now deprecated.

int **KINGetNumLinIters**(void \*kin\_mem, long int \*nliters)

The function *KINGetNumLinIters()* returns the cumulative number of linear iterations.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `nliters` – the current number of linear iterations.

**Return value:**

- `KINLS_SUCCESS` – The optional output value has been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.

**Warning:** The previous routine `KINSpilsGetNumLinIters()` is now deprecated.

int **KINGetNumLinConvFails**(void \*kin\_mem, long int \*nlcfails)

The function *KINGetNumLinConvFails()* returns the cumulative number of linear convergence failures.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `nlcfails` – the current number of linear convergence failures.

**Return value:**

- `KINLS_SUCCESS` – The optional output value has been successfully set.
- `KINLS_MEM_NULL` – The `kin_mem` pointer is NULL.
- `KINLS_LMEM_NULL` – The KINLS linear solver has not been initialized.

**Warning:** The previous routine `KINSpilsGetNumConvFails()` is now deprecated.

int **KINGetNumPrecEvals**(void \*kin\_mem, long int \*npevals)

The function *KINGetNumPrecEvals()* returns the cumulative number of preconditioner evaluations, i.e., the number of calls made to *psetup*.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL solver object.
- *npevals* – the cumulative number of calls to *psetup*.

**Return value:**

- *KINLS\_SUCCESS* – The optional output value has been successfully set.
- *KINLS\_MEM\_NULL* – The *kin\_mem* pointer is NULL.
- *KINLS\_LMEM\_NULL* – The KINLS linear solver has not been initialized.

**Warning:** The previous routine *KINSpilsGetNumPrecEvals()* is now deprecated.

int **KINGetNumPrecSolves**(void \*kin\_mem, long int \*npsolves)

The function *KINGetNumPrecSolves()* returns the cumulative number of calls made to the preconditioner solve function, *psolve*.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL solver object.
- *npsolves* – the cumulative number of calls to *psolve*.

**Return value:**

- *KINLS\_SUCCESS* – The optional output value has been successfully set.
- *KINLS\_MEM\_NULL* – The *kin\_mem* pointer is NULL.
- *KINLS\_LMEM\_NULL* – The KINLS linear solver has not been initialized.

**Warning:** The previous routine *KINSpilsGetNumPrecSolves()* is now deprecated.

int **KINGetNumJtimesEvals**(void \*kin\_mem, long int \*njvevals)

The function *KINGetNumJtimesEvals()* returns the cumulative number of calls made to the Jacobian-vector product function, *jtimes*.

**Arguments:**

- *kin\_mem* – pointer to the KINSOL solver object.
- *njvevals* – the cumulative number of calls to *jtimes*.

**Return value:**

- *KINLS\_SUCCESS* – The optional output value has been successfully set.
- *KINLS\_MEM\_NULL* – The *kin\_mem* pointer is NULL.
- *KINLS\_LMEM\_NULL* – The KINLS linear solver has not been initialized.

**Warning:** The previous routine *KINSpilsGetNumJtimesEvals()* is now deprecated.

int **KINGetLastLinFlag**(void \*kin\_mem, long int \*lsflag)

The function *KINGetLastLinFlag()* returns the last return value from an KINLS routine.

**Arguments:**

- kin\_mem – pointer to the KINSOL solver object.
- lsflag – the value of the last return flag from an KINLS function.

**Return value:**

- KINLS\_SUCCESS – The optional output value has been successfully set.
- KINLS\_MEM\_NULL – The kin\_mem pointer is NULL.
- KINLS\_LMEM\_NULL – The KINLS linear solver has not been initialized.

**Notes:**

If the KINLS setup function failed (i.e., KINSolve() returned KIN\_LSETUP\_FAIL) when using the *SUN-LINSOL\_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 KINLS setup function failed when using another SUNLinearSolver object, then lsflag will be SUNLS\_PSET\_FAIL\_UNREC, SUNLS\_ASET\_FAIL\_UNREC, or SUNLS\_PACKAGE\_FAIL\_UNREC.

If the KINLS solve function failed (KINSolve() returned KIN\_LSOLVE\_FAIL), 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  $J * v$  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 (generated only in SPGMR or SPFGMR); 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.

**Warning:** The previous routines KINDlsGetLastFlag() and KINSpilsGetLastFlag() are now deprecated.

char \***KINGetLinReturnFlagName**(long int lsflag)

The function *KINGetLinReturnFlagName()* returns the name of the KINLS constant corresponding to lsflag.

**Arguments:**

- flag – the flag returned by a call to an KINSOL function

**Return value:**

- char\* – the flag name string or if  $1 \leq lsflag \leq N$  (LU factorization failed), this function returns “NONE”.

**Warning:** The previous routines KINDlsGetReturnFlagName() and KINSpilsGetReturnFlagName() are now deprecated.

## 5.6 User-supplied functions

The user-supplied functions consist of one function defining the nonlinear system, (optionally) a function that handles error and warning messages, (optionally) a function that handles informational messages, (optionally) one or two functions that provides 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 Problem defining function

The user must provide a function of type *KINSysFn* defined as follows:

```
typedef int (*KINSysFn)(N_Vector u, N_Vector fval, void *user_data)
```

This function computes the  $F(u)$  (or  $G(u)$  for fixed-point iteration and Anderson acceleration) for a given value of the vector  $u$ .

**Arguments:**

- $u$  – is the current value of the dependent variable vector,  $u$
- $fval$  – is the output vector  $F(u)$
- $user\_data$  – is a pointer to user data, the same as the  $user\_data$  pointer parameter passed to *KINSetUserData()*

**Return value:**

An *KINSysFn* function type should return a value of 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if a nonrecoverable error occurred. In the last case, the integrator halts. If a recoverable error occurred, the integrator will attempt to correct and retry.

**Notes:**

Allocation of memory for  $fval$  is handled within KINSOL.

### 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 *KINSetErrFile()*), the user may provide a function of type *KINErrorHandlerFn* to process any such messages. The function type *KINErrorHandlerFn* is defined as follows:

```
typedef void (*KINErrorHandlerFn)(int error_code, const char *module, const char *function, char *msg, void *user_data)
```

This function processes error and warning messages from KINSOL and its sub-modules.

**Arguments:**

- $error\_code$  – is the error code
- $module$  – is the name of the KINSOL module reporting the error
- $function$  – is the name of the function in which the error occurred
- $eh\_data$  – is a pointer to user data, the same as the  $eh\_data$  parameter passed to *KINSetErrorHandlerFn()*

**Return value:**

This function has no return value.

**Notes:**

`error_code` is negative for errors and positive (`KIN_WARNING`) for warnings. If a function that returns a pointer to memory encounters an error, it sets `error_code` to 0.

### 5.6.3 Informational message handler function

As an alternative to the default behavior of directing informational (meaning non-error) messages to the file pointed to by `infofp` (see `KINSetInfoFile()`), the user may provide a function of type `KINInfoHandlerFn` to process any such messages. The function type `KINInfoHandlerFn` is defined as follows:

```
typedef void (*KINInfoHandlerFn)(const char *module, const char *function, char *msg, void *ih_data)
```

This function processes error and warning messages from KINSOL and its sub-modules.

**Arguments:**

- `error_code` – is the error code
- `module` – is the name of the KINSOL module reporting the error
- `function` – is the name of the function in which the error occurred
- `ih_data` – is a pointer to user data, the same as the `ih_data` parameter passed to `KINSetInfoHandlerFn()`

**Return value:**

This function has no return value.

### 5.6.4 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 `KINSetLinearSolver()`), the user may provide a function of type `KINLsJacFn` defined as follows:

```
typedef int (*KINLsJacFn)(N_Vector u, N_Vector fu, SUNMatrix J, void *user_data, N_Vector tmp1, N_Vector tmp2)
```

This function computes the Jacobian matrix  $J(u)$  (or an approximation to it).

**Arguments:**

- `u` – is the current (unscaled) iterate.
- `fu` – is the current value of the vector,  $F(u)$ .
- `J` – is the output (approximate) Jacobian matrix (of type `SUNMatrix`),  $F'(u)$ .
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.
- `tmp1`, `tmp2`, – are pointers to memory allocated for variables of type `N_Vector` which can be used by `KINLsJacFn` function as temporary storage or work space.

**Return value:**

An `KINLsJacFn` should return 0 if successful, or a non-zero value otherwise.

**Notes:**

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

With direct linear solvers (i.e., linear solvers with type `SUNLINEARSOLVER_DIRECT`), the Jacobian matrix  $J(u)$  is zeroed out prior to calling the user-supplied Jacobian function so only nonzero elements need to be loaded into  $J$ .

If the user's `KINLSJacFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These quantities may include the scale vectors and the unit roundoff. To obtain the scale vectors, the user will need to add to `user_data` pointers to `u_scale` and/or `f_scale` as needed. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

#### **dense:**

A user-supplied dense Jacobian function must load the  $N \times N$  dense matrix  $J$  with an approximation to the Jacobian matrix  $J(u)$  at the point  $(u)$ . 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  $J$  (with  $i, j = 0 \dots N-1$ ). This macro is meant for small problems for which efficiency of access is not a major concern. Thus, in terms of the indices  $m$  and  $n$  ranging from 1 to  $N$ , the Jacobian element  $J_{m,n}$  can be set using the statement `SM_ELEMENT_D(J, m-1, n-1) = Jm,n`. Alternatively, `SM_COLUMN_D(J, j)` returns a pointer to the first element of the  $j$ -th column of  $J$  (with  $j = 0 \dots N-1$ ), and the elements of the  $j$ -th column can then be accessed using ordinary array indexing. Consequently,  $J_{m,n}$  can be loaded using the statements `col_n = SM_COLUMN_D(J, n-1); col_n[m-1] = Jm,n`. For large problems, it is more efficient to use `SM_COLUMN_D` than to use `SM_ELEMENT_D`. Note that both of these macros number rows and columns starting from 0. The `SUNMATRIX_DENSE` type and accessor macros are documented in §7.3.

#### **banded:**

A user-supplied banded Jacobian function must load the  $N \times N$  banded matrix  $J$  with an approximation to the Jacobian matrix  $J(u)$  at the point  $(u)$ . The accessor macros `SM_ELEMENT_B`, `SM_COLUMN_B`, and `SM_COLUMN_ELEMENT_B` allow the user to read and write banded matrix elements without making specific references to the underlying representation of the `SUNMATRIX_BAND` type. `SM_ELEMENT_B(J, i, j)` references the  $(i, j)$ -th element of the banded matrix  $J$ , counting from 0. This macro is meant for use in small problems for which efficiency of access is not a major concern. Thus, in terms of the indices  $m$  and  $n$  ranging from 1 to  $N$  with  $(m, n)$  within the band defined by `mupper` and `mlower`, the Jacobian element  $J_{m,n}$  can be loaded using the statement `SM_ELEMENT_B(J, m-1, n-1) = Jm,n`. The elements within the band are those with  $-mupper \leq m-n \leq mlower$ . Alternatively, `SM_COLUMN_B(J, j)` returns a pointer to the diagonal element of the  $j$ -th column of  $J$ , 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);` and `SM_COLUMN_ELEMENT_B(col_n, m-1, n-1) = Jm,n`. The elements of the  $j$ -th column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type `SUNMATRIX_BAND`. The array `col_n` can be indexed from  $-mupper$  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  $N \times N$  compressed-sparse-column or compressed-sparse-row matrix  $J$  with an approximation to the Jacobian matrix  $J(u)$  at the point  $(u)$ . Storage for  $J$  already exists on entry to this function, although the user should ensure that sufficient space is allocated in  $J$  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.

**Warning:** The previous function type `KINDlsJacFn()` is identical to `KINLsJacFn`, 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.

### 5.6.5 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 `KINSetLinearSolver()`), the user may provide a function of type `KINLsJacTimesVecFn` 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 (*KINLsJacTimesVecFn)(N_Vector v, N_Vector Jv, N_Vector u, booleantype *new_u, void *user_data)
```

This function computes the product  $Jv$  (or an approximation to it).

**Arguments:**

- `v` – is the vector by which the Jacobian must be multiplied to the right.
- `Jv` – is the computed output vector.
- `u` – is the current value of the dependent variable vector.
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.

**Return value:**

The value returned by the Jacobian-times-vector function should be 0 if successful. If a recoverable failure occurred, the return value should be positive. In this case, KINSOL will attempt to correct by calling the preconditioner setup function. If this information is current, KINSOL halts. If the Jacobian-times-vector function encounters an unrecoverable error, it should return a negative value, prompting KINSOL to halt.

**Notes:**

If a user-defined routine is not given, then an internal `jtimes` function, using a difference quotient approximation, is used.

This function must return a value of  $J * v$  that uses the *current* value of  $J$ , i.e. as evaluated at the current  $u$ .

If the user's `KINLsJacTimesVecFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These might include the scale vectors and the unit roundoff. To obtain the scale vectors, the user will need to add to `user_data` pointers to `u_scale` and/or `f_scale` as needed. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

**Warning:** The previous function type `KINSpilsJacTimesVecFn` is identical to `KINLsJacTimesVecFn`, and may still be used for backward-compatibility. However, this will be removed in future releases, so we recommend that users transition to the new function type name soon.



### 5.6.6 Preconditioner solve (iterative linear solvers)

If a user-supplied preconditioner is to be used with a `SUNLinearSolver` solver module, then the user must provide a function to solve the linear system  $Pz = r$  where  $P$  is the preconditioner matrix which approximates (at least crudely) the Jacobian matrix  $J = F'(u)$ . This function must be of type `KINLSPrecSolveFn`, defined as follows:

```
typedef int (*KINLSPrecSolveFn)(N_Vector u, N_Vector uscale, N_Vector fval, N_Vector fscale, N_Vector v, void *user_data)
```

This function solves the preconditioning system  $Pz = r$ .

**Arguments:**

- `u` – is the current (unscaled) value of the iterate.
- `uscale` – is a vector containing diagonal elements of the scaling matrix `u`
- `fval` – is the vector  $F(u)$  evaluated at `u`
- `fscale` – is a vector containing diagonal elements of the scaling matrix for `fval`
- `v` – on input, `v` is set to the right-hand side vector of the linear system, `r`. On output, `v` must contain the solution `z` of the linear system  $Pz = r$
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.

**Return value:**

The value returned by the preconditioner solve function should be 0 if successful, positive for a recoverable error, or negative for an unrecoverable error.

**Notes:**

If the preconditioner solve function fails recoverably and if the preconditioner information (set by the preconditioner setup function) is out of date, KINSOL attempts to correct by calling the setup function. If the preconditioner data is current, KINSOL halts.

### 5.6.7 Preconditioner setup (iterative linear solvers)

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

```
typedef int (*KINLSPrecSetupFn)(N_Vector u, N_Vector uscale, N_Vector fval, N_Vector fscale, void *user_data)
```

This function evaluates and/or preprocesses Jacobian-related data needed by the preconditioner solve function.

**Arguments:**

- `u` – is the current (unscaled) value of the iterate.
- `uscale` – is a vector containing diagonal elements of the scaling matrix `u`
- `fval` – is the vector  $F(u)$  evaluated at `u`
- `fscale` – is a vector containing diagonal elements of the scaling matrix for `fval`
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.

**Return value:**

The value returned by the preconditioner 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:**

The user-supplied preconditioner setup subroutine should compute the right preconditioner matrix  $P$  (stored in the memory block referenced by the `user_data` pointer) used to form the scaled preconditioned linear system

$$(D_F J(u) P^{-1} D_u^{-1})(D_u P x) = -D_F F(u),$$

where  $D_u$  and  $D_F$  denote the diagonal scaling matrices whose diagonal elements are stored in the vectors `uscale` and `fscale`, respectively.

The preconditioner setup routine will not be called prior to every call made to the preconditioner solve function, but will instead be called only as often as necessary to achieve convergence of the Newton iteration.

If the user's `KINLSPrecSetupFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These might include the scale vectors and the unit roundoff. To obtain the scale vectors, the user will need to add to `user_data` pointers to `u_scale` and/or `f_scale` as needed. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

If the preconditioner solve routine requires no preparation, then a preconditioner setup function need not be given.

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

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, KINSOL provides a band-block-diagonal preconditioner module `KINBBDPRE`, to be used with the parallel `N_Vector` module described in §6.5.

This module provides a preconditioner matrix for KINSOL that is block-diagonal with banded blocks. The blocking corresponds to the distribution of the dependent variable vector  $u$  amongst the processes. Each preconditioner block is generated from the Jacobian of the local part (associated with the current process) of a given function  $G(u)$  approximating  $F(u)$  ( $G = F$  is allowed). The blocks are generated by each process via a difference quotient scheme, utilizing a specified band structure. This structure is given by upper and lower half-bandwidths, `mudq` and `ml dq`, defined as the number of non-zero diagonals above and below the main diagonal, respectively. However, from the resulting approximate Jacobian blocks, 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. Such an efficiency gain may occur if the couplings in the system outside a certain bandwidth are considerably weaker than those within the band. Reducing `mukeep` and `mlkeep` while keeping `mudq` and `ml dq` at their true values, discards the elements outside the narrower band. Reducing both pairs has the additional effect of lumping the outer Jacobian elements into the computed elements within the band, and requires more caution and experimentation to see whether the lower cost of narrower band matrices offsets the loss of accuracy in the blocks.

The `KINBBDPRE` module calls two user-provided functions to construct  $P$ : a required function `Gloc` (of type `KINBBDDLocalFn`) which approximates the nonlinear system function  $G(u) \approx F(u)$  and which is computed locally, and an optional function `Gcomm` (of type `KINBBDDCommFn`) which performs all interprocess communication necessary to evaluate the approximate function  $G$ . These are in addition to the user-supplied nonlinear system function that evaluates  $F(u)$ . Both functions take as input the same pointer `user_data` as that passed by the user to `KINSetUserData()` and passed to the user's function `func`, and neither function has a return value. The user is responsible for providing space (presumably within `user_data`) for components of  $u$  that are communicated by `Gcomm` from the other processes, and that are then used by `Gloc`, which should not do any communication.

```
typedef int (*KINBBDDLocalFn)(sunindextype Nlocal, N_Vector u, N_Vector gval, void *user_data)
```

This `Gloc` function computes  $G(u)$ , and outputs the resulting vector as `gval`.

**Arguments:**

- `Nlocal` – is the local vector length.
- `u` – is the current value of the iterate.
- `gval` – is the output vector.
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.

**Return value:**

An `KINBBDDLocalFn` function type should return 0 to indicate success, or non-zero if an error occurred.

**Notes:**

This function must assume that all inter-processor communication of data needed to calculate `gval` has already been done, and this data is accessible within `user_data`.

The case where  $G$  is mathematically identical to  $F$  is allowed.

```
typedef int (*KINBBDDCommFn)(sunindextype Nlocal, N_Vector u, void *user_data)
```

This `Gcomm` function performs all inter-processor communications necessary for the execution of the `Gloc` function above, using the input vectors `u`.

**Arguments:**

- `Nlocal` – is the local vector length.
- `u` – is the current value of the iterate.
- `user_data` – is a pointer to user data, the same as the `user_data` parameter passed to `KINSetUserData()`.

**Return value:**

An `KINBBDDLocalFn` function type should return 0 to indicate success, or non-zero if an error occurred.

**Notes:**

The `Gcomm` function is expected to save communicated data in space defined within the structure `user_data`.

Each call to the `Gcomm` function is preceded by a call to the residual function `func` with the same `u` argument. Thus `Gcomm` can omit any communications done by `func` if relevant to the evaluation of `Gloc`. If all necessary communication was done in `func`, then `Gcomm = NULL` can be passed in the call to `KINBBDDPrecInit()`.

Besides the header files required for the integration of the DAE problem (see §5.3), to use the `KINBBDDPRE` module, the main program must include the header file `kin_bbdpre.h` which declares the needed function prototypes.

The following is a summary of the usage of this module and describes the sequence of calls in the user main program. Steps that are unchanged from the user main program presented in §5.4 are not bold.

1. Initialize parallel or multi-threaded environment (*if appropriate*)
2. Create the SUNDIALS context object
3. Set the problem dimensions etc.
4. Create the vector with the initial guess
5. Create matrix object (*if appropriate*)
6. **Create linear solver object** (*if appropriate*)

When creating the iterative linear solver object, specify the use of right preconditioning (`SUN_PREC_RIGHT`) as KINSOL only supports right preconditioning.

7. Create nonlinear solver object (*if appropriate*)
8. Create KINSOL object
9. Initialize KINSOL solver
10. Attach the linear solver (*if appropriate*)
11. **Set linear solver optional inputs** (*if appropriate*)

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

12. **Initialize the KINBBDPRE preconditioner module**

Call `KINBBDPrecInit()` to allocate memory and initialize the internal preconditioner data. The last two arguments of `KINBBDPrecInit()` are the two user-supplied functions described above.

13. Set optional inputs
14. Solve problem
15. **Get optional outputs**

Additional optional outputs associated with KINBBDPRE are available by way of two routines described below, `KINBBDPrecGetWorkspace()` and `KINBBDPrecGetNumGfnEvals()`.

16. Deallocate memory
17. Finalize MPI, if used

The user-callable functions that initialize or re-initialize the KINBBDPRE preconditioner module are described next.

```
int KINBBDPrecInit(void *kin_mem, sunindextype Nlocal, sunindextype mudq, sunindextype mldq, sunindextype
    mukeep, sunindextype mlkeep, realtype dq_rel_u, KINBBDDLocalFn Gloc, KINBBDDCommFn
    Gcomm)
```

The function `KINBBDPrecInit()` initializes and allocates memory for the KINBBDPRE preconditioner.

#### Arguments:

- `kin_mem` – pointer to the KINSOL memory block.
- `Nlocal` – 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.
- `dq_rel_u` – the relative increment in components of  $u$  used in the difference quotient approximations. The default is  $dq\_rel\_u = \sqrt{\text{unit roundoff}}$ , which can be specified by passing `dq_rel_u= 0.0`.
- `Gloc` – the CC function which computes the approximation  $G(u) \approx F(u)$ .
- `Gcomm` – the optional CC function which performs all interprocess communication required for the computation of  $G(u)$ .

#### Return value:

- `KINLS_SUCCESS` – The call to `KINBBDPrecInit()` was successful.
- `KINLS_MEM_NULL` – The `kin_mem` pointer was NULL.
- `KINLS_MEM_FAIL` – A memory allocation request has failed.
- `KINLS_LMEM_NULL` – The KINLS linear solver interface has not been initialized.

- KINLS\_ILL\_INPUT – The supplied vector implementation was not compatible with the 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 `Nlocal-1`, it is replaced with 0 or `Nlocal-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 greater efficiency.

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

For all four half-bandwidths, the values need not be the same for every process.

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

int **KINBBDPrecGetWorkSpace**(void \*kin\_mem, long int \*lenrwBBDP, long int \*leniwBBDP)

The function `KINBBDPrecGetWorkSpace()` returns the local sizes of the KINBBDPRE real and integer workspaces.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `lenrwBBDP` – local number of real values in the KINBBDPRE workspace.
- `leniwBBDP` – local number of integer values in the KINBBDPRE workspace.

**Return value:**

- KINLS\_SUCCESS – The optional output value has been successfully set.
- KINLS\_MEM\_NULL – The `kin_mem` pointer was NULL.
- KINLS\_PMEM\_NULL – The KINBBDPRE preconditioner has not been initialized.

**Notes:**

The workspace requirements reported by this routine correspond only to memory allocated within the KINBBDPRE 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 `KINGetLinWorkSpace()` function.

int **KINBBDPrecGetNumGfnEvals**(void \*kin\_mem, long int \*ngevalsBBDP)

The function `KINBBDPrecGetNumGfnEvals()` returns the cumulative number of calls to the user `Gres` function due to the finite difference approximation of the Jacobian blocks used within KINBBDPRE's preconditioner setup function.

**Arguments:**

- `kin_mem` – pointer to the KINSOL solver object.
- `ngevalsBBDP` – the cumulative number of calls to the user `Gres` function.

**Return value:**

- KINLS\_SUCCESS – The optional output value has been successfully set.
- KINLS\_MEM\_NULL – The `kin_mem` pointer was NULL.
- KINLS\_PMEM\_NULL – The KINBBDPRE preconditioner has not been initialized.

In addition to the `ngevalsBBDP` evaluations of `Gres`, the costs associated with `KINBBDPRE` also includes `nlinsetups` LU factorizations, `nlinsetups` calls to `Gcomm`, `npsolves` banded backsolve calls, and `nrevalsLS` residual function evaluations, where `nlinsetups` is an optional KINSOL output (see §5.5.5.1), and `npsolves` and `nrevalsLS` are linear solver optional outputs (see §5.5.5.2).

## 5.8 Alternative to KINSOL for difficult systems

A nonlinear system  $F(u) = 0$  may be difficult to solve with KINSOL (or any other nonlinear system solver) for a variety of reasons. The possible reasons include high nonlinearity, small region of convergence, and lack of a good initial guess. For systems with such difficulties, there is an alternative approach that may be more successful. This is an old idea, but deserves some new attention.

If the nonlinear system is  $F(u) = 0$ , consider instead the ODE system  $du/dt = -M^{-1}F(u)$ , where  $M$  is a nonsingular matrix that is an approximation (even a crude approximation) to the system Jacobian  $F_u = dF/du$ . Whatever  $M$  is, if this ODE is solved until it reaches a steady state  $u^*$ , then  $u^*$  is a zero of the right-hand side of the ODE, and hence a solution to  $F(u) = 0$ . There is no issue of having a close enough initial guess.

A further basis for this choice of ODE is the following: If  $M$  approximates  $F_u$ , then the Jacobian of the ODE system,  $-M^{-1}F_u$ , is approximately equal to  $-I$  where  $I$  is the identity matrix. This means that (in a local approximation sense) the solution modes of the ODE behave like  $\exp(-t)$ , and that asymptotically the approach to the steady state goes as  $\exp(-t)$ . Of course, the closer  $M$  is to  $F_u$ , the better this basis applies.

Using (say) CVODE to solve the above ODE system requires, in addition to the objective function  $F(u)$ , the calculation of a suitable matrix  $M$  and its inverse, or at least a routine that solves linear systems  $Mx = b$ . This is similar to the KINSOL requirement of supplying the system Jacobian  $J$  (or solutions to  $Jx = b$ ), but differs in that  $M$  may be simpler than  $J$  and hence easier to deal with. Depending on the nature of  $M$ , this may be handled best with a direct solver, or with a preconditioned Krylov solver. The latter calls for the use of a preconditioner  $P$  that may be a crude approximation to  $M$ , hence even easier to solve. Note if using ARKODE, the ODE system may be posed in the linearly implicit form  $Mdu/dt = -F(u)$  where  $M$  is the “mass matrix” for the system. This use case requires supplying ARKODE with a function to evaluate  $M$  or to compute its action on a vector ( $Mv = w$ ) and attaching a linear solver (direct or iterative) to solve the linear systems  $Mx = b$ .

The solution of the ODE may be made easier by solving instead the equivalent DAE,  $Mdu/dt + F(u) = 0$ . Applying IDA to this system requires solutions to linear systems whose matrix is the DAE system Jacobian,  $J = F_u + \alpha M$ , where  $\alpha$  is the scalar coefficient  $c_j$  supplied to the user’s Jacobian or preconditioner routine. Selecting a preconditioned Krylov method requires an approximation to this Jacobian as preconditioner  $P$ . Given that  $M$  approximates  $F_u$  (possibly crudely), the appropriate approximation to  $J$  is  $P = M + \alpha M = (1 + \alpha)M$ . Again the user must supply a routine that solves linear systems  $Px = b$ , or  $Mx = b/(1 + \alpha)$ . If  $M$  is too difficult to solve, then an approximation  $M'$  that is easier can be substituted, as long as it achieves convergence. As always, there is a trade-off between the expense of solving  $M$  and the difficulty of achieving convergence in the linear solver.

For the solution of either the ODE or DAE system above, the chances for convergence can be improved with a piecewise constant choice for  $M$ . Specifically, starting from an initial guess  $u_0$ , an initial choice for  $M$  might be  $M_0 = F_u(u_0)$ , or some approximation to this Jacobian. Then one could integrate  $M_0 du/dt + F(u) = 0$  from  $t = 0$  to  $t = T$  for some sizable value  $T$ , evaluate  $F_u(u(T))$ , and take  $M_1$  to be an approximation to that Jacobian. Then integrate using  $M_1$  from  $t = T$  to  $t = 2T$ , and repeat the process until it converges to a steady state.

## 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 major SUNDIALS solvers (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 dense, banded and sparse-direct linear system solvers, 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);
```

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```

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      (*nvllnorm)(N_Vector);
void          (*nvcompare)(realtype, N_Vector, N_Vector);
boolean_t     (*nvinvtest)(N_Vector, N_Vector);
boolean_t     (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
realtype      (*nvminquotient)(N_Vector, N_Vector);
int          (*nvlinearcombination)(int, realtype *, N_Vector *, N_Vector);
int          (*nvscaleaddmulti)(int, realtype *, N_Vector, N_Vector *, N_Vector *);
int          (*nvdotprodmulti)(int, N_Vector, N_Vector *, realtype *);
int          (*nvlinearsumvectorarray)(int, realtype, N_Vector *, realtype,
                                         N_Vector *, N_Vector *);
int          (*nvscalevectorarray)(int, realtype *, N_Vector *, N_Vector *);
int          (*nvconstvectorarray)(int, realtype, N_Vector *);
int          (*nvwrmsnomrvectorarray)(int, N_Vector *, N_Vector *, realtype *);
int          (*nvwrmsnomrmaskvectorarray)(int, N_Vector *, N_Vector *, N_Vector,
                                         realtype *);
int          (*nvscaleaddmultivectorarray)(int, int, realtype *, N_Vector *,
                                         N_Vector **, N_Vector **);
int          (*nvlinearcombinationvectorarray)(int, int, realtype *, N_Vector **,
                                         N_Vector *);
realtype      (*nvdotprodlocal)(N_Vector, N_Vector);
realtype      (*nvmaxnormlocal)(N_Vector);
realtype      (*nvminlocal)(N_Vector);
realtype      (*nvllnormlocal)(N_Vector);
boolean_t     (*nvinvtestlocal)(N_Vector, N_Vector);
boolean_t     (*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);

```

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```

    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 this 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
<code>SUNDIALS_NVEC_SERIAL</code>	Serial	0
<code>SUNDIALS_NVEC_PARALLEL</code>	Distributed memory parallel (MPI)	1
<code>SUNDIALS_NVEC_OPENMP</code>	OpenMP shared memory parallel	2
<code>SUNDIALS_NVEC_PTHREADS</code>	PThreads shared memory parallel	3
<code>SUNDIALS_NVEC_PARHYP</code>	<i>hypre</i> ParHyp parallel vector	4
<code>SUNDIALS_NVEC_PETSC</code>	PETSc parallel vector	5
<code>SUNDIALS_NVEC_CUDA</code>	CUDA vector	6
<code>SUNDIALS_NVEC_HIP</code>	HIP vector	7
<code>SUNDIALS_NVEC_SYCL</code>	SYCL vector	8
<code>SUNDIALS_NVEC_RAJA</code>	RAJA vector	9
<code>SUNDIALS_NVEC_OPENMPDEV</code>	OpenMP vector with device offloading	10
<code>SUNDIALS_NVEC_TRILINOS</code>	Trilinos Tpetra vector	11
<code>SUNDIALS_NVEC_MANYVECTOR</code>	“ManyVector” vector	12
<code>SUNDIALS_NVEC_MPIMANYVECTOR</code>	MPI-enabled “ManyVector” vector	13
<code>SUNDIALS_NVEC_MPIPLUSX</code>	MPI+X vector	14
<code>SUNDIALS_NVEC_CUSTOM</code>	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.,  $m = \min_{0 \leq i < n} \text{real}(x_i)$ .
- `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  $0 \leq i < n$ .
- `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_VMinQuotientLocal()` are ill-defined due to the lack of a clear ordering in the complex plane. These routines should be set to NULL in the custom NVECTOR implementation.

While many SUNDIALS solver modules may be utilized on complex-valued data, others cannot. Specifically, although 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.

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 accessible 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*:

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

The output vector *z* can be the same as either of the input vectors (*x* or *y*).

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*:

$$z_i = c, \quad i = 0, \dots, n-1.$$

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*:

$$z_i = x_i y_i, \quad i = 0, \dots, n-1.$$

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*:

$$z_i = \frac{x_i}{y_i}, \quad i = 0, \dots, n-1.$$

The  $y_i$  may not be tested for 0 values. It should only be called with a *y* that is guaranteed to have all nonzero components.

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*:

$$z_i = c x_i, \quad i = 0, \dots, n-1.$$

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*:

$$z_i = |x_i|, \quad i = 0, \dots, n-1.$$

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*:

$$z_i = \frac{1}{x_i}, \quad i = 0, \dots, n-1.$$

This routine may not check for division by 0. It should be called only with an *x* which is guaranteed to have all nonzero components.

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*:

$$z_i = x_i + b, \quad i = 0, \dots, n-1.$$

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  $l_\infty$  norm of the *N\_Vector* *x*:

$$m = \max_{0 \leq i < n} |x_i|.$$

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*:

$$m = \sqrt{\left( \sum_{i=0}^{n-1} (x_i w_i H(id_i))^2 \right) / n},$$

$$\text{where } H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}.$$

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);
```

*boolean* **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);
```

*boolean* **N\_VConstrMask**(*N\_Vector* c, *N\_Vector* x, *N\_Vector* m)

Performs the following constraint tests based on the values in  $c_i$ :

$$\begin{aligned} x_i &> 0 & \text{if } c_i = 2, \\ x_i &\geq 0 & \text{if } c_i = 1, \\ x_i &< 0 & \text{if } c_i = -2, \\ x_i &\leq 0 & \text{if } c_i = -1. \end{aligned}$$

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  $\text{denom}$  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:

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

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:

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

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:

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

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:

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

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:

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

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:

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

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:

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

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:

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

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:

$$z_{k,j,i} = c_k x_{j,i} + y_{k,j,i}, \quad i = 0, \dots, n - 1 \quad j = 0, \dots, nv - 1, \quad k = 0, \dots, nsum - 1$$

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:

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

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  $x$ :

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

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

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  $x$ :

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

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

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

$$H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$$

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

Usage:

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

*boolean* **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:

$$z_i = \frac{1}{x_i}, i = 0, \dots, n_{local} - 1$$

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

*boolean* **N\_VConstrMaskLocal**(*N\_Vector* c, *N\_Vector* x, *N\_Vector* m)

Performs the following constraint tests based on the values in  $c_i$ :

$$\begin{aligned} x_i &> 0 & \text{if } c_i = 2, \\ x_i &\geq 0 & \text{if } c_i = 1, \\ x_i &< 0 & \text{if } c_i = -2, \\ x_i &\leq 0 & \text{if } c_i = -1. \end{aligned}$$

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  $y_j$ :

$$d_j = \sum_{i=0}^{n_{local}-1} x_i y_{j,i}, \quad j = 0, \dots, nv - 1,$$

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 KINSOL

In [Table 6.2](#) below, we list the vector functions used in the *N\_Vector* module used by the KINSOL package. The table also shows, for each function, which of the code modules uses the function. The KINSOL column shows function usage within the main integrator module, while the remaining columns show function usage within the KINLS linear solvers interface, and the KINBBDPRE preconditioner module.

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

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

Function name	KINSOL	KINLS	KINBBDPRE
<i>N_VGetVectorID()</i>			
<i>N_VGetLength()</i>	4		
<i>N_VClone()</i>	x	x	
<i>N_VCloneEmpty()</i>			
<i>N_VDestroy()</i>	x	x	
<i>N_VSpace()</i>	x	2	
<i>N_VGetArrayPointer()</i>	1	x	
<i>N_VSetArrayPointer()</i>	1		
<i>N_VLinearSum()</i>	x	x	
<i>N_VConst()</i>	x		
<i>N_VProd()</i>	x	x	
<i>N_VDiv()</i>	x		
<i>N_VScale()</i>	x	x	x
<i>N_VAbs()</i>	x		
<i>N_VInv()</i>	x		
<i>N_VDotProd()</i>	x	x	
<i>N_VMaxNorm()</i>	x		
<i>N_VMin()</i>	x		
<i>N_VWL2Norm()</i>	x	x	
<i>N_VL1Norm()</i>	3		
<i>N_VConstrMask()</i>	x		
<i>N_VMinQuotient()</i>	x		
<i>N_VLinearCombination()</i>	x	x	
<i>N_VDotProdMulti()</i>	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 IDA modules for user feedback.
3. These routines are only required if the internal difference-quotient routine for approximating the Jacobian-vector product is used.
4. This routine is only used when an iterative *SUNLinearSolver* module that does not support the *SUNLinearSolSetScalingVectors()* routine is supplied to KINSOL.

Each *SUNLinearSolver* object may require additional *N\_Vector* routines not listed in the table above. Please see the relevant descriptions of these modules in §8 for additional detail on their *N\_Vector* requirements.

The vector functions listed in §6.2 that are *not* used by KINSOL are *N\_VAddConst()*, *N\_VWrmsNorm()*, *N\_VWrmsNormMask()*, *N\_VCompare()*, *N\_VInvTest()*, and *N\_VGetCommunicator()*. Therefore a user-supplied *N\_Vector* module for KINSOL could omit these functions.

The optional function *N\_VLinearCombination()* is only used when Anderson acceleration is enabled or the SPBCG, SPTFQMR, SPGMR, or SPFGMR linear solvers are used. *N\_VDotProd()* is only used when Anderson acceleration is enabled or Classical Gram-Schmidt is used with SPGMR or SPFGMR. The remaining operations from §6.2.2 and §6.2.3 are unused and a user-supplied *N\_Vector* module for KINSOL could omit these operations.

## 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.

```
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:

```
#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:

```
#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:

```
#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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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 §10. 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;
    boolean_t 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean\_t* 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, *boolean\_t* 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, *boolean\_t* 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, *boolean\_t* 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 fnvector_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 §10. 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean\_t* 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 §10.

## 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;
    boolean_t 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, *boolean\_type* 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, *boolean\_type* 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, *boolean\_type* 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 §10.

## 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, *boolean\_t* 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, *boolean\_t* 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 {
    sunindex_t local_length;
    sunindex_t global_length;
    boolean_t own_data;
    Vec *pvec;
    MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_petsc.h`. 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 suffix *\_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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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 recommended to extract the PETSc vector via `x_vec = N_VGetVector_Petsc(v)`; and then access components using appropriate PETSc functions.
- The functions `N_VNewEmpty_Petsc()`, `N_VMake_Petsc()`, and `N_VCloneVectorArrayEmpty_Petsc()` set the field `own_data` to `SUNFALSE`. 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;
    boolean_t       own_helper;
    SUNMemory       host_data;
    SUNMemory       device_data;
    SUNCudaExecPolicy* stream_exec_policy;
```

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```

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 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, and a private data structure which holds additional 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\_VNewWithMemHelp\_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.

*boolean\_type* *N\_VIsManagedMemory\_Cuda*(*N\_Vector* v)

This function returns a boolean flag indicating 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 [32].

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*(*sunindex\_type* 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*(*sunindex\_type* 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, *boolean* 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

---

*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 recommended to use functions `N_VGetDeviceArrayPointer_Cuda()` or `N_VGetHostArrayPointer_Cuda()`. However, when using managed memory, the function `N_VGetArrayPointer()` may also be used.
- To maximize efficiency, vector operations in the NVECTOR\_CUDA implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.



## 6.10.2 The SUNCudaExecPolicy Class

In order to provide maximum flexibility to users, the CUDA kernel execution parameters used by kernels within SUNDIALS 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 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
```

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```

{
    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 individual 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 individual 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 additional 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 indicating 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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 recommended 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:

```
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:

```
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
    {
```

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```

    /* 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 individual 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 individual 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:

```

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;
    boolean_t         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\_VNewWithMemHelp\_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\_nvecscyl.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 [SUNSyclExecPolicy](#) 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, boolean\_t 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, boolean\_t 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, boolean\_t 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, boolean\_t 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, boolean\_t 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, boolean\_t 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, boolean\_t 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 SUNDIALS 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 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 `SUNSYCLBlockReduceExecPolicy` 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);

```

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```
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\_raj.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\_nvesyclraja.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 [32].

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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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, *boolean* 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 [24, 44] 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 §10.1.4. 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::HostMirror` 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 contiguous data array on the host, a pointer to the beginning of a contiguous data array on the device, and a boolean flag *own\_data* which specifies the ownership of host and device data arrays.

```
struct _N_VectorContent_OpenMPDEV
{
    sunindextype length;
    booleantype  own_data;
    realtype     *host_data;
    realtype     *dev_data;
};
```

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

### 6.15.1 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, *realttype* \*h\_vdata, *realttype* \*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.

*realttype* \***N\_VGetHostArrayPointer\_OpenMPDEV**(*N\_Vector* v)

This function returns a pointer to the host data array.

*realttype* \***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, *booleanttype* 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, *boolean*type tf)

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

int **N\_VEnableScaleAddMulti\_OpenMPDEV**(*N\_Vector* v, *boolean*type 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, *boolean*type tf)

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

int **N\_VEnableLinearSumVectorArray\_OpenMPDEV**(*N\_Vector* v, *boolean*type tf)

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

int **N\_VEnableScaleVectorArray\_OpenMPDEV**(*N\_Vector* v, *boolean*type 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, *boolean*type tf)

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

int **N\_VEnableWrmsNormVectorArray\_OpenMPDEV**(*N\_Vector* v, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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 suffix `_Trilinos` (e.g. `N_VDestroy_Trilinos`). Vector operations call existing `Tpetra::Vector` methods when available. Vector operations specific to SUNDIALS are implemented as standalone functions in the namespace `sundials::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 recommended to extract the Trilinos vector object via `x_vec = N_VGetVector_Trilinos(v)` and then access components using the appropriate Trilinos functions.
- The functions `N_VDestroy_Trilinos` and `N_VDestroyVectorArray_Trilinos` only delete the `N_Vector` wrapper. The underlying Tpetra vector object will exist for as long as there is at least one reference to it.

## 6.17 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 `sunindex_type` 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 */
    boolean_type  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_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\_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, *boolean\_t* 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_MPI-MANYVECTOR`. Three potential use cases for this module include:

- 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*.
- 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.
- 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 `sunindex_t` 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     */
    boolean_type  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 user-callable 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, *boolean*type 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, NVECTOR\_PARHYP, NVECTOR\_PETSC, or NVECTOR\_TRILINOS implementations underneath the NVECTOR\_MPIPLUSX 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\_MPIMANYVECTOR (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, its compatibility with the SUNDIALS direct solvers and preconditioners depends on the local vector implementation.

The module NVECTOR\_MPIPLUSX provides the following additional user-callable routines:

`N_Vector N_VMake_MPIplusX(MPI_Comm comm, N_Vector *local_vector, SUNContext sunctx)`

This function creates a MPIplusX vector from an existing local (i.e. on node) NVECTOR object, and a user-created MPI communicator.

The input `comm` should be this user-created MPI communicator. This routine will internally call `MPI_Comm_dup` to create a copy of the input `comm`, so the user-supplied `comm` argument need not be retained after the call to `N_VMake_MPIplusX()`.

This routine will copy the 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\_VSetArrayPointer()* 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 each implementation. 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_VBufSize`: Tests for accuracy in the reported buffer size.
- `Test_N_VBufPack`: Tests for accuracy in the buffer packing routine.
- `Test_N_VBufUnpack`: 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 at least two `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);
```

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```

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 this 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 *SUNDIALS*

Matrix ID	Matrix type
<i>SUNMATRIX_BAND</i>	Band $M \times M$ matrix
<i>SUNMATRIX_CUSPARSE</i>	CUDA sparse CSR matrix
<i>SUNMATRIX_CUSTOM</i>	User-provided custom matrix
<i>SUNMATRIX_DENSE</i>	Dense $M \times N$ matrix
<i>SUNMATRIX_GINKGO</i>	<i>SUNMatrix</i> wrapper for Ginkgo matrices
<i>SUNMATRIX_MAGMADENSE</i>	Dense $M \times N$ matrix
<i>SUNMATRIX_ONEMKLDENSE</i>	oneMKL dense $M \times N$ matrix
<i>SUNMATRIX_SLUNRLOC</i>	<i>SUNMatrix</i> wrapper for SuperLU_DIST SuperMatrix
<i>SUNMATRIX_SPARSE</i>	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:

$$A_{i,j} = 0, \quad i = 1, \dots, m, \quad j = 1, \dots, n.$$

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:

$$B_{i,j} = A_{i,j}, \quad i = 1, \dots, m, \quad j = 1, \dots, n.$$

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:

$$A_{i,j} = cA_{i,j} + B_{i,j}, \quad i = 1, \dots, m, \quad j = 1, \dots, n.$$

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:

$$A_{i,j} = cA_{i,j} + \delta_{i,j}, \quad i, j = 1, \dots, n.$$

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  $y \leftarrow Ax$ . 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:

$$y_i = \sum_{j=1}^n A_{i,j} x_j, \quad i = 1, \dots, m.$$

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 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  $0 \leq j < N$ ). The type of the expression `SM_COLUMN_D(A, j)` is `realtype *`. The pointer returned by the call `SM_COLUMN_D(A, j)` can be treated as an array which is indexed from 0 to  $M-1$ .

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  $0 \leq i < M$  and  $0 \leq j < N$ ).

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: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

*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 *j*th 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 [42]. 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 `SUNMatrix`.

**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  $M_{block} \times nblocks$ .

**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  $N_{block} \times nblocks$ .

**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  $nblocks * N_{block}$ .

---

*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

*sunindex*type **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*.

*sunindex*type **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*.

*sunindex*type **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

*sunindex*type **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*.

*real*type \***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*.

*real*type \***SUNMatrix\_OneMklDense\_Column**(*SUNMatrix* A, *sunindex*type 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_BlockData(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  $N_{\text{block}}$ .

---

### 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;
```

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```

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 *SUNLINSOL\_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  $\min(N-1, \text{mu}+\text{ml})$  because of partial pivoting. The **smu** field holds the upper half-bandwidth allocated for the band matrix.
- **ldim** - leading dimension ( $\text{ldim} \geq \text{smu} + \text{ml} + 1$ )
- **data** - pointer to a contiguous block of **realtype** variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. **data** is a pointer to **ldata** contiguous locations which hold the elements within the banded matrix.
- **ldata** - length of the data array ( $= \text{ldim} \cdot N$ )
- **cols** - array of pointers. **cols[j]** is a pointer to the uppermost element within the band in the *j*-th column. This pointer may be treated as an array indexed from **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:

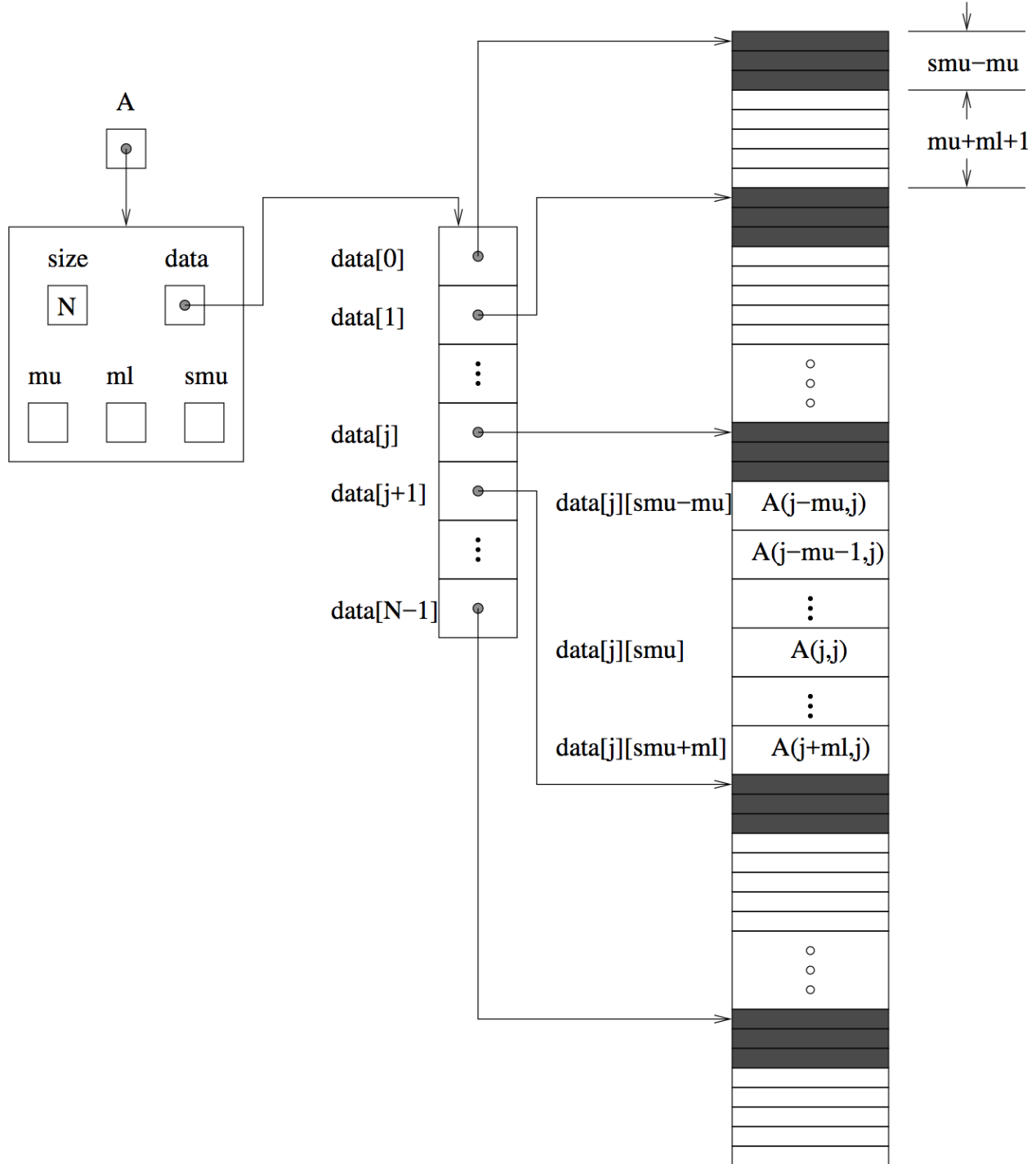


Fig. 7.1: Diagram of the storage for the SUNMATRIX\_BAND module. Here  $A$  is an  $N \times N$  band matrix with upper and lower half-bandwidths  $\mu$  and  $ml$ , respectively. The rows and columns of  $A$  are numbered from 0 to  $N-1$  and the  $(i, j)$ -th element of  $A$  is denoted  $A(i, j)$ . 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 `realttype *`. 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  $j - \mu \leq i \leq j + \text{ml}$ .

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  $j - \mu \leq i \leq j + \text{ml}$ .

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  $A\_data = \text{SUNBandMatrix\_Data}(A)$ , or equivalently  $A\_data = \text{SM\_DATA\_B}(A)$ , and then access  $A\_data[i]$  within the loop.
  - First obtain the array of column pointers via  $A\_cols = \text{SUNBandMatrix\_Cols}(A)$ , or equivalently  $A\_cols = \text{SM\_COLS\_B}(A)$ , and then access  $A\_cols[j][i]$  within the loop.
  - Within a loop over the columns, access the column pointer via  $A\_colj = \text{SUNBandMatrix\_Column}(A, j)$  and then to access the entries within that column using  $\text{SM\_COLUMN\_ELEMENT\_B}(A\_colj, i, j)$ .

All three of these are more efficient than using  $\text{SM\_ELEMENT\_B}(A, i, j)$  within a double loop.

- Within the  $\text{SUNMatMatvec\_Band}$  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  $\text{SUNMATRIX\_CUSPARSE}$  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  $\text{sunmatrix/sunmatrix\_cusparses.h}$ . The installed library to link to is  $\text{libsundials\_sunmatrixcusparses.lib}$  where  $\text{.lib}$  is typically  $\text{.so}$  for shared libraries and  $\text{.a}$  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

$$A = \begin{bmatrix} A_0 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{n-1} \end{bmatrix},$$

where all the block matrices  $A_j$  share the same sparsity pattern. We will refer to this format as BCSR (not to be confused with the canonical BSR format where each block is stored as dense). In this format, the CSR column indices and row pointers are only stored for the first block and are computed only as necessary for other blocks. This can drastically reduce the amount of storage required compared to the regular CSR format when the number of blocks is large. This format is well-suited for, and intended to be used with, the  $\text{SUNLinearSolver\_cuSolverSp\_batchQR}$  linear solver (see §8.17).

**The  $\text{SUNMATRIX\_CUSPARSE}$  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 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, *boolean*type 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 `cusparseSetStream` 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 **real** type 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  $5 \times 4$  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;
```

(continues on next page)

(continued from previous page)

```
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, 28, 36, 37]. 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\_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 [24, 44] and KokkosKernels [43] 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 §10.1.4. For instructions on building and using Kokkos and KokkosKernels, refer to the [Kokkos](#) and [KokkosKernels](#). documentation.

### 7.10.1 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).

### 7.10.2 SUNMATRIX\_KOKKOSDENSE API

In this section we list the public API of the `sundials::kokkos::DenseMatrix` class.

```
template<class ExecutionSpace = 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

## 7.11 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  $z = Ax$  using `SUNMatMatvec()`, and verifies that  $y = z$ .
- `Test_SUNMatSpace`: verifies that `SUNMatSpace()` can be called, and outputs the results to `stdout`.

## 7.12 SUNMatrix functions used by KINSOL

In [Table 7.2](#), we list the matrix functions in the SUNMatrix module used within the KINSOL package. The table also shows, for each function, which of the code modules uses the function. The main KINSOL integrator does not call any SUNMatrix functions directly, so the table columns are specific to the KINLS and KINBBDPRE preconditioner modules. We further note that the KINLS interface only utilizes these routines when supplied with a *matrix-based* linear solver, i.e., the SUNMatrix object passed to `KINSetLinearSolver()` was not NULL.

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

Table 7.2: List of matrix functions usage by KINSOL code modules

	KINLS	KINBBDPRE
<i>SUNMatGetID()</i>	x	
<i>SUNMatDestroy()</i>		x
<i>SUNMatZero()</i>	x	x
<i>SUNMatSpace()</i>		†

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 KINSOL are: *SUNMatCopy()*, *SUNMatClone()*, *SUNMatScaleAdd()*, *SUNMatScaleAddI()* and *SUNMatMatvec()*. Therefore a user-supplied `SUNMatrix` module for KINSOL could omit these functions.

We note that the KINBBDPRE preconditioner module is 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 KINLS 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  $P_2x$ .

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_linear_solver.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 *SUNMatrix* 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 = SUNLinSolLastFlag(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 (\***SUNTimesFn**)(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

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

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_UNREC	-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_UNREC	-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*, *\*hypr\**, *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_SPGMR	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 discussed 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 SUNMATRIX 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 reused 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 *hypr* library; this may be used as a template for other customized implementations (see `examples/arkode/CXX_parhyp/ark_heat2D_hypr.cpp`).

### Matrix-based iterative linear solvers (current *A*)

For users who wish to utilize a matrix-based iterative linear solver 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* `SUNLinSolSetATimes()` routine, then each SUNDIALS package will call that routine to attach its package-specific matrix-vector product routine to the SUNLinSol object. The SUNDIALS package will then call the SUNLinSol-provided `SUNLinSolSetup()` routine (infrequently) to update matrix information, but will provide current matrix-vector products to the SUNLinSol implementation through the package-supplied `SUNATimesFn` routine.

## Application-specific linear solvers with embedded matrix structure

Many applications can exploit additional linear system structure arising from 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 KINSOL SUNLinearSolver interface

Table 8.3 below lists the `SUNLinearSolver` module linear solver functions used within the KINLS interface. As with the `SUNMatrix` module, we emphasize that the KINSOL user does not need to know detailed usage of linear solver functions by the KINSOL code modules in order to use KINSOL. 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 KINLS will consider all solves as requiring zero iterations.
2. Although `SUNLinSolResNorm()` is optional, if it is not implemented by the `SUNLinearSolver` then KINLS will consider all solves as being *exact*.
3. Although KINLS does not call `SUNLinSolLastFlag()` directly, this routine is available for users to query linear solver issues directly.
4. Although KINLS 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 KINLS interface

SUNLinSolGetType	x	x	x
SUNLinSolSetATimes	†	x	†
SUNLinSolSetPreconditioner	†	†	†
SUNLinSolSetScalingVectors	†	†	†
SUNLinSolInitialize	x	x	x
SUNLinSolSetup	x	x	x
SUNLinSolSolve	x	x	x
<sup>1</sup> SUNLinSolNumIters		†	†
<sup>2</sup> SUNLinSolResNorm		†	†
<sup>3</sup> SUNLinSolLastFlag			
<sup>4</sup> SUNLinSolFree			
SUNLinSolSpace	†	†	†

Since there are a wide range of potential `SUNLinearSolver` use cases, the following subsections describe some details of the KINLS 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. As a result, KINSOL can perform its optional residual monitoring scheme, described in §2.8.

### 8.2.2 Iterative linear solver tolerance

If the `SUNLinearSolver` object self-identifies as having type `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE` then KINLS will adjust the linear solver tolerance `delta` as described in §2.9 during the course of the nonlinear solve process. However, if the iterative linear solver does not support scaling matrices (i.e., the `SUNLinSolSetScalingVectors` routine is `NULL`), then KINLS will be unable to fully handle ill-conditioning in the nonlinear solve process through the solution and residual scaling operators described in §2.4. In this case, KINLS 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 residual components have similar magnitude; hence the scaling matrix  $D_F$  used in computing the linear residual norm (see §2.4) should satisfy the assumption

$$(D_F)_{i,i} \approx D_{F,mean}, \quad \text{for } i = 0, \dots, n-1.$$

2. The `SUNLinearSolver` object uses a standard 2-norm to measure convergence.

Since KINSOL uses  $D_F$  as the left-scaling matrix,  $S_1 = D_F$ , then the linear solver convergence requirement is con-



verted as follows (using the notation from equations (8.1) – (8.2):

$$\begin{aligned}
& \|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \text{tol} \\
\Leftrightarrow & \|D_F P_1^{-1} b - D_F P_1^{-1} A x\|_2 < \text{tol} \\
\Leftrightarrow & \sum_{i=0}^{n-1} [(D_F)_{i,i} (P_1^{-1}(b - Ax))_i]^2 < \text{tol}^2 \\
\Leftrightarrow & D_{F,mean}^2 \sum_{i=0}^{n-1} [(P_1^{-1}(b - Ax))_i]^2 < \text{tol}^2 \\
\Leftrightarrow & \sum_{i=0}^{n-1} [(P_1^{-1}(b - Ax))_i]^2 < \left(\frac{\text{tol}}{D_{F,mean}}\right)^2 \\
\Leftrightarrow & \|P_1^{-1}(b - Ax)\|_2 < \frac{\text{tol}}{D_{F,mean}}
\end{aligned}$$

Therefore the tolerance scaling factor

$$D_{F,mean} = \frac{1}{\sqrt{n}} \left( \sum_{i=0}^{n-1} (D_F)_{i,i}^2 \right)^{1/2}$$

is computed and the scaled tolerance  $\text{delta} = \text{tol} / D_{F,mean}$  is supplied to the `SUNLinearSolver` object.

### 8.2.3 Matrix-embedded solver incompatibility

At present, KINLS is incompatible with `SUNLinearSolver` objects that self-identify as having type `SUNLINEAR-SOLVER_MATRIX_EMBEDDED`. Support for such user-supplied linear solvers may be added in a future release. Users interested in such support are recommended to contact the SUNDIALS development team.

## 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  $m_l$ , then the upper triangular factor  $U$  can have upper bandwidth as big as  $\text{smu} = \text{MIN}(N-1, \mu+m_l)$ . The lower triangular factor  $L$  has lower bandwidth  $m_l$ .

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 `SUNMatrix` implementations. These are currently limited to the `SUNMATRIX_DENSE` matrix type and the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

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 `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.

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 nonzeros 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 is compiled with 64-bit indices (`SUNDIALS_INDEX_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_INDEX_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, 19]). 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 §10.1.4 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 “condst”, routine(s). If these estimates of the condition number are larger than  $\varepsilon^{-2/3}$  (where  $\varepsilon$  is the double-precision unit roundoff), then a new factorization is performed.
- The module includes the routine `SUNKLUREInit`, that can be called by the user to force a full refactorization at the next “setup” call.
- The “solve” call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The `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 §10.1.4 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  $smu = \text{MIN}(N-1, mu+mL)$ . 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 SUNMatrix implementations. These are currently limited to the SUNMATRIX\_DENSE matrix type and the NVECTOR\_SERIAL, NVECTOR\_OPENMP, and NVECTOR\_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

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 §10.1.4 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 [42]. 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;  
    boolean_t      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 [30]) 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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{8.3}$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \tag{8.4}$$

The scaling matrix must be chosen so that the vectors  $SP^{-1}b$  and  $S^{-1}Px$  have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

$$\begin{aligned} & \|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta \\ \Leftrightarrow & \|SP^{-1}b - SP^{-1}Ax\|_2 < \delta \\ \Leftrightarrow & \|P^{-1}b - P^{-1}Ax\|_S < \delta \end{aligned}$$

where  $\|v\|_S = \sqrt{v^T S^T S v}$ , with an input tolerance  $\delta$ .

### 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* suncctx)

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.
- suncctx – 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  $\leq 0$  will result in the default value (5).

Since the PCG algorithm is designed to only support symmetric preconditioning, then any of the `pre-type` 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 SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL), PCG should *only* be used with these packages when the linear systems are known to be *symmetric*. Since the scaling of matrix rows and columns must be identical in a symmetric matrix, symmetric preconditioning should work appropriately even for packages designed with one-sided preconditioning in mind.

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 §10.1.2 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 §10.1.2 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;
```

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```

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 [45] 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  $\leq 0$  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\_SPBCGS*SetPrecType(*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\_SPBCGS*SetMaxl(*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 §10.1.2 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 §10.1.2 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 **SUNSPBCGSsetMax1**(*SUNLinearSolver* S, int max1)  
 Wrapper function for *SUNLinSol\_SPBCGSsetMax1()*

### 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 max1;
    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:

- max1 - 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 [40] 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  $\leq 0$  will result in the default value (5).

Since the FGMRES algorithm is designed to only support right preconditioning, then any of the pretype inputs 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\_SPFGMRSetGType**(*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 §10.1.2 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 §10.1.2 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  $v_1, \dots, v_{\text{maxl}+1}$ , stored in `V[0]`, ..., `V[maxl]`. Each  $v_i$  is a vector of type `N_Vector`,
- `Z` - the array of preconditioned Krylov basis vectors  $z_1, \dots, z_{\text{maxl}+1}$ , 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  $F_0, F_1, \dots, F_j$ , where

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

are represented in the `givens` vector as `givens[0] = c0`, `givens[1] = s0`, `givens[2] = c1`, `givens[3] = s1`, ..., `givens[2j] = cj`, `givens[2j+1] = sj`,

- `xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,
- `yg` - a length  $(\text{maxl} + 1)$  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_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`

## 8.13 The `SUNLinSol_SPGMR` Module

The `SUNLinSol_SPGMR` implementation of the `SUNLinearSolver` class performs a Scaled, Preconditioned, Generalized Minimum Residual [41] 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 `SUNLinSol_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  $\leq 0$  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 §10.1.2 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 §10.1.2 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  $v_1, \dots, v_{\maxl+1}$ , stored in  $V[0], \dots, V[\maxl]$ . Each  $v_i$  is a vector of type N\_Vector,
- Hes - the  $(\maxl + 1) \times \maxl$  Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by  $Hes[i][j]$ ,
- givens - a length 2  $\maxl$  array which represents the Givens rotation matrices that arise in the GMRES algorithm. These matrices are  $F_0, F_1, \dots, F_j$ , where

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

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

- xcor - a vector which holds the scaled, preconditioned correction to the initial guess,
- yg - a length  $(\maxl + 1)$  array of `realtype` values used to hold “short” vectors (e.g.  $y$  and  $g$ ),
- vtemp - temporary vector storage.
- 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 [27] 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_SPTFQMR` 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  $\leq 0$  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 §10.1.2 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 §10.1.2 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_sunlinsol_superludist.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 unprefix 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 stores 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 structure 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, 28, 36, 37]. The package uses a SPMD parallel programming model and multithreading to enhance efficiency in distributed-memory parallel environments with multi-core 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 §10.1.4 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, 21, 35]. 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 §10.1.4 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 `SUNMatrix` 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 argument `cuSolverWorkspace`. The size of the internal buffer is proportional to the number of matrix blocks while the size of the workspace is almost independent of the number of blocks.

### 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 [11]. 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 `SUNMatrix.Ginkgo`. Instructions on building SUNDIALS with Ginkgo enabled are given in §10.1.4. 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 interoperability 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 `SUNMatrix.Ginkgo.CompatibleNVectors`) and creating a Ginkgo-enabled `SUNMatrix` (see `SUNMatrix.Ginkgo`) 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 criterion that matches the default SUNDIALS stopping criterion. Namely, it checks if the max iterations (5 by default) were reached or if the absolute residual norm was below a specified tolerance. The criterion 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 criterion, 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, suncctx};
```

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 CVMODE.
//
// Implicit conversion from sundials::ginkgo::LinearSolver<GkoSolverType, GkoMatrixType>
// to a SUNLinearSolver object is done.
//
// For details about creating A see the SUNMATRIX_GINKGO module.
CVMODESetLinearSolver(cvmode_mem, LS, A);

// Alternatively with explicit conversion of LS to a SUNLinearSolver
// and A to a SUNMatrix:
CVMODESetLinearSolver(cvmode_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 suncctx)

Constructs a new `LinearSolver` from a Ginkgo solver factory.

#### Parameters

- **gko\_solver\_factory** – The Ginkgo solver factory (typically `gko::matrix::<type>::Factory`)
- **suncctx** – 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 `DefaultStop` 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 [43] 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 §10.1.4. 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 §7.10).

### 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

# Tools for Memory Management

To support applications which leverage memory pools, or utilize a memory abstraction layer, sundials provides a set of utilities we will 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.

### 9.1 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 to 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;
    boolean_t  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 accessible 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 structure 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_allocations,
                         unsigned long* num_deallocations, size_t* bytes_allocated,
                         size_t* bytes_high_watermark);
    SUNMemoryHelper (*clone)(SUNMemoryHelper);
    int (*destroy)(SUNMemoryHelper);
};

```

### 9.1.1 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).

## 9.1.2 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).

### 9.1.3 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.

---

### 9.1.4 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`.

## 9.2 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`.

### 9.2.1 `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).

## 9.3 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`.

### 9.3.1 `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).

## 9.4 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.

### 9.4.1 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 10

# SUNDIALS 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 §10.1 and §10.2.

## 10.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Make-files, 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.

### 10.1.1 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
```

#### 10.1.1.1 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 Makefiles).
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
Press [c] to configure
Press [h] for help Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
CMake Version 3.12.1

```

Fig. 10.1: 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
Press [c] to configure
Press [h] for help          Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
CMake Version 3.12.1

```

Fig. 10.2: Changing the INSTDIR for SUNDIALS and corresponding EXAMPLES.

### 10.1.1.2 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
```

### 10.1.2 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\_CCODE**

Build the CCODE library

Default: ON

#### **BUILD\_CCODES**

Build the CCODES 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 §10.1.4.

---

**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

---

output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by `EXAMPLES_INSTALL_PATH`. A CMake configuration script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by `EXAMPLES_INSTALL_PATH`.

---

#### **EXAMPLES\_INSTALL\_PATH**

Output directory for installing example files

Default: `/usr/local/examples`

---

**Note:** The actual default value for this option will be an `examples` subdirectory created under `CMAKE_INSTALL_PREFIX`.

---

#### **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 architectures/executors to build for. Options currently 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 §10.1.4.

---

**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 §10.1.4.

---

**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 §10.1.4.

---

**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**

mpi f90 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 §10.1.4.

---

**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 directories. 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 with SuperLU\_DIST enabled in §10.1.4.

---

#### **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 §10.1.4.

---

**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 capabilities 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 capabilities for fine-grained profiling.

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\_ADIK**

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

### 10.1.3 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 \  
>
```

(continues on next page)



(continued from previous page)

```
> -DENABLE_MPI=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/srcdir

% make install
```

### 10.1.4 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.

#### 10.1.4.1 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 architectures/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`.

#### 10.1.4.2 Building with Kokkos

**Kokkos** is a modern C++ (requires at least C++14) programming model for writing 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.

---

#### 10.1.4.3 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 `SUNDIALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were lower and one, respectively.

---

SUNDIALS has been tested with OpenBLAS 0.3.18.

#### 10.1.4.4 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`, `COLAMD_LIBRARY_DIR`, and `KLU_LIBRARY`.

SUNDIALS has been tested with SuiteSparse version 5.10.1.

#### 10.1.4.5 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.

#### 10.1.4.6 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.

#### 10.1.4.7 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 v6.6.2. SUNDIALS requires PETSc 3.5.0 or newer.

#### 10.1.4.8 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 v6.6.2.

#### 10.1.4.9 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.

#### 10.1.4.10 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 §10.1.4.3.

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.

#### 10.1.4.11 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.

#### 10.1.4.12 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.

#### 10.1.4.13 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.

#### 10.1.4.14 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.

#### 10.1.5 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
```

#### 10.1.6 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.

---

### 10.1.7 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.

## 10.2 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.

## 10.2.1 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::ccode`. 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::ccode SUNDIALS::nvecpetsc)
```

Table 10.1: 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
OPENMP	Libraries	libsundials_nvecopenmp.LIB

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Table 10.1 – continued from previous page

	Headers	nvector/nvector_openmp.h
PTHREADS	Libraries	libsundials_nvecpthread.LIB
	Headers	nvector/nvector_pthreads.h
PARHYP	Libraries	libsundials_nvecparhyp.LIB
	Headers	nvector/nvector_parp.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
<b>SUNMATRIX Modules</b>		
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
<b>SUNLINSOL Modules</b>		
BAND	Libraries	libsundials_sunlinsolband.LIB
	Headers	sunlinsol/sunlinsol_band.h
CUSOLVERS_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
LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.LIB

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Table 10.1 – continued from previous page

	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
<b>SUNNONLINSOL Modules</b>		
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
<b>SUNMEMORY Modules</b>		
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
<b>SUNDIALS Packages</b>		
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
		cvodes/cvodes_diag.h

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Table 10.1 – continued from previous page

		cvmodes/cvmodes_direct.h
		cvmodes/cvmodes_impl.h
		cvmodes/cvmodes_ls.h
		cvmodes/cvmodes_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 11

## KINSOL 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.

### 11.1 KINSOL input constants

Table 11.1: KINSOL Main Solver Input Constants

Constant Name	Value	Description
KIN_ETACHOICE1	1	Use Eisenstat and Walker Choice 1 for $\eta$ .
KIN_ETACHOICE2	2	Use Eisenstat and Walker Choice 2 for $\eta$ .
KIN_ETACONSTANT	3	Use constant value for $\eta$ .
KIN_NONE	0	Use Newton iteration.
KIN_LINESEARCH	1	Use Newton iteration with linesearch globalization.
KIN_PICARD	2	Use Picard iteration.

Table 11.2: Iterative Linear Solver Constants

Constant Name	Value	Description
SUN_PREC_NONE	0	No preconditioning
SUN_PREC_RIGHT	2	Preconditioning on the right.
SUN_MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
SUN_CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

Table 11.3: Anderson Acceleration Orthogonalization Method Constants

Constant Name	Value	Description
KIN_ORTH_MGS	0	Use Modified Gram-Schmidt for Anderson acceleration.
KIN_ORTH_ICWY	1	Use Inverse Compact WY Modified Gram-Schmidt for Anderson acceleration.
KIN_ORTH_CGS2	2	Use Classical Gram-Schmidt with Reorthogonalization (CGS-2) for Anderson Acceleration.
KIN_ORTH_DCGS2	3	Use CGS-2 with Delayed Reorthogonalization for Anderson acceleration.

## 11.2 KINSOL output constants

Table 11.4: KINSOL Main Solver Output Constants

Constant Name	Value	Description
KIN_SUCCESS	0	Successful function return.
KIN_INITIAL_GUESS_OK	1	The initial user-supplied guess already satisfies the stopping criterion.
KIN_STEP_LT_STPTOL	2	The stopping tolerance on scaled step length was satisfied.
KIN_WARNING	99	A non-fatal warning. The solver will continue.
KIN_MEM_NULL	-1	The <code>kin_mem</code> argument was NULL.
KIN_ILL_INPUT	-2	One of the function inputs is illegal.
KIN_NO_MALLOC	-3	The KINSOL memory was not allocated by a call to <code>KINMalloc</code> .
KIN_MEM_FAIL	-4	A memory allocation failed.
KIN_LINESEARCH_NONCONV	-5	The linesearch algorithm was unable to find an iterate sufficiently distinct from the current iterate.
KIN_MAXITER_REACHED	-6	The maximum number of nonlinear iterations has been reached.
KIN_MXNEWT_5X_EXCEEDED	-7	Five consecutive steps have been taken that satisfy a scaled step length test.
KIN_LINESEARCH_BCFAIL	-8	The linesearch algorithm was unable to satisfy the $\beta$ -condition for <code>nbcfails</code> iterations.
KIN_LINSOLV_NO_RECOVERY	-9	The user-supplied routine preconditioner <code>slve</code> function failed recoverably, but the preconditioner is already current.
KIN_LINIT_FAIL	-10	The linear solver's initialization function failed.
KIN_LSETUP_FAIL	-11	The linear solver's setup function failed in an unrecoverable manner.
KIN_LSOLVE_FAIL	-12	The linear solver's solve function failed in an unrecoverable manner.
KIN_SYSFUNC_FAIL	-13	The system function failed in an unrecoverable manner.
KIN_FIRST_SYSFUNC_ERR	-14	The system function failed with a recoverable error at the first call.
KIN_REPTD_SYSFUNC_ERR	-15	The system function had repeated recoverable errors.

Table 11.5: KINLS Linear Solver Interface Output Constants

Constant Name	Value	Description
KINLS_SUCCESS	0	Successful function return.
KINLS_MEM_NULL	-1	The <code>kin_mem</code> argument was NULL.
KINLS_LMEM_NULL	-2	The KINLS linear solver has not been initialized.
KINLS_ILL_INPUT	-3	The KINLS solver is not compatible with the current <code>N_Vector</code> module, or an input value was illegal.
KINLS_MEM_FAIL	-4	A memory allocation request failed.
KINLS_PMEM_NULL	-5	The preconditioner module has not been initialized.
KINLS_JACFUNC_ERR	-6	The Jacobian function failed
KINLS_SUNMAT_FAIL	-7	An error occurred with the current <code>SUNMatrix</code> module.
KINLS_SUNLS_FAIL	-8	An error occurred with the current <code>SUNLinearSolver</code> module.

## Chapter 12

# Appendix: SUNDIALS Release History

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
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
Aug 2015	2.6.2	1.0.2	2.8.2	2.8.2	2.8.2	1.2.2	2.8.2

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Table 12.1 – continued from previous page

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
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 <sup>3</sup>	–	–	–	–
Feb 1999	–	–	–	–	1.0.0 <sup>4</sup>	–	–
Aug 1998	–	–	–	–	–	–	1.0.0 <sup>5</sup>
Jul 1997	–	–	1.0.0 <sup>2</sup>	–	–	–	–
Sep 1994	–	–	1.0.0 <sup>1</sup>	–	–	–	–

1. CVODE written
2. PVODE written
3. CVODE and PVODE combined
4. IDA written
5. KINSOL written

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# Index

## B

booleantype (*C type*), 63

## C

ccmake, 296

cmake, 297

CMake options

adiak\_DIR, 310

AMDGPU\_TARGETS, 304

BUILD\_ARKODE, 300

BUILD\_CCODE, 300

BUILD\_CCODES, 300

BUILD\_FORTRAN\_MODULE\_INTERFACE, 304

BUILD\_IDA, 300

BUILD\_IDAS, 300

BUILD\_KINSOL, 300

BUILD\_SHARED\_LIBS, 300

BUILD\_STATIC\_LIBS, 300

CALIPER\_DIR, 310

CMAKE\_BUILD\_TYPE, 300

CMAKE\_C\_COMPILER, 301

CMAKE\_C\_EXTENSIONS, 301

CMAKE\_C\_FLAGS, 301

CMAKE\_C\_FLAGS\_DEBUG, 301

CMAKE\_C\_FLAGS\_MINSIZEREL, 301

CMAKE\_C\_FLAGS\_RELEASE, 301

CMAKE\_C\_STANDARD, 301

CMAKE\_CUDA\_ARCHITECTURES, 303

CMAKE\_CXX\_COMPILER, 301

CMAKE\_CXX\_EXTENSIONS, 302

CMAKE\_CXX\_FLAGS, 301

CMAKE\_CXX\_FLAGS\_DEBUG, 301

CMAKE\_CXX\_FLAGS\_MINSIZEREL, 302

CMAKE\_CXX\_FLAGS\_RELEASE, 302

CMAKE\_CXX\_STANDARD, 302

CMAKE\_Fortran\_COMPILER, 302

CMAKE\_Fortran\_FLAGS, 302

CMAKE\_Fortran\_FLAGS\_DEBUG, 302

CMAKE\_Fortran\_FLAGS\_MINSIZEREL, 302

CMAKE\_Fortran\_FLAGS\_RELEASE, 302

CMAKE\_INSTALL\_LIBDIR, 302

CMAKE\_INSTALL\_PREFIX, 302

ENABLE\_ADIK, 310

ENABLE\_CALIPER, 310

ENABLE\_CUDA, 303

ENABLE\_GINKGO, 304

ENABLE\_HIP, 304

ENABLE\_HYPRE, 305

ENABLE\_KLU, 305

ENABLE\_KOKKOS, 304

ENABLE\_KOKKOS\_KERNELS, 304

ENABLE\_LAPACK, 305

ENABLE\_MAGMA, 305

ENABLE\_MPI, 306

ENABLE\_ONEMKL, 306

ENABLE\_OPENMP, 307

ENABLE\_PETSC, 307

ENABLE\_PTHREAD, 307

ENABLE\_RAJA, 307

ENABLE\_SUPERLUDIST, 308

ENABLE\_SUPERLUMT, 309

ENABLE\_SYCL, 309

ENABLE\_XBRAID, 303

EXAMPLES\_ENABLE\_C, 303

EXAMPLES\_ENABLE\_CUDA, 303

EXAMPLES\_ENABLE\_CXX, 303

EXAMPLES\_ENABLE\_F2003, 303

EXAMPLES\_INSTALL, 303

EXAMPLES\_INSTALL\_PATH, 304

Ginkgo\_DIR, 304

HYPRE\_INCLUDE\_DIR, 305

HYPRE\_LIBRARY, 305

KLU\_INCLUDE\_DIR, 305

KLU\_LIBRARY\_DIR, 305

Kokkos\_DIR, 304

KokkosKernels\_DIR, 304

LAPACK\_LIBRARIES, 305

MAGMA\_DIR, 306

MPI\_C\_COMPILER, 306

MPI\_CXX\_COMPILER, 306

MPI\_Fortran\_COMPILER, 306

MPICH\_EXECUTABLE, 306

ONEMKL\_DIR, 307

PETSC\_DIR, 307

PETSC\_INCLUDES, 307

PETSC\_LIBRARIES, 307

SUNDIALS\_BUILD\_WITH\_MONITORING, 310

SUNDIALS\_BUILD\_WITH\_PROFILING, 310

SUNDIALS\_F77\_FUNC\_CASE, 310

SUNDIALS\_F77\_FUNC\_UNDERSCORES, 311

SUNDIALS\_GINKGO\_BACKENDS, 304  
SUNDIALS\_INDEX\_SIZE, 311  
SUNDIALS\_INDEX\_TYPE, 311  
SUNDIALS\_INSTALL\_CMAKEDIR, 311  
SUNDIALS\_LOGGING\_ENABLE\_MPI, 310  
SUNDIALS\_LOGGING\_LEVEL, 309  
SUNDIALS\_MAGMA\_BACKENDS, 306  
SUNDIALS\_MATH\_LIBRARY, 311  
SUNDIALS\_ONEMKL\_USE\_GETRF\_LOOP, 307  
SUNDIALS\_ONEMKL\_USE\_GETRS\_LOOP, 307  
SUNDIALS\_PRECISION, 311  
SUNDIALS\_RAJA\_BACKENDS, 308  
SUNDIALS\_SYCL\_2020\_UNSUPPORTED, 309  
SUPERLUDIST\_DIR, 308  
SUPERLUDIST\_INCLUDE\_DIR, 308  
SUPERLUDIST\_INCLUDE\_DIRS, 308  
SUPERLUDIST\_LIBRARIES, 308  
SUPERLUDIST\_LIBRARY\_DIR, 308  
SUPERLUDIST\_OpenMP, 308  
SUPERLUMT\_INCLUDE\_DIR, 309  
SUPERLUMT\_LIBRARY\_DIR, 309  
SUPERLUMT\_THREAD\_TYPE, 309  
USE\_GENERIC\_MATH, 312  
USE\_XSDK\_DEFAULTS, 312  
XBRAID\_DIR, 312  
XBRAID\_INCLUDES, 312  
XBRAID\_LIBRARIES, 312

cmake-gui, 296

CopyFromDevice (C++ function), 162

CopyToDevice (C++ function), 162

## D

DenseLinearSolver (C++ class), 281

DenseLinearSolver::~DenseLinearSolver (C++ function), 281

DenseLinearSolver::Convert (C++ function), 281

DenseLinearSolver::DenseLinearSolver (C++ function), 281

DenseLinearSolver::operator SUNLinearSolver (C++ function), 281

DenseLinearSolver::operator= (C++ function), 281

DenseMatrix (C++ class), 213

DenseMatrix::~DenseMatrix (C++ function), 214

DenseMatrix::BlockCols (C++ function), 214

DenseMatrix::BlockRows (C++ function), 214

DenseMatrix::Blocks (C++ function), 214

DenseMatrix::Cols (C++ function), 214

DenseMatrix::Convert (C++ function), 214

DenseMatrix::DenseMatrix (C++ function), 213, 214

DenseMatrix::ExecSpace (C++ function), 214

DenseMatrix::operator SUNMatrix (C++ function), 214

DenseMatrix::operator= (C++ function), 214

DenseMatrix::Rows (C++ function), 214

DenseMatrix::View (C++ function), 214

## G

GetDenseMat (C++ function), 214

GetVec (C++ function), 162

## K

KINBBDDCommFn (C type), 99

KINBBDDLocalFn (C type), 98

KINBBDPrecGetNumGfnEvals (C function), 101

KINBBDPrecGetWorkSpace (C function), 101

KINBBDPrecInit (C function), 100

KINCreate (C function), 66

KINErrorHandlerFn (C type), 93

KINFree (C function), 66

KINGetFuncNorm (C function), 86

KINGetJac (C function), 88

KINGetJacNumIters (C function), 88

KINGetLastLinFlag (C function), 91

KINGetLinReturnFlagName (C function), 92

KINGetLinWorkSpace (C function), 89

KINGetNumBacktrackOps (C function), 86

KINGetNumBetaCondFails (C function), 86

KINGetNumFuncEvals (C function), 86

KINGetNumJacEvals (C function), 89

KINGetNumJtimesEvals (C function), 91

KINGetNumLinConvFails (C function), 90

KINGetNumLinFuncEvals (C function), 89

KINGetNumLinIters (C function), 90

KINGetNumNonlinSolvIters (C function), 86

KINGetNumPrecEvals (C function), 90

KINGetNumPrecSolves (C function), 91

KINGetReturnFlagName (C function), 88

KINGetStepLength (C function), 87

KINGetUserData (C function), 87

KINGetWorkSpace (C function), 85

KINInfoHandlerFn (C type), 94

KINInit (C function), 66

KINLsJacFn (C type), 94

KINLsJacTimesVecFn (C type), 96

KINLsPrecSetupFn (C type), 97

KINLsPrecSolveFn (C type), 97

KINPrintAllStats (C function), 87

KINSetConstraints (C function), 78

KINSetDamping (C function), 80

KINSetDampingAA (C function), 80

KINSetDelayAA (C function), 81

KINSetErrFile (C function), 70

KINSetErrHandlerFn (C function), 71

KINSetEtaConstValue (C function), 75

KINSetEtaForm (C function), 74

KINSetEtaParams (C function), 75

KINSetFuncNormTol (C function), 78

KINSetInfoFile (C function), 71

KINSetInfoHandlerFn (C function), 71  
 KINSetJacFn (C function), 82  
 KINSetJacTimesVecFn (C function), 83  
 KINSetJacTimesVecSysFn (C function), 83  
 KINSetLinearSolver (C function), 67  
 KINSetMAA (C function), 80  
 KINSetMaxBetaFails (C function), 77  
 KINSetMaxNewtonStep (C function), 77  
 KINSetMaxSetupCalls (C function), 74  
 KINSetMaxSubSetupCalls (C function), 74  
 KINSetNoInitSetup (C function), 73  
 KINSetNoMinEps (C function), 77  
 KINSetNoResMon (C function), 73  
 KINSetNumMaxIters (C function), 73  
 KINSetOrthAA (C function), 81  
 KINSetPreconditioner (C function), 84  
 KINSetPrintLevel (C function), 72  
 KINSetRelErrFunc (C function), 77  
 KINSetResMonConstValue (C function), 76  
 KINSetResMonParams (C function), 76  
 KINSetReturnNewest (C function), 79  
 KINSetScaledStepTol (C function), 78  
 KINSetSysFunc (C function), 79  
 KINSetUserData (C function), 72  
 KINSol (C function), 68  
 KINSysFn (C type), 93

## L

LinearSolver (C++ class), 279  
 LinearSolver::~~LinearSolver (C++ function), 279  
 LinearSolver::Convert (C++ function), 279  
 LinearSolver::GkoExec (C++ function), 279  
 LinearSolver::GkoFactory (C++ function), 279  
 LinearSolver::GkoSolver (C++ function), 279  
 LinearSolver::LinearSolver (C++ function), 279  
 LinearSolver::NumIters (C++ function), 279  
 LinearSolver::operator SUNLinearSolver (C++ function), 279  
 LinearSolver::operator= (C++ function), 279  
 LinearSolver::ResNorm (C++ function), 280  
 LinearSolver::Setup (C++ function), 280  
 LinearSolver::Solve (C++ function), 280

## N

N\_VAbs (C function), 112  
 N\_VAddConst (C function), 112  
 N\_VBufPack (C function), 121  
 N\_VBufSize (C function), 121  
 N\_VBufUnpack (C function), 121  
 N\_VClone (C function), 110  
 N\_VCloneEmpty (C function), 110  
 N\_VCloneVectorArray (C function), 105  
 N\_VCloneVectorArrayEmpty (C function), 106  
 N\_VCompare (C function), 114

N\_VConst (C function), 111  
 N\_VConstrMask (C function), 114  
 N\_VConstrMaskLocal (C function), 119  
 N\_VConstVectorArray (C function), 116  
 N\_VCopyFromDevice\_Cuda (C function), 143  
 N\_VCopyFromDevice\_Hip (C function), 148  
 N\_VCopyFromDevice\_OpenMPDEV (C function), 164  
 N\_VCopyFromDevice\_Raja (C function), 158  
 N\_VCopyFromDevice\_Sycl (C++ function), 153  
 N\_VCopyOps (C function), 108  
 N\_VCopyToDevice\_Cuda (C function), 143  
 N\_VCopyToDevice\_Hip (C function), 148  
 N\_VCopyToDevice\_OpenMPDEV (C function), 164  
 N\_VCopyToDevice\_Raja (C function), 158  
 N\_VCopyToDevice\_Sycl (C++ function), 153  
 N\_VDestroy (C function), 110  
 N\_VDestroyVectorArray (C function), 106  
 N\_VDiv (C function), 112  
 N\_VDotProd (C function), 113  
 N\_VDotProdLocal (C function), 118  
 N\_VDotProdMulti (C function), 115  
 N\_VDotProdMultiAllReduce (C function), 120  
 N\_VDotProdMultiLocal (C function), 120  
 N\_Vector (C type), 103  
 N\_VEnableConstVectorArray\_Cuda (C function), 144  
 N\_VEnableConstVectorArray\_Hip (C function), 149  
 N\_VEnableConstVectorArray\_ManyVector (C function), 169  
 N\_VEnableConstVectorArray\_MPIManyVector (C function), 173  
 N\_VEnableConstVectorArray\_OpenMP (C function), 132  
 N\_VEnableConstVectorArray\_OpenMPDEV (C function), 165  
 N\_VEnableConstVectorArray\_Parallel (C function), 128  
 N\_VEnableConstVectorArray\_ParHyp (C function), 138  
 N\_VEnableConstVectorArray\_Petsc (C function), 141  
 N\_VEnableConstVectorArray\_Pthreads (C function), 136  
 N\_VEnableConstVectorArray\_Raja (C function), 159  
 N\_VEnableConstVectorArray\_Serial (C function), 125  
 N\_VEnableConstVectorArray\_Sycl (C++ function), 154  
 N\_VEnableDotProdMulti\_Cuda (C function), 144  
 N\_VEnableDotProdMulti\_Hip (C function), 149  
 N\_VEnableDotProdMulti\_ManyVector (C function), 169  
 N\_VEnableDotProdMulti\_MPIManyVector (C function), 173  
 N\_VEnableDotProdMulti\_OpenMP (C function), 132

`N_VEnableDotProdMulti_OpenMPDEV` (*C function*), 165

`N_VEnableDotProdMulti_Parallel` (*C function*), 128

`N_VEnableDotProdMulti_ParHyp` (*C function*), 138

`N_VEnableDotProdMulti_Petsc` (*C function*), 140

`N_VEnableDotProdMulti_Pthreads` (*C function*), 135

`N_VEnableDotProdMulti_Serial` (*C function*), 125

`N_VEnableFusedOps_Cuda` (*C function*), 144

`N_VEnableFusedOps_Hip` (*C function*), 149

`N_VEnableFusedOps_ManyVector` (*C function*), 169

`N_VEnableFusedOps_MPIManyVector` (*C function*), 172

`N_VEnableFusedOps_OpenMP` (*C function*), 132

`N_VEnableFusedOps_OpenMPDEV` (*C function*), 164

`N_VEnableFusedOps_Parallel` (*C function*), 128

`N_VEnableFusedOps_ParHyp` (*C function*), 138

`N_VEnableFusedOps_Petsc` (*C function*), 140

`N_VEnableFusedOps_Pthreads` (*C function*), 135

`N_VEnableFusedOps_Raja` (*C function*), 159

`N_VEnableFusedOps_Serial` (*C function*), 124

`N_VEnableFusedOps_Sycl` (*C++ function*), 154

`N_VEnableLinearCombination_Cuda` (*C function*), 144

`N_VEnableLinearCombination_Hip` (*C function*), 149

`N_VEnableLinearCombination_ManyVector` (*C function*), 169

`N_VEnableLinearCombination_MPIManyVector` (*C function*), 173

`N_VEnableLinearCombination_OpenMP` (*C function*), 132

`N_VEnableLinearCombination_OpenMPDEV` (*C function*), 164

`N_VEnableLinearCombination_Parallel` (*C function*), 128

`N_VEnableLinearCombination_ParHyp` (*C function*), 138

`N_VEnableLinearCombination_Petsc` (*C function*), 140

`N_VEnableLinearCombination_Pthreads` (*C function*), 135

`N_VEnableLinearCombination_Raja` (*C function*), 159

`N_VEnableLinearCombination_Serial` (*C function*), 124

`N_VEnableLinearCombination_Sycl` (*C++ function*), 154

`N_VEnableLinearCombinationVectorArray_Cuda` (*C function*), 144

`N_VEnableLinearCombinationVectorArray_Hip` (*C function*), 149

`N_VEnableLinearCombinationVectorArray_OpenMP` (*C function*), 132

`N_VEnableLinearCombinationVectorArray_OpenMPDEV` (*C function*), 165

`N_VEnableLinearCombinationVectorArray_Parallel` (*C function*), 129

`N_VEnableLinearCombinationVectorArray_ParHyp` (*C function*), 139

`N_VEnableLinearCombinationVectorArray_Petsc` (*C function*), 141

`N_VEnableLinearCombinationVectorArray_Pthreads` (*C function*), 136

`N_VEnableLinearCombinationVectorArray_Raja` (*C function*), 159

`N_VEnableLinearCombinationVectorArray_Serial` (*C function*), 125

`N_VEnableLinearCombinationVectorArray_Sycl` (*C++ function*), 154

`N_VEnableLinearSumVectorArray_Cuda` (*C function*), 144

`N_VEnableLinearSumVectorArray_Hip` (*C function*), 149

`N_VEnableLinearSumVectorArray_ManyVector` (*C function*), 169

`N_VEnableLinearSumVectorArray_MPIManyVector` (*C function*), 173

`N_VEnableLinearSumVectorArray_OpenMP` (*C function*), 132

`N_VEnableLinearSumVectorArray_OpenMPDEV` (*C function*), 165

`N_VEnableLinearSumVectorArray_Parallel` (*C function*), 128

`N_VEnableLinearSumVectorArray_ParHyp` (*C function*), 138

`N_VEnableLinearSumVectorArray_Petsc` (*C function*), 140

`N_VEnableLinearSumVectorArray_Pthreads` (*C function*), 136

`N_VEnableLinearSumVectorArray_Raja` (*C function*), 159

`N_VEnableLinearSumVectorArray_Serial` (*C function*), 125

`N_VEnableLinearSumVectorArray_Sycl` (*C++ function*), 154

`N_VEnableScaleAddMulti_Cuda` (*C function*), 144

`N_VEnableScaleAddMulti_Hip` (*C function*), 149

`N_VEnableScaleAddMulti_ManyVector` (*C function*), 169

`N_VEnableScaleAddMulti_MPIManyVector` (*C function*), 173

`N_VEnableScaleAddMulti_OpenMP` (*C function*), 132

`N_VEnableScaleAddMulti_OpenMPDEV` (*C function*), 165

`N_VEnableScaleAddMulti_Parallel` (*C function*), 128

`N_VEnableScaleAddMulti_ParHyp` (*C function*), 138

`N_VEnableScaleAddMulti_Petsc` (*C function*), 140

`N_VEnableScaleAddMulti_Pthreads` (*C function*), 136



- 135
- `N_VEnableScaleAddMulti_Raja` (*C function*), 159
- `N_VEnableScaleAddMulti_Serial` (*C function*), 124
- `N_VEnableScaleAddMulti_Sycl` (*C++ function*), 154
- `N_VEnableScaleAddMultiVectorArray_Cuda` (*C function*), 144
- `N_VEnableScaleAddMultiVectorArray_Hip` (*C function*), 149
- `N_VEnableScaleAddMultiVectorArray_OpenMP` (*C function*), 132
- `N_VEnableScaleAddMultiVectorArray_OpenMPDEV` (*C function*), 165
- `N_VEnableScaleAddMultiVectorArray_Parallel` (*C function*), 129
- `N_VEnableScaleAddMultiVectorArray_ParHyp` (*C function*), 138
- `N_VEnableScaleAddMultiVectorArray_Petsc` (*C function*), 141
- `N_VEnableScaleAddMultiVectorArray_Pthreads` (*C function*), 136
- `N_VEnableScaleAddMultiVectorArray_Raja` (*C function*), 159
- `N_VEnableScaleAddMultiVectorArray_Serial` (*C function*), 125
- `N_VEnableScaleAddMultiVectorArray_Sycl` (*C++ function*), 154
- `N_VEnableScaleVectorArray_Cuda` (*C function*), 144
- `N_VEnableScaleVectorArray_Hip` (*C function*), 149
- `N_VEnableScaleVectorArray_ManyVector` (*C function*), 169
- `N_VEnableScaleVectorArray_MPIManyVector` (*C function*), 173
- `N_VEnableScaleVectorArray_OpenMP` (*C function*), 132
- `N_VEnableScaleVectorArray_OpenMPDEV` (*C function*), 165
- `N_VEnableScaleVectorArray_Parallel` (*C function*), 128
- `N_VEnableScaleVectorArray_ParHyp` (*C function*), 138
- `N_VEnableScaleVectorArray_Petsc` (*C function*), 140
- `N_VEnableScaleVectorArray_Pthreads` (*C function*), 136
- `N_VEnableScaleVectorArray_Raja` (*C function*), 159
- `N_VEnableScaleVectorArray_Serial` (*C function*), 125
- `N_VEnableScaleVectorArray_Sycl` (*C++ function*), 154
- `N_VEnableWrmsNormMaskVectorArray_Cuda` (*C function*), 144
- `N_VEnableWrmsNormMaskVectorArray_Hip` (*C function*), 149
- `N_VEnableWrmsNormMaskVectorArray_ManyVector` (*C function*), 169
- `N_VEnableWrmsNormMaskVectorArray_MPI-ManyVector` (*C function*), 173
- `N_VEnableWrmsNormMaskVectorArray_OpenMP` (*C function*), 132
- `N_VEnableWrmsNormMaskVectorArray_OpenMPDEV` (*C function*), 165
- `N_VEnableWrmsNormMaskVectorArray_Parallel` (*C function*), 129
- `N_VEnableWrmsNormMaskVectorArray_ParHyp` (*C function*), 138
- `N_VEnableWrmsNormMaskVectorArray_Petsc` (*C function*), 141
- `N_VEnableWrmsNormMaskVectorArray_Pthreads` (*C function*), 136
- `N_VEnableWrmsNormMaskVectorArray_Serial` (*C function*), 125
- `N_VEnableWrmsNormVectorArray_Cuda` (*C function*), 144
- `N_VEnableWrmsNormVectorArray_Hip` (*C function*), 149
- `N_VEnableWrmsNormVectorArray_ManyVector` (*C function*), 169
- `N_VEnableWrmsNormVectorArray_MPIManyVector` (*C function*), 173
- `N_VEnableWrmsNormVectorArray_OpenMP` (*C function*), 132
- `N_VEnableWrmsNormVectorArray_OpenMPDEV` (*C function*), 165
- `N_VEnableWrmsNormVectorArray_Parallel` (*C function*), 128
- `N_VEnableWrmsNormVectorArray_ParHyp` (*C function*), 138
- `N_VEnableWrmsNormVectorArray_Petsc` (*C function*), 141
- `N_VEnableWrmsNormVectorArray_Pthreads` (*C function*), 136
- `N_VEnableWrmsNormVectorArray_Serial` (*C function*), 125
- `N_VFreeEmpty` (*C function*), 108
- `N_VGetArrayPointer` (*C function*), 110
- `N_VGetArrayPointer_MPIPlusX` (*C function*), 175
- `N_VGetCommunicator` (*C function*), 111
- `N_VGetDeviceArrayPointer` (*C function*), 110
- `N_VGetDeviceArrayPointer_Cuda` (*C function*), 142
- `N_VGetDeviceArrayPointer_Hip` (*C function*), 147
- `N_VGetDeviceArrayPointer_OpenMPDEV` (*C function*), 164
- `N_VGetDeviceArrayPointer_Raja` (*C function*), 158
- `N_VGetDeviceArrayPointer_Sycl` (*C++ function*), 153
- `N_VGetHostArrayPointer_Cuda` (*C function*), 142
- `N_VGetHostArrayPointer_Hip` (*C function*), 147
- `N_VGetHostArrayPointer_OpenMPDEV` (*C function*),

- 164
- N\_VGetHostArrayPointer\_Raja (C function), 158
- N\_VGetHostArrayPointer\_Sycl (C++ function), 153
- N\_VGetLength (C function), 111
- N\_VGetLocalLength (C function), 111
- N\_VGetLocalLength\_MPIPlusX (C function), 174
- N\_VGetLocalLength\_Parallel (C function), 128
- N\_VGetLocalVector\_MPIPlusX (C function), 174
- N\_VGetNumSubvectors\_ManyVector (C function), 169
- N\_VGetNumSubvectors\_MPIManyVector (C function), 172
- N\_VGetSubvector\_ManyVector (C function), 168
- N\_VGetSubvector\_MPIManyVector (C function), 172
- N\_VGetSubvectorArrayPointer\_ManyVector (C function), 168
- N\_VGetSubvectorArrayPointer\_MPIManyVector (C function), 172
- N\_VGetSubvectorLocalLength\_ManyVector (C function), 168
- N\_VGetSubvectorLocalLength\_MPIManyVector (C function), 172
- N\_VGetVecAtIndexVectorArray (C function), 106
- N\_VGetVector\_ParHyp (C function), 138
- N\_VGetVector\_Petsc (C function), 140
- N\_VGetVector\_Trilinos (C++ function), 166
- N\_VGetVectorID (C function), 109
- N\_VInv (C function), 112
- N\_VInvTest (C function), 114
- N\_VInvTestLocal (C function), 119
- N\_VIsManagedMemory\_Cuda (C function), 142
- N\_VIsManagedMemory\_Hip (C function), 147
- N\_VIsManagedMemory\_Raja (C function), 158
- N\_VIsManagedMemory\_Sycl (C++ function), 153
- N\_VL1Norm (C function), 114
- N\_VL1NormLocal (C function), 118
- N\_VLinearCombination (C function), 115
- N\_VLinearCombinationVectorArray (C function), 117
- N\_VLinearSum (C function), 111
- N\_VLinearSumVectorArray (C function), 116
- N\_VMake\_Cuda (C function), 143
- N\_VMake\_Hip (C function), 148
- N\_VMake\_MPIManyVector (C function), 171
- N\_VMake\_MPIPlusX (C function), 174
- N\_VMake\_OpenMP (C function), 131
- N\_VMake\_OpenMPDEV (C function), 164
- N\_VMake\_Parallel (C function), 128
- N\_VMake\_ParHyp (C function), 137
- N\_VMake\_Petsc (C function), 140
- N\_VMake\_Pthreads (C function), 135
- N\_VMake\_Raja (C function), 158
- N\_VMake\_Serial (C function), 124
- N\_VMake\_Sycl (C++ function), 153
- N\_VMake\_Trilinos (C++ function), 166
- N\_VMakeManaged\_Cuda (C function), 143
- N\_VMakeManaged\_Hip (C function), 148
- N\_VMakeManaged\_Raja (C function), 158
- N\_VMakeManaged\_Sycl (C++ function), 153
- N\_VMakeWithManagedAllocator\_Cuda (C function), 143
- N\_VMaxNorm (C function), 113
- N\_VMaxNormLocal (C function), 118
- N\_VMin (C function), 113
- N\_VMinLocal (C function), 118
- N\_VMinQuotient (C function), 115
- N\_VMinQuotientLocal (C function), 120
- N\_VNew\_Cuda (C function), 142
- N\_VNew\_Hip (C function), 147
- N\_VNew\_ManyVector (C function), 168
- N\_VNew\_MPIManyVector (C function), 171
- N\_VNew\_OpenMP (C function), 131
- N\_VNew\_OpenMPDEV (C function), 164
- N\_VNew\_Parallel (C function), 127
- N\_VNew\_Pthreads (C function), 135
- N\_VNew\_Raja (C function), 158
- N\_VNew\_Serial (C function), 124
- N\_VNew\_Sycl (C++ function), 152
- N\_VNewEmpty (C function), 107
- N\_VNewEmpty\_Cuda (C function), 143
- N\_VNewEmpty\_Hip (C function), 148
- N\_VNewEmpty\_OpenMP (C function), 131
- N\_VNewEmpty\_OpenMPDEV (C function), 164
- N\_VNewEmpty\_Parallel (C function), 128
- N\_VNewEmpty\_ParHyp (C function), 137
- N\_VNewEmpty\_Petsc (C function), 140
- N\_VNewEmpty\_Pthreads (C function), 135
- N\_VNewEmpty\_Raja (C function), 158
- N\_VNewEmpty\_Serial (C function), 124
- N\_VNewEmpty\_Sycl (C++ function), 153
- N\_VNewManaged\_Cuda (C function), 142
- N\_VNewManaged\_Hip (C function), 148
- N\_VNewManaged\_Raja (C function), 158
- N\_VNewManaged\_Sycl (C++ function), 152
- N\_VNewVectorArray (C function), 106
- N\_VNewWithMemHelp\_Cuda (C function), 142
- N\_VNewWithMemHelp\_Hip (C function), 148
- N\_VNewWithMemHelp\_Raja (C function), 158
- N\_VNewWithMemHelp\_Sycl (C++ function), 153
- N\_VPrint\_Cuda (C function), 143
- N\_VPrint\_Hip (C function), 148
- N\_VPrint\_OpenMP (C function), 131
- N\_VPrint\_OpenMPDEV (C function), 164
- N\_VPrint\_Parallel (C function), 128
- N\_VPrint\_ParHyp (C function), 138
- N\_VPrint\_Petsc (C function), 140
- N\_VPrint\_Pthreads (C function), 135
- N\_VPrint\_Raja (C function), 158
- N\_VPrint\_Serial (C function), 124



N\_VPrint\_Sycl (C++ function), 154  
 N\_VPrintFile\_Cuda (C function), 143  
 N\_VPrintFile\_Hip (C function), 148  
 N\_VPrintFile\_OpenMP (C function), 132  
 N\_VPrintFile\_OpenMPDEV (C function), 164  
 N\_VPrintFile\_Parallel (C function), 128  
 N\_VPrintFile\_ParHyp (C function), 138  
 N\_VPrintFile\_Petsc (C function), 140  
 N\_VPrintFile\_Pthreads (C function), 135  
 N\_VPrintFile\_Raja (C function), 159  
 N\_VPrintFile\_Serial (C function), 124  
 N\_VPrintFile\_Sycl (C++ function), 154  
 N\_VProd (C function), 111  
 N\_VScale (C function), 112  
 N\_VScaleAddMulti (C function), 115  
 N\_VScaleAddMultiVectorArray (C function), 117  
 N\_VScaleVectorArray (C function), 116  
 N\_VSetArrayPointer (C function), 111  
 N\_VSetArrayPointer\_MPIPlusX (C function), 175  
 N\_VSetDeviceArrayPointer\_Sycl (C++ function), 153  
 N\_VSetHostArrayPointer\_Sycl (C++ function), 153  
 N\_VSetKernelExecPolicy\_Cuda (C function), 143  
 N\_VSetKernelExecPolicy\_Hip (C function), 148  
 N\_VSetKernelExecPolicy\_Sycl (C++ function), 153  
 N\_VSetSubvectorArrayPointer\_ManyVector (C function), 169  
 N\_VSetSubvectorArrayPointer\_MPIManyVector (C function), 172  
 N\_VSetVecAtIndexVectorArray (C function), 107  
 N\_VSpace (C function), 110  
 N\_VWl2Norm (C function), 114  
 N\_VWrmsNorm (C function), 113  
 N\_VWrmsNormMask (C function), 113  
 N\_VWrmsNormMaskVectorArray (C function), 117  
 N\_VWrmsNormVectorArray (C function), 117  
 N\_VWSqrSumLocal (C function), 119  
 N\_VWSqrSumMaskLocal (C function), 119  
 NV\_COMM\_P (C macro), 127  
 NV\_CONTENT\_OMP (C macro), 130  
 NV\_CONTENT\_OMPDEV (C macro), 163  
 NV\_CONTENT\_P (C macro), 126  
 NV\_CONTENT\_PT (C macro), 134  
 NV\_CONTENT\_S (C macro), 123  
 NV\_DATA\_DEV\_OMPDEV (C macro), 163  
 NV\_DATA\_HOST\_OMPDEV (C macro), 163  
 NV\_DATA\_OMP (C macro), 130  
 NV\_DATA\_P (C macro), 126  
 NV\_DATA\_PT (C macro), 134  
 NV\_DATA\_S (C macro), 123  
 NV\_GLOBLLENGTH\_P (C macro), 127  
 NV\_Ith\_OMP (C macro), 131  
 NV\_Ith\_P (C macro), 127  
 NV\_Ith\_PT (C macro), 134

NV\_Ith\_S (C macro), 124  
 NV\_LENGTH\_OMP (C macro), 131  
 NV\_LENGTH\_OMPDEV (C macro), 163  
 NV\_LENGTH\_PT (C macro), 134  
 NV\_LENGTH\_S (C macro), 123  
 NV\_LOCLENGTH\_P (C macro), 127  
 NV\_NUM\_THREADS\_OMP (C macro), 131  
 NV\_NUM\_THREADS\_PT (C macro), 134  
 NV\_OWN\_DATA\_OMP (C macro), 130  
 NV\_OWN\_DATA\_OMPDEV (C macro), 163  
 NV\_OWN\_DATA\_P (C macro), 126  
 NV\_OWN\_DATA\_PT (C macro), 134  
 NV\_OWN\_DATA\_S (C macro), 123

## R

realtype (C type), 62

## S

SM\_COLS\_B (C macro), 199  
 SM\_COLS\_D (C macro), 185  
 SM\_COLUMN\_B (C macro), 199  
 SM\_COLUMN\_D (C macro), 185  
 SM\_COLUMN\_ELEMENT\_B (C macro), 199  
 SM\_COLUMNS\_B (C macro), 198  
 SM\_COLUMNS\_D (C macro), 184  
 SM\_COLUMNS\_S (C macro), 206  
 SM\_CONTENT\_B (C macro), 196  
 SM\_CONTENT\_D (C macro), 184  
 SM\_CONTENT\_S (C macro), 206  
 SM\_DATA\_B (C macro), 198  
 SM\_DATA\_D (C macro), 185  
 SM\_DATA\_S (C macro), 208  
 SM\_ELEMENT\_B (C macro), 199  
 SM\_ELEMENT\_D (C macro), 185  
 SM\_INDEXPTRS\_S (C macro), 208  
 SM\_INDEXVALS\_S (C macro), 208  
 SM\_LBAND\_B (C macro), 198  
 SM\_LDATA\_B (C macro), 198  
 SM\_LDATA\_D (C macro), 184  
 SM\_LDIM\_B (C macro), 198  
 SM\_NNZ\_S (C macro), 206  
 SM\_NP\_S (C macro), 208  
 SM\_ROWS\_B (C macro), 196  
 SM\_ROWS\_D (C macro), 184  
 SM\_ROWS\_S (C macro), 206  
 SM\_SPARSETYPE\_S (C macro), 208  
 SM\_SUBAND\_B (C macro), 198  
 SM\_UBAND\_B (C macro), 198  
 SUN\_LOGLEVEL\_ALL (C enumerator), 43  
 SUN\_LOGLEVEL\_DEBUG (C enumerator), 43  
 SUN\_LOGLEVEL\_ERROR (C enumerator), 43  
 SUN\_LOGLEVEL\_INFO (C enumerator), 43  
 SUN\_LOGLEVEL\_NONE (C enumerator), 43  
 SUN\_LOGLEVEL\_WARNING (C enumerator), 43

- SUN\_OUTPUTFORMAT\_CSV (*C enumerator*), 63  
 SUN\_OUTPUTFORMAT\_TABLE (*C enumerator*), 63  
 SUNATimesFn (*C type*), 223  
 SUNBandLinearSolver (*C function*), 233  
 SUNBandMatrix (*C function*), 199  
 SUNBandMatrix\_Cols (*C function*), 200  
 SUNBandMatrix\_Column (*C function*), 200  
 SUNBandMatrix\_Columns (*C function*), 200  
 SUNBandMatrix\_Data (*C function*), 200  
 SUNBandMatrix\_LData (*C function*), 200  
 SUNBandMatrix\_LDim (*C function*), 200  
 SUNBandMatrix\_LowerBandwidth (*C function*), 200  
 SUNBandMatrix\_Print (*C function*), 200  
 SUNBandMatrix\_Rows (*C function*), 200  
 SUNBandMatrix\_StoredUpperBandwidth (*C function*), 200  
 SUNBandMatrix\_UpperBandwidth (*C function*), 200  
 SUNBandMatrixStorage (*C function*), 199  
 SUNContext (*C type*), 37  
 SUNContext\_Create (*C function*), 37  
 SUNContext\_Free (*C function*), 38  
 SUNContext\_GetLogger (*C function*), 39  
 SUNContext\_GetProfiler (*C function*), 38  
 SUNContext\_SetLogger (*C function*), 38  
 SUNContext\_SetProfiler (*C function*), 38  
 SUNCudaBlockReduceAtomicExecPolicy (*C++ function*), 146  
 SUNCudaBlockReduceExecPolicy (*C++ function*), 146  
 SUNCudaExecPolicy (*C++ type*), 145  
 SUNCudaGridStrideExecPolicy (*C++ function*), 146  
 SUNCudaThreadDirectExecPolicy (*C++ function*), 146  
 SUNDenseLinearSolver (*C function*), 234  
 SUNDenseMatrix (*C function*), 185  
 SUNDenseMatrix\_Cols (*C function*), 186  
 SUNDenseMatrix\_Column (*C function*), 186  
 SUNDenseMatrix\_Columns (*C function*), 186  
 SUNDenseMatrix\_Data (*C function*), 186  
 SUNDenseMatrix\_LData (*C function*), 186  
 SUNDenseMatrix\_Print (*C function*), 185  
 SUNDenseMatrix\_Rows (*C function*), 185  
 SUNDIALSFileClose (*C function*), 56  
 SUNDIALSFileOpen (*C function*), 56  
 SUNDIALSGetVersion (*C function*), 49  
 SUNDIALSGetVersionNumber (*C function*), 49  
 SUNHipBlockReduceAtomicExecPolicy (*C++ function*), 151  
 SUNHipBlockReduceExecPolicy (*C++ function*), 151  
 SUNHipExecPolicy (*C++ type*), 150  
 SUNHipGridStrideExecPolicy (*C++ function*), 151  
 SUNHipThreadDirectExecPolicy (*C++ function*), 151  
 sunindextype (*C type*), 63  
 SUNKLU (*C function*), 237  
 SUNKLUReInit (*C function*), 237  
 SUNKLUSetOrdering (*C function*), 237  
 SUNLapackBand (*C function*), 239  
 SUNLapackDense (*C function*), 241  
 SUNLinearSolver (*C type*), 225  
 SUNLinSol\_Band (*C function*), 232  
 SUNLinSol\_cuSolverSp\_batchQR (*C function*), 276  
 SUNLinSol\_cuSolverSp\_batchQR\_GetDescription (*C function*), 277  
 SUNLinSol\_cuSolverSp\_batchQR\_GetDeviceSpace (*C function*), 277  
 SUNLinSol\_cuSolverSp\_batchQR\_SetDescription (*C function*), 277  
 SUNLinSol\_Dense (*C function*), 234  
 SUNLinSol\_KLU (*C function*), 235  
 SUNLinSol\_KLUGetCommon (*C function*), 237  
 SUNLinSol\_KLUGetNumeric (*C function*), 237  
 SUNLinSol\_KLUGetSymbolic (*C function*), 237  
 SUNLinSol\_KLUReInit (*C function*), 236  
 SUNLinSol\_KLUSetOrdering (*C function*), 236  
 SUNLinSol\_LapackBand (*C function*), 239  
 SUNLinSol\_LapackDense (*C function*), 241  
 SUNLinSol\_MagmaDense (*C function*), 243  
 SUNLinSol\_MagmaDense\_SetAsync (*C function*), 243  
 SUNLinSol\_OneMklDense (*C function*), 244  
 SUNLinSol\_PCG (*C function*), 246  
 SUNLinSol\_PCGSetMaxl (*C function*), 247  
 SUNLinSol\_PCGSetPrecType (*C function*), 246  
 SUNLinSol\_SPBCGS (*C function*), 250  
 SUNLinSol\_SPBCGSSetMaxl (*C function*), 251  
 SUNLinSol\_SPBCGSSetPrecType (*C function*), 251  
 SUNLinSol\_SPFQMR (*C function*), 255  
 SUNLinSol\_SPFQMRSetGSType (*C function*), 256  
 SUNLinSol\_SPFQMRSetMaxRestarts (*C function*), 256  
 SUNLinSol\_SPFQMRSetPrecType (*C function*), 255  
 SUNLinSol\_SPGMR (*C function*), 260  
 SUNLinSol\_SPGMRSetGSType (*C function*), 261  
 SUNLinSol\_SPGMRSetMaxRestarts (*C function*), 261  
 SUNLinSol\_SPGMRSetPrecType (*C function*), 261  
 SUNLinSol\_SPTFQMR (*C function*), 265  
 SUNLinSol\_SPTFQMRSetMaxl (*C function*), 266  
 SUNLinSol\_SPTFQMRSetPrecType (*C function*), 266  
 SUNLinSol\_SuperLUDIST (*C function*), 270  
 SUNLinSol\_SuperLUDIST\_GetBerr (*C function*), 270  
 SUNLinSol\_SuperLUDIST\_GetGridinfo (*C function*), 271  
 SUNLinSol\_SuperLUDIST\_GetLUstruct (*C function*), 271  
 SUNLinSol\_SuperLUDIST\_GetScalePermstruct (*C function*), 271  
 SUNLinSol\_SuperLUDIST\_GetSOLVEstruct (*C function*), 271  
 SUNLinSol\_SuperLUDIST\_GetSuperLUOptions (*C function*), 271

- SUNLinSol\_SuperLUDIST\_GetSuperLUStat (*C function*), 271
- SUNLinSol\_SuperLUMT (*C function*), 273
- SUNLinSol\_SuperLUMTSetOrdering (*C function*), 273
- SUNLinSolFree (*C function*), 220
- SUNLinSolFreeEmpty (*C function*), 227
- SUNLinSolGetID (*C function*), 219
- SUNLinSolGetType (*C function*), 218
- SUNLinSolInitialize (*C function*), 219
- SUNLinSolLastFlag (*C function*), 222
- SUNLinSolNewEmpty (*C function*), 227
- SUNLinSolNumIters (*C function*), 222
- SUNLinSolResid (*C function*), 222
- SUNLinSolResNorm (*C function*), 222
- SUNLinSolSetATimes (*C function*), 221
- SUNLinSolSetInfoFile\_PCG (*C function*), 247
- SUNLinSolSetInfoFile\_SPBCGS (*C function*), 251
- SUNLinSolSetInfoFile\_SPGMR (*C function*), 256
- SUNLinSolSetInfoFile\_SPGMR (*C function*), 261
- SUNLinSolSetInfoFile\_SPTFQMR (*C function*), 266
- SUNLinSolSetPreconditioner (*C function*), 221
- SUNLinSolSetPrintLevel\_PCG (*C function*), 248
- SUNLinSolSetPrintLevel\_SPBCGS (*C function*), 252
- SUNLinSolSetPrintLevel\_SPGMR (*C function*), 257
- SUNLinSolSetPrintLevel\_SPGMR (*C function*), 262
- SUNLinSolSetPrintLevel\_SPTFQMR (*C function*), 267
- SUNLinSolSetScalingVectors (*C function*), 221
- SUNLinSolSetup (*C function*), 219
- SUNLinSolSetZeroGuess (*C function*), 221
- SUNLinSolSolve (*C function*), 220
- SUNLinSolSpace (*C function*), 222
- SUNLogger (*C type*), 43
- SUNLogger\_Create (*C function*), 43
- SUNLogger\_CreateFromEnv (*C function*), 43
- SUNLogger\_Destroy (*C function*), 45
- SUNLogger\_Flush (*C function*), 45
- SUNLogger\_GetOutputRank (*C function*), 45
- SUNLogger\_QueueMsg (*C function*), 44
- SUNLogger\_SetDebugFilename (*C function*), 44
- SUNLogger\_SetErrorFilename (*C function*), 44
- SUNLogger\_SetInfoFilename (*C function*), 44
- SUNLogger\_SetWarningFilename (*C function*), 44
- SUNLogLevel (*C enum*), 43
- SUNMatClone (*C function*), 181
- SUNMatCopy (*C function*), 182
- SUNMatCopyOps (*C function*), 180
- SUNMatDestroy (*C function*), 182
- SUNMatFreeEmpty (*C function*), 181
- SUNMatGetID (*C function*), 181
- SUNMatMatvec (*C function*), 183
- SUNMatMatvecSetup (*C function*), 183
- SUNMatNewEmpty (*C function*), 180
- SUNMatrix (*C type*), 179
- SUNMatrix\_cuSparse\_BlockColumns (*C function*), 203
- SUNMatrix\_cuSparse\_BlockData (*C function*), 203
- SUNMatrix\_cuSparse\_BlockNNZ (*C function*), 203
- SUNMatrix\_cuSparse\_BlockRows (*C function*), 203
- SUNMatrix\_cuSparse\_Columns (*C function*), 202
- SUNMatrix\_cuSparse\_CopyFromDevice (*C function*), 203
- SUNMatrix\_cuSparse\_CopyToDevice (*C function*), 203
- SUNMatrix\_cuSparse\_Data (*C function*), 203
- SUNMatrix\_cuSparse\_IndexPointers (*C function*), 203
- SUNMatrix\_cuSparse\_IndexValues (*C function*), 203
- SUNMatrix\_cuSparse\_MakeCSR (*C function*), 202
- SUNMatrix\_cuSparse\_MatDescr (*C function*), 203
- SUNMatrix\_cuSparse\_NewBlockCSR (*C function*), 202
- SUNMatrix\_cuSparse\_NewCSR (*C function*), 202
- SUNMatrix\_cuSparse\_NNZ (*C function*), 202
- SUNMatrix\_cuSparse\_NumBlocks (*C function*), 203
- SUNMatrix\_cuSparse\_Rows (*C function*), 202
- SUNMatrix\_cuSparse\_SetFixedPattern (*C function*), 203
- SUNMatrix\_cuSparse\_SetKernelExecPolicy (*C function*), 204
- SUNMatrix\_cuSparse\_SparseType (*C function*), 202
- SUNMatrix\_MagmaDense (*C function*), 187
- SUNMatrix\_MagmaDense\_Block (*C function*), 189
- SUNMatrix\_MagmaDense\_BlockColumn (*C function*), 189
- SUNMatrix\_MagmaDense\_BlockColumns (*C function*), 188
- SUNMatrix\_MagmaDense\_BlockData (*C function*), 189
- SUNMatrix\_MagmaDense\_BlockRows (*C function*), 188
- SUNMatrix\_MagmaDense\_Column (*C function*), 189
- SUNMatrix\_MagmaDense\_Columns (*C function*), 188
- SUNMatrix\_MagmaDense\_CopyFromDevice (*C function*), 190
- SUNMatrix\_MagmaDense\_CopyToDevice (*C function*), 190
- SUNMatrix\_MagmaDense\_Data (*C function*), 189
- SUNMatrix\_MagmaDense\_LData (*C function*), 188
- SUNMatrix\_MagmaDense\_NumBlocks (*C function*), 189
- SUNMatrix\_MagmaDense\_Rows (*C function*), 188
- SUNMatrix\_MagmaDenseBlock (*C function*), 187
- SUNMatrix\_OneMklDense (*C++ function*), 191
- SUNMatrix\_OneMklDense\_Block (*C function*), 194
- SUNMatrix\_OneMklDense\_BlockColumn (*C function*), 194
- SUNMatrix\_OneMklDense\_BlockColumns (*C function*), 193
- SUNMatrix\_OneMklDense\_BlockData (*C function*), 194

`SUNMatrix_OneMklDense_BlockLData` (C function), 194

`SUNMatrix_OneMklDense_BlockRows` (C function), 193

`SUNMatrix_OneMklDense_Column` (C function), 193

`SUNMatrix_OneMklDense_Columns` (C function), 192

`SUNMatrix_OneMklDense_CopyFromDevice` (C function), 195

`SUNMatrix_OneMklDense_CopyToDevice` (C function), 195

`SUNMatrix_OneMklDense_Data` (C function), 193

`SUNMatrix_OneMklDense_LData` (C function), 193

`SUNMatrix_OneMklDense_NumBlocks` (C function), 193

`SUNMatrix_OneMklDense_Rows` (C function), 192

`SUNMatrix_OneMklDenseBlock` (C++ function), 192

`SUNMatrix_SLUNRloc` (C function), 211

`SUNMatrix_SLUNRloc_OwnData` (C function), 211

`SUNMatrix_SLUNRloc_Print` (C function), 211

`SUNMatrix_SLUNRloc_ProcessGrid` (C function), 211

`SUNMatrix_SLUNRloc_SuperMatrix` (C function), 211

`SUNMatScaleAdd` (C function), 182

`SUNMatScaleAddI` (C function), 182

`SUNMatSpace` (C function), 182

`SUNMatZero` (C function), 182

`SUNMemory` (C type), 283

`SUNMemoryHelper` (C type), 283

`SUNMemoryHelper_Alias` (C function), 285

`SUNMemoryHelper_Alloc` (C function), 284

`SUNMemoryHelper_Alloc_Cuda` (C function), 288

`SUNMemoryHelper_Alloc_Hip` (C function), 290

`SUNMemoryHelper_Alloc_Sycl` (C function), 292

`SUNMemoryHelper_Clone` (C function), 287

`SUNMemoryHelper_Copy` (C function), 285

`SUNMemoryHelper_Copy_Cuda` (C function), 288

`SUNMemoryHelper_Copy_Hip` (C function), 290

`SUNMemoryHelper_Copy_Sycl` (C function), 292

`SUNMemoryHelper_CopyAsync` (C function), 286

`SUNMemoryHelper_CopyAsync_Cuda` (C function), 289

`SUNMemoryHelper_CopyAsync_Hip` (C function), 291

`SUNMemoryHelper_CopyAsync_Sycl` (C function), 293

`SUNMemoryHelper_CopyOps` (C function), 286

`SUNMemoryHelper_Cuda` (C function), 288

`SUNMemoryHelper_Dealloc` (C function), 284

`SUNMemoryHelper_Dealloc_Cuda` (C function), 288

`SUNMemoryHelper_Dealloc_Hip` (C function), 290

`SUNMemoryHelper_Dealloc_Sycl` (C function), 292

`SUNMemoryHelper_Destroy` (C function), 287

`SUNMemoryHelper_GetAllocStats` (C function), 286

`SUNMemoryHelper_GetAllocStats_Cuda` (C function), 289

`SUNMemoryHelper_GetAllocStats_Hip` (C function), 291

`SUNMemoryHelper_GetAllocStats_Sycl` (C function), 293

`SUNMemoryHelper_Hip` (C function), 290

`SUNMemoryHelper_NewEmpty` (C function), 286

`SUNMemoryHelper_Ops` (C type), 284

`SUNMemoryHelper_Sycl` (C function), 292

`SUNMemoryHelper_Wrap` (C function), 285

`SUNMemoryType` (C enum), 283

`SUNOutputFormat` (C enum), 63

`SUNPCG` (C function), 248

`SUNPCGSetMaxl` (C function), 248

`SUNPCGSetPrecType` (C function), 248

`SUNProfiler` (C type), 47

`SUNProfiler_Begin` (C function), 47

`SUNProfiler_Create` (C function), 47

`SUNProfiler_End` (C function), 48

`SUNProfiler_Free` (C function), 47

`SUNProfiler_Print` (C function), 48

`SUNProfiler_Reset` (C function), 48

`SUNPSetupFn` (C type), 223

`SUNPSolveFn` (C type), 223

`SUNSparseFromBandMatrix` (C function), 209

`SUNSparseFromDenseMatrix` (C function), 209

`SUNSparseMatrix` (C function), 208

`SUNSparseMatrix_Columns` (C function), 209

`SUNSparseMatrix_Data` (C function), 209

`SUNSparseMatrix_IndexPointers` (C function), 210

`SUNSparseMatrix_IndexValues` (C function), 210

`SUNSparseMatrix_NNZ` (C function), 209

`SUNSparseMatrix_NP` (C function), 209

`SUNSparseMatrix_Print` (C function), 209

`SUNSparseMatrix_Realloc` (C function), 209

`SUNSparseMatrix_Rows` (C function), 209

`SUNSparseMatrix_SparseType` (C function), 209

`SUNSPBCGS` (C function), 252

`SUNSPBCGSSetMaxl` (C function), 252

`SUNSPBCGSSetPrecType` (C function), 252

`SUNSPFGMR` (C function), 257

`SUNSPFGMRSetGStype` (C function), 257

`SUNSPFGMRSetMaxRestarts` (C function), 257

`SUNSPFGMRSetPrecType` (C function), 257

`SUNSPGMR` (C function), 262

`SUNSPGMRSetGStype` (C function), 263

`SUNSPGMRSetMaxRestarts` (C function), 263

`SUNSPGMRSetPrecType` (C function), 262

`SUNSPTFQMR` (C function), 267

`SUNSPTFQMRSetMaxl` (C function), 267

`SUNSPTFQMRSetPrecType` (C function), 267

`SUNSuperLUMT` (C function), 274

`SUNSuperLUMTSetOrdering` (C function), 274

`SUNSyclBlockReduceExecPolicy` (C++ function), 156

`SUNSyclExecPolicy` (C++ type), 155

`SUNSyclGridStrideExecPolicy` (C++ function), 156

SUNSYclThreadDirectExecPolicy (C++ *function*),  
[156](#)

## V

Vector (C++ *class*), [161](#)

Vector::~~Vector (C++ *function*), [161](#)

Vector::Convert (C++ *function*), [162](#)

Vector::HostView (C++ *function*), [162](#)

Vector::Length (C++ *function*), [161](#)

Vector::operator N\_Vector (C++ *function*), [162](#)

Vector::operator= (C++ *function*), [161](#)

Vector::Vector (C++ *function*), [161](#)

Vector::View (C++ *function*), [162](#)

vector\_type (C++ *type*), [166](#)