User Documentation for KINSOL v5.0.0-dev.1 (SUNDIALS v5.0.0-dev.1)

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Chapter 1

Introduction

KINSOL is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [19]. 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 [7]. 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) [31], FGMRES (Flexible Generalized Miniman RESidual) [30], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [32], TFQMR (Transpose-Free Quasi-Minimal Residual) [16], and PCG (Preconditioned Conjugate Gradient) [18] 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 matrix, 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 three, especially if encountering convergence failures with GMRES. Bi-CGStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size. 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 the sparse direct solvers KLU [10, 1], and the threaded sparse direct solver, SuperLU_MT [24, 12, 3].

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 multiprosessor environments with minimal impact on the rest of the solver. The vector module design is shared across the SUNDIALS suite. This NVECTOR module is written in terms of abstract vector operations with the actual routines attached by a particular implementation (such as serial or parallel) of NVECTOR. This abstraction allows writing the SUNDIALS solvers in a manner independent of the actual NVECTOR implementation (which can be user-supplied), as well as allowing more than one NVECTOR module linked into an executable file. SUNDIALS (and thus KINSOL) is supplied with serial, MPI-parallel, and both OpenMP and Pthreads thread-parallel NVECTOR implementations.

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

Changes in v5.0.0-dev.1

Several new functions were added to aid in creating custom NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL objects. The constructors N_VNewEmpty(), SUNMatNewEmpty(), SUNLinSolNewEmpty(), and SUNNonlinSolNewEmpty() allocate "empty" generic NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL objects respectively 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 these functions will ease the introduction of any new optional operations to the NVECTOR, SUNMATRIX, SUNLINSOL, or SUNNONLINSOL APIs by ensuring only required operations need to be set. Additionally, the functions N_VCopyOps(w, v) and SUNMatCopyOps(A, B) have been added to copy the operation function pointers between vector and matrix objects respectively. When used in clone routines for custom vector and matrix objects these functions also will ease the introduction of any new optional operations to the NVECTOR or SUNMATRIX APIs by ensuring all operations are copied when cloning objects.

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

Fixed a bug in the build system that prevented the NVECTOR_PTHREADS module from being built. Fixed a memory leak in the NVECTOR_PETSC clone function.

The NVECTOR_MANYVECTOR module has been split into two versions: one that requires MPI (NVECTOR_MPIMANYVECTOR) and another that does not use MPI at all (NVECTOR_MANYVECTOR). The associated example problems have been similarly updated to reflect this new structure.

An additional NVECTOR implementation, NVECTOR_MPIPLUSX, was 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.

The *_MPICuda and *_MPIRaja functions were 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 with NVECTOR_CUDA or NVECTOR_RAJA to replace the functionality. The necessary changes are minimal and should require few code modifications.

A new Fortran 2003 interface to KINSOL was added. This includes Fortran 2003 interfaces to all generic SUNDIALS types (i.e. NVECTOR, SUNMATRIX, SUNLINSOL, SUNNONLINSOL), and many of the module implementations. See Section 5 for more details.

Changes in v5.0.0-dev.0

An additional NVECTOR implementation, NVECTOR_MANYVECTOR, was created to support flexible partitioning of solution data among different processing elements (e.g., CPU + GPU) or for multiphysics problems that couple distinct MPI-based simulations together (see Section 6.13 for more details). This implementation is accompanied by additions to user documentation and SUNDIALS examples.

Eleven new optional vector operations have been added to the NVECTOR API to support the new NVECTOR_MANYVECTOR implementation (see Chapter 6 for more details). Two of the operations, N_VGetCommunicator and N_VGetLength, must be implemented by subvectors that are combined to create an NVECTOR_MANYVECTOR, but are 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 NVECTOR implementation defines any of the local operations as NULL, then the NVECTOR_MANYVECTOR will call standard NVECTOR operations to complete the computation.

A new SUNMATRIX and SUNLINSOL implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS.

A new operation, SUNMatMatvecSetup, was added to the SUNMATRIX API. 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.

The generic SUNMATRIX API now defines error codes to be returned by SUNMATRIX operations. Operations which return an integer flag indiciating success/failure may return different values than previously.

Changes in v4.1.0

An additional NVECTOR 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 NVECTOR 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.

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.

Changes in v4.0.1

No changes were made in this release.

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 SUNLINSOL 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 SUNLINSOL 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 SUNLINSOL 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_SPFGMR, 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 ${\tt SUNBandMatrix}$ 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 NVECTOR API. These *optional* operations are disabled by default and may be activated by calling vector specific routines after creating an NVECTOR (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 NVECTOR implementation defines any of these operations as NULL, then standard NVECTOR 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 NVECTOR implementation for leveraging OpenMP 4.5+ device offloading has been added, NVECTOR_OPENMPDEV. See §6.11 for more details.

Changes in v3.2.1

The changes in this minor release include the following:

- Fixed a bug in the CUDA NVECTOR 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 modified.

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 NVECTOR 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>_COMPILER can compile MPI programs before trying to locate and use an MPI installation.
- The previous options for setting MPI compiler wrappers and the executable for running MPI programs have been have been depreated. The new options that align with those used in native CMake FindMPI module are MPI_C_COMPILER, MPI_CXX_COMPILER, MPI_Fortran_COMPILER, and MPIEXEC_EXECUTABLE.
- When a Fortran name-mangling scheme is needed (e.g., LAPACK_ENABLE is ON) the build system will infer the scheme from the Fortran compiler. If a Fortran compiler is not available or the inferred or default scheme needs to be overridden, the advanced options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES can be used to manually set the name-mangling scheme and bypass trying to infer the scheme.
- Parts of the main CMakeLists.txt file were moved to new files in the src and example directories to make the CMake configuration file structure more modular.

Changes in v3.1.2

The changes in this minor release include the following:

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

- Fixed Windows specific problem where sunindextype was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows sunindextype is now defined as the MSVC basic type __int64.
- Added sparse SUNMatrix "Reallocate" routine to allow specification of the nonzero storage.
- Updated the KLU SUNLinearSolver module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.
- Updated the "ScaleAdd" and "ScaleAddl" 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.

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 NVECTOR and SUNMATRIX header files.
- Fixed an indexing bug in the CUDA NVECTOR implementation of N_VWrmsNormMask and revised the RAJA NVECTOR implementation of N_VWrmsNormMask to work with mask arrays using values other than zero or one. Replaced double with realtype in the RAJA vector test functions.
- Fixed compilation issue with GCC 7.3.0 and Fortran programs that do not require a SUNMATRIX or SUNLINSOL module (e.g., iterative linear solvers or fixed pointer solver).

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

Changes in v3.1.0

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

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

Changes in v3.0.0

All interfaces to matrix structures and linear solvers have been reworked, and all example programs have been updated. The goal of the redesign of these interfaces was to provide more encapsulation and ease in 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 Dls and Sls matrix structures in a single objectoriented 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, SPTFQMR, 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 (Dls) interfaces and scaled, preconditioned, iterative linear solver (Spils) interfaces to utilize generic SUNMATRIX and SUNLINEARSOLVER objects.
- Removed package-specific, linear solver-specific, solver modules (e.g. CVDENSE, KINBAND, IDAKLU, ARKSPGMR) since their functionality is entirely replicated by the generic Dls/Spils interfaces and SUNLINEARSOLVER/SUNMATRIX modules. The exception is CVDIAG, a diagonal approximate Jacobian solver available to CVODE and CVODES.
- Converted all SUNDIALS example problems to utilize new generic SUNMATRIX and SUNLIN-EARSOLVER objects, along with updated Dls and Spils linear solver interfaces.
- Added Spils interface routines to ARKode, CVODE, CVODES, IDA and IDAS to allow specification of a user-provided "JTSetup" routine. This change supports users who wish to set up data structures for the user-provided Jacobian-times-vector ("JTimes") routine, and where the cost of one JTSetup setup per Newton iteration can be amortized between multiple JTimes calls

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

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

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

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

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

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.

Changes in v2.9.0

Two additional NVECTOR 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 NVECTOR module now includes a function, N_VGetVectorID, that returns the NVECTOR 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 lamba 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 linit function. This ensures that these solver counters are initialized upon linear solver instantiation as well as at the beginning of the problem solution.

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

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.

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 NVECTOR 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 mxnewtstep 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+ml) was changed to smu = mu + ml 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 NVECTOR modules have been added for thread-parallel computing environments — one for OpenMP, denoted NVECTOR_OPENMP, and one for Pthreads, denoted NVECTOR_PTHREADS.

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

Changes in v2.7.0

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

A large number of 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.

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.

Changes in v2.5.0

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

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

Changes in v2.4.0

KINSPBCG, KINSPTFQMR, KINDENSE, and KINBAND modules have been added to interface with the Scaled Preconditioned Bi-CGStab (SPBCGS), Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR), DENSE, and BAND linear solver modules, respectively. (For details see Chapter 4.) 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 A.

Changes in v2.3.0

The user interface has been further refined. Several functions used for setting optional inputs were combined into a single one. 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.

Changes in v2.2.1

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

Changes in v2.2.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the iopt and ropt arrays. Instead, 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 4.

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 4 through §4.5.3 only, and looking at examples in [9]. In a different direction, a more expert user with a nonlinear system may want to (a) use a package preconditioner (§4.7), (b) supply his/her own Jacobian or preconditioner routines (§4.6), (c) supply a new NVECTOR module (Chapter 6), or even (d) supply a different linear solver module (§3.2 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 (§3.1) and the software organization of the KINSOL solver (§3.2).
- Chapter 4 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.
- In Chapter 5.1.5, we describe FKINSOL, an interface module for the use of KINSOL with FORTRAN applications.
- Chapter 6 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, and details on the four NVECTOR implementations provided with SUNDIALS.
- Chapter 7 gives a brief overview of the generic SUNMATRIX module shared among the various components of SUNDIALS, and details on the SUNMATRIX implementations provided with SUNDIALS: a dense implementation (§7.3), a banded implementation (§7.4) and a sparse implementation (§7.5).
- Chapter 8 gives a brief overview of the generic Sunlinsol module shared among the various components of Sundials. This chapter contains details on the Sunlinsol implementations provided with Sundials. The chapter also contains details on the Sunlinsol implementations provided with Sundials that interface with external linear solver libraries.
- Finally, in the appendices, we provide detailed instructions for the installation of KINSOL, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from KINSOL functions (Appendix B).

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 installation instructions that constitute important warnings are marked with a triangular symbol in the margin.



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

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<u>!</u>

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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)

Chapter 2

Mathematical Considerations

KINSOL solves nonlinear algebraic systems in real N-space.

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

$$F(u) = 0, \quad F: \mathbf{R}^N \to \mathbf{R}^N, \tag{2.1}$$

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

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

given an initial guess u_0 .

Basic Newton iteration

Depending on the linear solver used, KINSOL can employ either an Inexact Newton method [5, 7, 11, 13, 23], or a Modified Newton method. At the highest level, KINSOL implements the following iteration scheme:

- 1. Set $u_0 = \text{an initial guess}$
- 2. For $n = 0, 1, 2, \dots$ until convergence do:
 - (a) Solve $J(u_n)\delta_n = -F(u_n)$
 - (b) Set $u_{n+1} = u_n + \lambda \delta_n$, $0 < \lambda \le 1$
 - (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 δ_n , is added to u_n to produce a new iterate, u_{n+1} . A test for convergence is made before the iteration continues.

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, using either the KLU sparse solver library [10, 1], or the threadenabled SuperLU_MT sparse solver library [24, 12, 3] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT 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,
- SPBCGS, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver,
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver, or
- PCG, a scaled preconditioned CG (Conjugate Gradient method) solver.

When using a direct linear solver, the linear system in 2(a) is solved exactly, thus resulting in a Modified Newton method (the Jacobian matrix is normally out of date; see below¹). Note that the dense, band, and sparse direct linear solvers can only be used with the serial and threaded vector representations.

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.

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,
- $\|\lambda \delta_{n-1}\|_{D_{n,\infty}} > 1.5$ (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
- $\|\lambda \delta_n\|_{D_u,\infty}$ < STEPTOL with outdated Jacobian or preconditioner information.

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.

 $^{^{1}}$ KINSOL allows the user to enforce a Jacobian evaluation at each iteration thus allowing for an Exact Newton iteration.

Scaling

To address the case of ill-conditioned nonlinear systems, KINSOL allows prescribing 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. In the text below, we use the following scaled norms:

$$||z||_{D_u} = ||D_u z||_2, \quad ||z||_{D_F} = ||D_F z||_2, \quad ||z||_{D_u,\infty} = ||D_u z||_\infty, \quad \text{and} \quad ||z||_{D_F,\infty} = ||D_F z||_\infty$$
 (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 (2.7) and (2.9) below.

Globalization strategy

Two methods of applying a computed step δ_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 λ always set to 1. The other method is a global strategy, which attempts to use the direction implied by δ_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 α and β conditions of the Goldstein-Armijo linesearch given in [13] for step 2(b), where λ 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 the value λ such that $u_n + \lambda \delta_n$ satisfies the sufficient decrease condition (or α -condition)

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

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

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

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

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

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

For more details, the reader is referred to [13].

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 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

$$\|\lambda \delta_n\|_{D_{\infty,\infty}} < \text{STEPTOL},$$

where 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.

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 δ_n in Step 2(b) is scaled to take a step of that length.

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 ω is given by

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

with ρ defined as

$$\rho = \frac{\|F(u_n)\|_{D_F}}{\text{FTOL}}\,,\tag{2.5}$$

where FTOL is the input scalar tolerance discussed before. Optionally, a constant value ω_{const} can be used for the parameter ω .

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

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 [14]. More precisely, the Krylov iteration must pass a stopping test

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

where η_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 γ and α are 0.9 and 2, respectively.

Constant η

$$\eta_n = constant,$$

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 η does not decrease too quickly [14].

Difference quotient Jacobian approximations

With the dense and banded matrix-based linear solvers, 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

$$J^{ij} = [F^i(u + \sigma_i e^j) - F^i(u)]/\sigma_i.$$
 (2.6)

The increments σ_i are given by

$$\sigma_j = \sqrt{U} \, \max \{ |u^j|, 1/D_u^j \} \,.$$
 (2.7)

In the dense case, this scheme requires N evaluations of F, one for each column of J. In the band case, the columns of J are computed in groups, by the Curtis-Powell-Reid algorithm, with the number of F evaluations equal to the bandwidth. 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

$$J(u)v \approx [F(u+\sigma v) - F(u)]/\sigma, \qquad (2.8)$$

where u is the current approximation to a root of (2.1), and σ is a scalar. The choice of σ is taken from [7] and is given by

$$\sigma = \frac{\max\{|u^T v|, u_{typ}^T | v|\}}{\|v\|_2^2} \operatorname{sign}(u^T v) \sqrt{U}, \qquad (2.9)$$

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 σ remains appropriately small, as shown in [5].

Basic Fixed Point iteration

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

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

Here, u_n is the *n*th iterate to u. At each stage in the iteration process, function G is applied to the current iterate 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 $u_0 = \text{an initial guess}$
- 2. For $n = 0, 1, 2, \dots$ until convergence do:
 - (a) Set $u_{n+1} = G(u_n) = u_n L^{-1}F(u_n)$.
 - (b) 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 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 p. 182 of [28].

Anderson Acceleration

The Picard and fixed point methods can be significantly accelerated using Anderson's method [4, 33, 15, 27]. Anderson acceleration can be formulated as follows:

- 1. Set $u_0 =$ an initial guess and $m \ge 1$
- 2. Set $u_1 = G(u_0)$
- 3. For $n = 0, 1, 2, \dots$ until convergence do:
 - (a) Set $m_n = \min\{m, n\}$
 - (b) Set $F_n = (f_{n-m_n}, ..., f_n)$, 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 $u_{n+1} = \sum_{i=0}^{m_n} \alpha_i^{(n)} G(u_{n-m_n+i})$
 - (e) Test for convergence

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

- 1. Set $u_0 = \text{an initial guess and } m \geq 1$
- 2. Set $u_1 = G(u_0)$
- 3. For $n = 0, 1, 2, \dots$ 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 $u_{n+1} = G(u_n) \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i}$ with $\Delta g_i = G(u_{i+1}) G(u_i)$
 - (e) Test for convergence

The least-squares problem in (c) is solved by applying a QR factorization to $\Delta F_n = Q_n R_n$ and solving $R_n \gamma = Q_n^T f_n$.

Fixed-point - Anderson Acceleration Stopping Criterion

The default stopping criterion is

$$||G(u_{n+1}) - u_{n+1}||_{D_{F,\infty}} < \text{GTOL},$$

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.

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

3.1 SUNDIALS organization

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

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

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

3.2 KINSOL organization

The KINSOL package is written in the ANSI C language. This section 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 Figure 3.3. The central solver module, implemented in the files kinsol.h, kinsol_impl.h and kinsol.c, deals with the solution of a nonlinear algebraic system using either an Inexact Newton method or a line search method for the global strategy. Although this module contains logic for the Newton iteration, it has no knowledge of the method used to solve the linear systems that arise. For any given user problem, one of the linear system solver modules is specified, and is then invoked as needed.

KINSOL now has a single unified linear solver interface, KINLS, supporting both direct and iterative linear solvers built using the generic SUNLINSOL API (see Chapter 8). These solvers may utilize a SUNMATRIX object (see Chapter 7) for storing Jacobian information, or they may be matrix-free. Since KINSOL can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to KINSOL will expand as new SUNLINSOL modules are developed.

For users employing dense or banded Jacobian matrices, KINLS includes algorithms for their approximation through difference quotients, but the user also has the option of supplying the Jacobian

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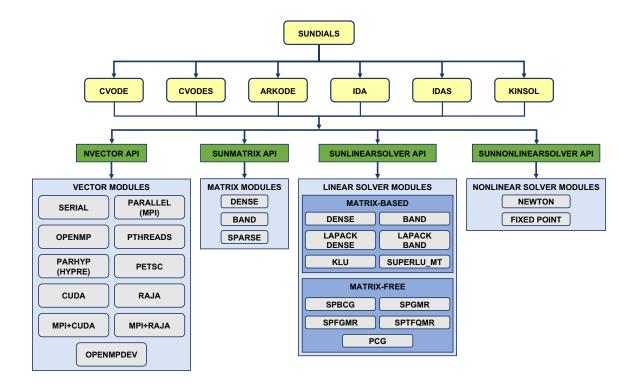


Figure 3.1: High-level diagram of the SUNDIALS suite

(or an approximation to it) directly. This user-supplied routine is required when using sparse or user-supplied Jacobian matrices.

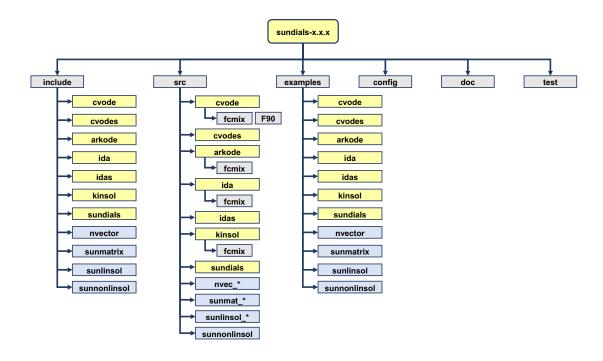
For users employing matrix-free iterative linear solvers, KINLS includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector, Jv. Again, the user has the option of providing routines for this operation, in two phases: setup (preprocessing 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 [6, 8], 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 solution, as required to achieve convergence. The call list within the central KINSOL module to each of the associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

KINSOL also provides a preconditioner module called KINBBDPRE for use with any of the Krylov iterative linear solvers. It works in conjunction with NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a banded matrix, as further described in §4.7.

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



(a) Directory structure of the SUNDIALS source tree



(b) Directory structure of the Sundials examples

Figure 3.2: Organization of the SUNDIALS suite

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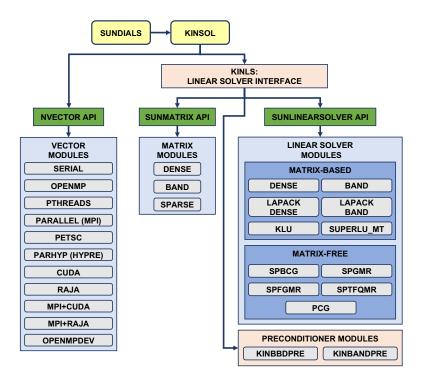


Figure 3.3: Overall structure diagram of the KINSOL package. Modules specific to KINSOL are distinguished by rounded boxes, while generic solver and auxiliary modules are in rectangular boxes. Grayed boxes refer to the encompassing SUNDIALS structure. Note also that the LAPACK, KLU and SUPERLUMT support is through interfaces to external packages. Users will need to download and compile those packages independently.

Chapter 4

Using KINSOL for C Applications

This chapter is concerned with the use of KINSOL for the solution of nonlinear systems. The following subsections treat the header files, the layout of the user's main program, description of the KINSOL user-callable routines, and user-supplied functions. The sample programs described in the companion document [9] may also be helpful. Those codes may be used as templates (with the removal of some lines involved in testing), and are included in the KINSOL package.

Users with applications written in FORTRAN should see Chapter 5.1.5, which describes the FORTRAN/C interface module.

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

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 Appendix B.

4.1 Access to library and header files

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

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

- *libdir*/libsundials_kinsol. *lib*,
- libdir/libsundials_nvec*. lib (one to four files),

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

- incdir/include/kinsol
- incdir/include/sundials
- incdir/include/nvector
- incdir/include/sunmatrix

• incdir/include/sunlinsol

The directories *libdir* and *incdir* are the install library and include directories, respectively. For a default installation, these are *builddir*/lib and *builddir*/include, respectively, where *builddir* was defined in Appendix A.

4.2 Data types

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

4.2.1 Floating point types

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

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

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

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

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

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

4.2.2 Integer types used for vector and matrix indices

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

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

4.3 Header files 29

4.3 Header files

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

• kinsol/kinsol.h, the header file for KINSOL, which defines several types and various constants, and includes function prototypes. This includes the header file for KINLS, kinsol/kinsol.ls.h.

kinsol.h also includes sundials_types.h, which defines the types realtype, sunindextype, and booleantype and constants SUNFALSE and SUNTRUE.

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

If using a Newton or Picard nonlinear solver that requires the solution of a linear system, then a linear solver module header file will be required. The header files corresponding to the various SUNDIALS-provided linear solver modules available for use with KINSOL are:

• Direct linear solvers:

- sunlinsol/sunlinsol_dense.h, which is used with the dense linear solver module, SUN-LINSOL_DENSE;
- sunlinsol/sunlinsol_band.h, which is used with the banded linear solver module, SUN-LINSOL_BAND;
- sunlinsol/sunlinsol_lapackdense.h, which is used with the LAPACK package dense linear solver module, SUNLINSOL_LAPACKDENSE;
- sunlinsol/sunlinsol_lapackband.h, which is used with the LAPACK package banded linear solver module, SUNLINSOL_LAPACKBAND;
- sunlinsol/sunlinsol_klu.h, which is used with the KLU sparse linear solver module, SUNLINSOL_KLU;
- sunlinsol/sunlinsol_superlumt.h, which is used with the SUPERLUMT sparse linear solver module, SUNLINSOL_SUPERLUMT;

• Iterative linear solvers:

- sunlinsol/sunlinsol_spgmr.h, which is used with the scaled, preconditioned GMRES Krylov linear solver module, SUNLINSOL_SPGMR;
- sunlinsol/sunlinsol_spfgmr.h, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, SUNLINSOL_SPFGMR;
- sunlinsol/sunlinsol_spbcgs.h, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, SUNLINSOL_SPBCGS;
- sunlinsol/sunlinsol_sptfqmr.h, which is used with the scaled, preconditioned TFQMR
 Krylov linear solver module, SUNLINSOL_SPTFQMR;
- sunlinsol/sunlinsol_pcg.h, which is used with the scaled, preconditioned CG Krylov linear solver module, SUNLINSOL_PCG;

The header files for the SUNLINSOL_DENSE and SUNLINSOL_LAPACKDENSE linear solver modules include the file sunmatrix_dense.h, which defines the SUNMATRIX_DENSE matrix module, as as well as various functions and macros acting on such matrices.

The header files for the SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND linear solver modules include the file sunmatrix/sunmatrix_band.h, which defines the SUNMATRIX_BAND matrix module, as as well as various functions and macros acting on such matrices.

The header files for the SUNLINSOL_KLU and SUNLINSOL_SUPERLUMT sparse linear solvers include the file sunmatrix_sparse.h, which defines the SUNMATRIX_SPARSE matrix module, as well as various functions and macros acting on such matrices.

The header files for the Krylov iterative solvers include the file sundials_sundials_iterative.h, which enumerates the kind of preconditioning, and (for the SPGMR and SPFGMR solvers) the choices for the Gram-Schmidt process.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the kinFoodWeb_kry_p example (see [9]), preconditioning is done with a block-diagonal matrix. For this, even though the SUNLINSOL_SPGMR linear solver is used, the header sundials/sundials_dense.h is included for access to the underlying generic dense matrix arithmetic routines.

4.4 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the solution of a nonlinear system problem. Most of the steps are independent of the NVECTOR, SUNMATRIX, and SUNLINSOL implementations used. For the steps that are not, refer to Chapter 6, 7, and 8 for the specific name of the function to be called or macro to be referenced.

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

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

2. Set problem dimensions etc.

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

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

3. Set vector with initial guess

To set the vector **u** of initial guess values, use the appropriate functions defined by the particular NVECTOR implementation.

For native SUNDIALS vector implementations (except the CUDA and RAJA-based ones), use a call of the form $\mathbf{u} = \mathbf{N}_{\text{VMake}} ****(..., \mathbf{udata})$ if the realtype array udata containing the initial values of u already exists. Otherwise, create a new vector by making a call of the form $\mathbf{u} = \mathbf{N}_{\text{VNew}} ***(...)$, and then set its elements by accessing the underlying data with a call of the form $\mathbf{ydata} = \mathbf{N}_{\text{VGetArrayPointer}}(\mathbf{u})$. See §6.3-6.6 for details.

For the hypre and PETSc vector wrappers, first create and initialize the underlying vector and then create an NVECTOR wrapper with a call of the form u = N_VMake_***(uvec), where uvec is a hypre or PETSc vector. Note that calls like N_VNew_***(...) and N_VGetArrayPointer(...) are not available for these vector wrappers. See §6.7 and §6.8 for details.

If using either the CUDA- or RAJA-based vector implementations use a call of the form u = N_VMake_***(..., c) where c is a pointer to a suncudavec or sunrajavec vector class if this class already exists. Otherwise, create a new vector by making a call of the form u = N_VNew_***(...), and then set its elements by accessing the underlying data where it is located with a call of the form N_VGetDeviceArrayPointer_*** or N_VGetHostArrayPointer_***. Note that the vector class will allocate memory on both the host and device when instantiated. See §6.9-6.10 for details.

4. Create KINSOL object

Call kin_mem = KINCreate() to create the KINSOL memory block. KINCreate returns a pointer to the KINSOL memory structure. See §4.5.1 for details.

5. Allocate internal memory

Call KINInit(...) to specify the problem defining function F, allocate internal memory for KINSOL, and initialize KINSOL. KINInit returns a flag to indicate success or an illegal argument value. See §4.5.1 for details.

6. Create matrix object

If a matrix-based linear solver is to be used within a Newton or Picard iteration, then a template Jacobian matrix must be created by using the appropriate functions defined by the particular SUNMATRIX implementation.

For the SUNDIALS-supplied SUNMATRIX implementations, the matrix object may be created using a call of the form

```
SUNMatrix J = SUNBandMatrix(...);
or
SUNMatrix J = SUNDenseMatrix(...);
or
SUNMatrix J = SUNSparseMatrix(...);
```

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

7. Create linear solver object

If a Newton or Picard iteration is chosen, then the desired linear solver object must be created by using the appropriate functions defined by the particular SUNLINSOL implementation.

For any of the SUNDIALS-supplied SUNLINSOL implementations, the linear solver object may be created using a call of the form

```
SUNLinearSolver LS = SUNLinSol_*(...);
```

where * can be replaced with "Dense", "SPGMR", or other options, as discussed in §4.5.2 and Chapter 8.

8. Set linear solver optional inputs

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

9. Attach linear solver module

If a Newton or Picard iteration is chosen, initialize the KINLS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with one of the following calls (for details see §4.5.2):

```
ier = KINSetLinearSolver(...);
```

10. Set optional inputs

Call KINSet* routines to change from their default values any optional inputs that control the behavior of KINSOL. See §4.5.4 for details.

11. Solve problem

Call ier = KINSol(...) to solve the nonlinear problem for a given initial guess. See §4.5.3 for details.

12. Get optional outputs

Call KINGet* functions to obtain optional output. See §4.5.5 for details.

13. Deallocate memory for solution vector

Upon completion of the solution, deallocate memory for the vector **u** by calling the appropriate destructor function defined by the NVECTOR implementation:

```
N_VDestroy(u);
```

14. Free solver memory

Call KINFree(&kin_mem) to free the memory allocated for KINSOL.

15. Free linear solver and matrix memory

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

16. Finalize MPI, if used

Call MPI_Finalize() to terminate MPI.

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

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

Linear Solver	Serial	Parallel (MPI)	OpenMP	pThreads	hypre	PETSC	CUDA	RAJA	User Supp.
Dense	√		√	√					√
Band	√		√	√					√
LapackDense	√		√	√					√
LapackBand	√		√	√					√
KLU	√		√	√					\checkmark
SUPERLUMT	√		√	√					\checkmark
SPGMR	\checkmark	✓	√	√	√	\checkmark	\checkmark	√	\checkmark
SPFGMR	√	✓	√	√	√	√	√	√	\checkmark
SPBCGS	√	✓	√	√	√	√	√	√	√
SPTFQMR	√	√	√	√	√	√	√	√	√
PCG	√	√	√	√	√	√	√	√	√
User Supp.	√	✓	√	√	√	√	√	√	√

4.5 User-callable functions

This section describes the KINSOL functions that are called by the user to set up and solve a nonlinear problem. Some of these are required. However, starting with §4.5.4, the functions listed involve optional inputs/outputs or restarting, and those paragraphs can be skipped for a casual use of KINSOL. In any case, refer to §4.4 for the correct order of these calls.

The return flag (when present) for each of these routines is a negative integer if an error occurred, and non-negative otherwise.

4.5.1 KINSOL initialization and deallocation functions

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

Call kin_mem = KINCreate();

Description The function KINCreate instantiates a KINSOL solver object.

Arguments This function has no arguments.

Return value If successful, KINCreate returns a pointer to the newly created KINSOL memory block

(of type void *). If an error occurred, KINCreate prints an error message to stderr

and returns NULL.

KINInit

Call flag = KINInit(kin_mem, func, tmpl);

Description The function KINInit specifies the problem-defining function, allocates internal mem-

ory, and initializes KINSOL.

Arguments kin_mem (void *) pointer to the KINSOL memory block returned by KINCreate.

func (KINSysFn) is the C function which computes the system function F (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 §4.6.1.)

tmpl (N_Vector) 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 The return value flag (of type int) will be one of the following:

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.

KINFree

Call KINFree(&kin_mem);

Description The function KINFree frees the memory allocated by a previous call to KINCreate.

Arguments The argument is the address of the pointer to the KINSOL memory block returned by

KINCreate (of type void *).

Return value The function KINFree has no return value.

4.5.2 Linear solver specification function

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 Sunlinsol modules. Here, matrix-based sunlinsol modules utilize sunmatrix objects to store the Jacobian matrix $J = \partial F/\partial u$ and factorizations used throughout the solution process. Conversely, matrix-free sunlinsol 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 §4.5.4 and §4.6. 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 SUNLINSOL object and call the function KINSetLinearSolver, as documented below. To create the SUNLinearSolver object, the user may call one of the SUNDIALS-packaged SUNLINSOL module constructor routines via a call of the form

```
SUNLinearSolver LS = SUNLinSol_*(...);
```

The current list of such constructor routines includes SUNLinSol_Dense, SUNLinSol_Band, SUNLinSol_LapackDense, SUNLinSol_LapackBand, SUNLinSol_KLU, SUNLinSol_SuperLUMT, SUNLinSol_SPGMR, SUNLinSol_SPFGMR, SUNLinSol_SPTFQMR, and SUNLinSol_PCG.

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 SUNLINSOL 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 SUNLINSOL object to use for solving Newton or Picard systems. The third argument is an optional SUNMATRIX object to accompany matrix-based SUNLINSOL 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.

KINSetLinearSolver

Call flag = KINSetLinearSolver(kin_mem, LS, J);

Description The function KINSetLinearSolver attaches a g

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 (void *) pointer to the KINSOL memory block.

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

J (SUNMatrix) SUNMATRIX object for used as a template for the Jacobian (or NULL if not applicable).

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

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.

4.5.3 KINSOL solver function

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

KINSol

Call flag = KINSol(kin_mem, u, strategy, u_scale, f_scale);

Description The function KINSol computes an approximate solution to the nonlinear system.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

u (N_Vector) 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 (int) 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 (N_Vector) 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 (N_Vector) vector containing diagonal elements of scaling matrix D_F for F(u) chosen so that the components of $D_F \cdot F(u)$ (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 On return, KINSol returns the approximate solution in the vector **u** if successful. The return value flag (of type int) will be one of the following:

KIN_SUCCESS

KINSol succeeded; the scaled norm of F(u) is less than fnormtol.

KIN_INITIAL_GUESS_OK

The guess $\mathbf{u} = u_0$ satisfied the system F(u) = 0 within the tolerances specified (the scaled norm of $F(u_0)$ is less than 0.01 *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 §4.5.4 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 scsteptol 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 $||D_u p||_{L^2} > 0.99$ 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.

4.5.4 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 4.2 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. For the most casual use of KINSOL, the reader can skip to §4.6.

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 flag < 0 will catch any error.

Table 4.2: Optional inputs for KINSOL and KINLS

Optional input	Function name	Default						
KINSOL main solver								
Error handler function	KINSetErrHandlerFn	internal fn.						
Pointer to an error file	KINSetErrFile	stderr						
Info handler function	KINSetInfoHandlerFn	internal fn.						
Pointer to an info file	KINSetInfoFile	stdout						
Data for problem-defining function	KINSetUserData	NULL						
Verbosity level of output	KINSetPrintLevel	0						
Max. number of nonlinear iterations	KINSetNumMaxIters	200						
No initial matrix setup	KINSetNoInitSetup	SUNFALSE						
No residual monitoring*	KINSetNoResMon	SUNFALSE						
Max. iterations without matrix setup	KINSetMaxSetupCalls	10						
Max. iterations without residual check*	KINSetMaxSubSetupCalls	5						
Form of η coefficient	KINSetEtaForm	KIN_ETACHOICE1						
Constant value of η	KINSetEtaConstValue	0.1						
Values of γ and α	KINSetEtaParams	0.9 and 2.0						
Values of ω_{min} and ω_{max}^*	KINSetResMonParams	0.00001 and 0.9						
Constant value of ω^*	KINSetResMonConstValue	0.9						
Lower bound on ϵ	KINSetNoMinEps	SUNFALSE						
Max. scaled length of Newton step	KINSetMaxNewtonStep	$ 1000 D_uu_0 _2$						
Max. number of β -condition failures	KINSetMaxBetaFails	10						
Rel. error for D.Q. Jv	KINSetRelErrFunc	$\sqrt{\text{uround}}$						
Function-norm stopping tolerance	KINSetFuncNormTol	$uround^{1/3}$						
Scaled-step stopping tolerance	KINSetScaledSteptol	$uround^{2/3}$						
Inequality constraints on solution	KINSetConstraints	NULL						
Nonlinear system function	KINSetSysFunc	none						
Anderson Acceleration subspace size	KINSetMAA	0						
KINLS linear solver interface								
Jacobian function	KINSetJacFn	DQ						
Preconditioner functions and data	KINSetPreconditioner	NULL, NULL, NULL						
Jacobian-times-vector function and data	KINSetJacTimesVecFn	internal DQ,						
		NULL						

4.5.4.1 Main solver optional input functions

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

KINSetErrFile

Call flag = KINSetErrFile(kin_mem, errfp);

 $\label{thm:local_problem} \textbf{Description} \quad \text{The function $\tt KINSol$ messages} \\$

should be directed when the default KINSOL error handler function is used.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

errfp (FILE *) pointer to output file.

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

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.

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.

KINSetErrHandlerFn

Call flag = KINSetErrHandlerFn(kin_mem, ehfun, eh_data);

Description The function KINSetErrHandlerFn specifies the optional user-defined function to be

used in handling error messages.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

ehfun (KINErrHandlerFn) is the user's C error handler function (see §4.6.2).

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

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

KIN_SUCCESS The function enfun 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.

KINSetInfoFile

Call flag = KINSetInfoFile(kin_mem, infofp);

Description The function KINSetInfoFile specifies the pointer to the file where all informative

(non-error) messages should be directed.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

infofp (FILE *) pointer to output file.

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

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.



KINSetInfoHandlerFn

Call flag = KINSetInfoHandlerFn(kin_mem, ihfun, ih_data);

Description The function KINSetInfoHandlerFn specifies the optional user-defined function to be

used in handling informative (non-error) messages.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

ihfun (KINInfoHandlerFn) is the user's C information handler function (see §4.6.3).

ih_data (void *) pointer to user data passed to ihfun every time it is called.

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

KIN_SUCCESS The function infun and data pointer in_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) mes-

sages to the file specified by the file pointer infofp (see KINSetInfoFile above).

KINSetPrintLevel

Call flag = KINSetPrintLevel(kin_mem, printfl);

Description The function KINSetPrintLevel specifies the level of verbosity of the output.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

printfl (int) flag indicating the level of verbosity. Must be one of:

0 no information displayed.

1 for each nonlinear iteration display the following information: the scaled Euclidean ℓ_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 The return value flag (of type int) is one of:

KIN_SUCCESS The optional value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KIN_ILL_INPUT The argument printfl had an illegal value.

Notes The default value for printfl is 0.

KINSetUserData

Call flag = KINSetUserData(kin_mem, user_data);

Description The function KINSetUserData specifies the pointer to user-defined memory that is to

be passed to all user-supplied functions.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

user_data (void *) pointer to the user-defined memory.

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

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.

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.



KINSetNumMaxIters

Call flag = KINSetNumMaxIters(kin_mem, mxiter);

Description The function KINSetNumMaxIters specifies the maximum number of nonlinear iterations

allowed.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

mxiter (long int) maximum number of nonlinear iterations.

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

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.

KINSetNoInitSetup

Call flag = KINSetNoInitSetup(kin_mem, noInitSetup);

Description The function KINSetNoInitSetup specifies whether an initial call to the preconditioner

or Jacobian setup function should be made or not.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

noInitSetup (booleantype) flag controlling whether an initial call to the precondi-

tioner or Jacobian setup function is made (pass SUNFALSE) or not made

(pass SUNTRUE).

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

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.

KINSetNoResMon

Call flag = KINSetNoResMon(kin_mem, noNNIResMon);

Description The function KINSetNoResMon specifies whether or not the nonlinear residual monitoring

scheme is used to control Jacobian updating

Arguments kin_mem (void *) pointer to the KINSOL memory block.

noNNIResMon (booleantype) flag controlling whether residual monitoring is used (pass

SUNFALSE) or not used (pass SUNTRUE).

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

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.

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

KINSetMaxSetupCalls

Call flag = KINSetMaxSetupCalls(kin_mem, msbset);

Description 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 (void *) pointer to the KINSOL memory block.

msbset (long int) maximum number of nonlinear iterations without a call to the preconditioner or Jacobian setup function. Pass 0 to indicate the default.

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

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).

KINSetMaxSubSetupCalls

Call flag = KINSetMaxSubSetupCalls(kin_mem, msbsetsub);

 $\label{thm:condition} \textbf{Description} \quad \text{The function $\tt KINSetMaxSubSetupCalls} \ \ \text{specifies the maximum number of nonlinear} \\$

iterations between checks by the residual monitoring algorithm.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

msbsetsub (long int) maximum number of nonlinear iterations without checking the nonlinear residual. Pass 0 to indicate the default.

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

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.

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

KINSetEtaForm

Call flag = KINSetEtaForm(kin_mem, etachoice);

Description The function KINSetEtaForm specifies the method for computing the value of the η

coefficient used in the calculation of the linear solver convergence tolerance.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

etachoice (int) flag indicating the method for computing η . The value must be one of KIN_ETACHOICE1, KIN_ETACHOICE2, or KIN_ETACONSTANT (see Chapter 2 for details).

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

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 $\eta_{\rm safe} > 0.1$. For KIN_ETACHOICE1

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

and for KIN_ETACHOICE2

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

where γ and α 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 $\eta_{\max} = 0.9$.

KINSetEtaConstValue

Call flag = KINSetEtaConstValue(kin_mem, eta);

Description The function KINSetEtaConstValue specifies the constant value for η in the case etachoice = KIN_ETACONSTANT.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

eta (realtype) constant value for η . Pass 0.0 to indicate the default.

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

KIN_SUCCESS The optional value has been successfully set.

 ${\tt KIN_MEM_NULL} \quad {\tt The \; kin_mem \; pointer \; is \; NULL}.$

KIN_ILL_INPUT The argument eta had an illegal value

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

KINSetEtaParams

Call flag = KINSetEtaParams(kin_mem, egamma, ealpha);

Description The function KINSetEtaParams specifies the parameters γ and α in the formula for η , in the case etachoice = KIN_ETACHOICE2.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

egamma (realtype) value of the γ parameter. Pass 0.0 to indicate the default. ealpha (realtype) value of the α parameter. Pass 0.0 to indicate the default.

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

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 $0.0 < \text{egamma} \le 1.0 \text{ and } 1.0 < \text{ealpha} \le 2.0.$

KINSetResMonConstValue

Call flag = KINSetResMonConstValue(kin_mem, omegaconst);

Description The function KINSetResMonConstValue specifies the constant value for ω when using

residual monitoring.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

omegaconst (realtype) constant value for ω . Passing 0.0 results in using Eqn. (2.4).

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

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 < omegaconst < 1.0.

KINSetResMonParams

Call flag = KINSetResMonParams(kin_mem, omegamin, omegamax);

Description The function KINSetResMonParams specifies the parameters ω_{min} and ω_{max} in the for-

mula (2.4) for ω .

Arguments kin_mem (void *) pointer to the KINSOL memory block.

omegamin (realtype) value of the ω_{min} parameter. Pass 0.0 to indicate the default. omegamax (realtype) value of the ω_{max} parameter. Pass 0.0 to indicate the default.

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

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 < omegamin < omegamax < 1.0.

${\tt KINSetNoMinEps}$

Call flag = KINSetNoMinEps(kin_mem, noMinEps);

Description The function KINSetNoMinEps specifies a flag that controls whether or not the value of

 ϵ , the scaled linear residual tolerance, is bounded from below.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

noMinEps (booleantype) flag controlling the bound on ϵ . If SUNFALSE is passed the value of ϵ is constrained and if SUNTRUE is passed then ϵ is not constrained.

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

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*fnormtol, is applied to ϵ (see KINSetFuncNormTol below).

KINSetMaxNewtonStep

Call flag = KINSetMaxNewtonStep(kin_mem, mxnewtstep);

Description The function KINSetMaxNewtonStep specifies the maximum allowable scaled length of

the Newton step.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

mxnewtstep (realtype) maximum scaled step length (≥ 0.0). Pass 0.0 to indicate the default.

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

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 mxnewtstep is $1000 \|u_0\|_{D_u}$, where u_0 is the initial guess.

KINSetMaxBetaFails

Call flag = KINSetMaxBetaFails(kin_mem, mxnbcf);

Description The function KINSetMaxBetaFails specifies the maximum number of β -condition fail-

ures in the linesearch algorithm.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

mxnbcf (realtype) maximum number of β -condition failures. Pass 0.0 to indicate the

default.

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

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.

KINSetRelErrFunc

Call flag = KINSetRelErrFunc(kin_mem, relfunc);

Description 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.(2.7)]

or the Jacobian-vector product [see Eq.(2.9)]. The value stored is $\sqrt{\text{relfunc}}$.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

relfunc (realtype) relative error in F(u) (relfunc ≥ 0.0). Pass 0.0 to indicate the

default.

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

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 = unit roundoff.

KINSetFuncNormTol

Call flag = KINSetFuncNormTol(kin_mem, fnormtol);

Description 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 (void *) pointer to the KINSOL memory block.

fnormtol (realtype) tolerance for stopping based on scaled function norm (≥ 0.0).

Pass 0.0 to indicate the default.

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

 ${\tt KIN_SUCCESS} \quad \text{ The optional value has been successfully set.}$

KIN_MEM_NULL The kin_mem pointer is NULL.

KIN_ILL_INPUT The tolerance was negative.

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

KINSetScaledStepTol

Call flag = KINSetScaledStepTol(kin_mem, scsteptol);

 $\label{prop:condition} \textbf{Description} \quad \text{The function $\tt KINSetScaledStepTol specifies the scalar used as a stopping tolerance on the scalar used as a stopping tolerance of the scalar used as a sc$

the minimum scaled step length.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

scsteptol (realtype) tolerance for stopping based on scaled step length (≥ 0.0). Pass

0.0 to indicate the default.

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

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 (unit roundoff) $^{2/3}$.

KINSetConstraints

Call flag = KINSetConstraints(kin_mem, constraints);

Description The function KINSetConstraints specifies a vector that defines inequality constraints

for each component of the solution vector u.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

constraints (N_Vector) 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 $u_i > 0.0$.

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

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.

KINSetSysFunc

Call flag = KINSetSysFunc(kin_mem, func);

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

Arguments kin_mem (void *) pointer to the KINSOL memory block.

func (KINSysFn) user-supplied function that evaluates F(u) (or G(u) for fixed-point iteration).

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

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.

KINSetMAA

Call flag = KINSetMAA(kin_mem, maa);

Description The function KINSetMAA specifies the size of the subspace used with Anderson acceler-

ation in conjunction with Picard or fixed-point iteration.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

maa (long int) subspace size for various methods. A value of 0 means no acceler-

ation, while a positive value means acceleration will be done.

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

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 ${\tt maa}$ is 0, indicating no acceleration. The value of ${\tt maa}$ 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.

4.5.4.2 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 a dense or banded matrix 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.

KINSetJacFn

Call flag = KINSetJacFn(kin_mem, jac);

Description The function KINSetJacFn specifies the Jacobian approximation function to be used.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

jac (KINLsJacFn) user-defined Jacobian approximation function.

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

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

By default, KINLS uses an internal difference quotient function for dense and band matrices. If NULL is passed to jac, this default function is used. An error will occur if no jac is supplied when using a sparse or user-supplied matrix.

This function must be called *after* the KINLS linear solver interface has been initialized through a call to KINSetLinearSolver.

The function type KINLsJacFn is described in §4.6.4.

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 §4.6.5 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.

KINSetJacTimesVecFn

Call flag = KINSetJacTimesVecFn(kin_mem, jtimes);

Description The function KINSetJacTimesVecFn specifies the Jacobian-vector product function.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

jtimes (KINLsJacTimesVecFn) user-defined Jacobian-vector product function.

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

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 §4.6.5.

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 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 §4.6. 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.

KINSetPreconditioner

Call flag = KINSetPreconditioner(kin_mem, psetup, psolve);

Description The function KINSetPreconditioner specifies the preconditioner setup and solve func-

tions.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

psetup (KINLsPrecSetupFn) user-defined function to set up the preconditioner. Pass

NULL if no setup operation is necessary.

psolve (KINLsPrecSolveFn) user-defined preconditioner solve function.

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

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 SUNLINSOL

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.

The function type KINLsPrecSolveFn is described in $\S4.6.6$.

The function type KINLsPrecSetupFn is described in §4.6.7.

The previous routine KINSpilsSetPreconditioner 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.

4.5.5 Optional output functions

KINSOL provides an extensive list of functions that can be used to obtain solver performance information. Table 4.3 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).

4.5.5.1 SUNDIALS version information

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

SUNDIALSGetVersion

Call flag = SUNDIALSGetVersion(version, len);

Description The function SUNDIALSGetVersion fills a character array with SUNDIALS version infor-

mation.

Arguments version (char *) character array to hold the SUNDIALS version information.

len (int) allocated length of the version character array.

Return value If successful, SUNDIALSGetVersion returns 0 and version contains the SUNDIALS ver-

sion information. Otherwise, it returns -1 and version is not set (the input character

array is too short).

Notes A string of 25 characters should be sufficient to hold the version information. Any

trailing characters in the version array are removed.

Optional output Function name KINSOL main solver Size of Kinsol real and integer workspaces KINGetWorkSpace Number of function evaluations KINGetNumFuncEvals Number of nonlinear iterations KINGetNumNolinSolvIters Number of β -condition failures KINGetNumBetaCondFails Number of backtrack operations KINGetNumBacktrackOps Scaled norm of FKINGetFuncNorm Scaled norm of the step KINGetStepLength KINLS linear solver interface Size of real and integer workspaces KINGetLinWorkSpace No. of Jacobian evaluations KINGetNumJacEvals No. of F calls for D.Q. Jacobian[-vector] evals. KINGetNumLinFuncEvals No. of linear iterations KINGetNumLinIters No. of linear convergence failures KINGetNumLinConvFails No. of preconditioner evaluations KINGetNumPrecEvals No. of preconditioner solves KINGetNumPrecSolves No. of Jacobian-vector product evaluations KINGetNumJtimesEvals Last return from a kinls function KINGetLastLinFlag Name of constant associated with a return flag KINGetLinReturnFlagName

Table 4.3: Optional outputs from KINSOL and KINLS

SUNDIALSGetVersionNumber

Call flag = SUNDIALSGetVersionNumber(&major, &minor, &patch, label, len);

Description The function SUNDIALSGetVersionNumber set integers for the SUNDIALS major, minor,

and patch release numbers and fills a character array with the release label if applicable.

Arguments major (int) SUNDIALS release major version number.

minor (int) SUNDIALS release minor version number.

patch (int) SUNDIALS release patch version number.

label (char *) character array to hold the SUNDIALS release label.

len (int) allocated length of the label character array.

Return value If successful, SUNDIALSGetVersionNumber returns 0 and the major, minor, patch, and

 ${\tt label}$ values are set. Otherwise, it returns -1 and the values are not set (the input

character array is too short).

Notes A string of 10 characters should be sufficient to hold the label information. If a label

is not used in the release version, no information is copied to label. Any trailing

characters in the label array are removed.

4.5.5.2 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.

KINGetWorkSpace

Call flag = KINGetWorkSpace(kin_mem, &lenrw, &leniw);

Description The function KINGetWorkSpace returns the KINSOL integer and real workspace sizes.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

lenrw (long int) the number of realtype values in the KINSOL workspace.

leniw (long int) the number of integer values in the KINSOL workspace.

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

KIN_SUCCESS The optional output values have been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

Notes

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).

KINGetNumFuncEvals

Call flag = KINGetNumFuncEvals(kin_mem, &nfevals);

Description The function KINGetNumFuncEvals returns the number of evaluations of the system

function.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nfevals (long int) number of calls to the user-supplied function that evaluates F(u).

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KINGetNumNonlinSolvIters

Call flag = KINGetNumNonlinSolvIters(kin_mem, &nniters);

Description The function KINGetNumNonlinSolvIters returns the number of nonlinear iterations.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nniters (long int) number of nonlinear iterations.

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KINGetNumBetaCondFails

Call flag = KINGetNumBetaCondFails(kin_mem, &nbcfails);

Description The function KINGetNumBetaCondFails returns the number of β -condition failures.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nbcfails (long int) number of β -condition failures.

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KINGetNumBacktrackOps

Call flag = KINGetNumBacktrackOps(kin_mem, &nbacktr);

Description The function KINGetNumBacktrackOps returns the number of backtrack operations (step

length adjustments) performed by the line search algorithm.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nbacktr (long int) number of backtrack operations.

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KINGetFuncNorm

Call flag = KINGetFuncNorm(kin_mem, &fnorm);

Description The function KINGetFuncNorm returns the scaled Euclidean ℓ_2 norm of the nonlinear

system function F(u) evaluated at the current iterate.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

fnorm (realtype) current scaled norm of F(u).

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

KINGetStepLength

Call flag = KINGetStepLength(kin_mem, &steplength);

Description The function KINGetStepLength returns the scaled Euclidean ℓ_2 norm of the step used

during the previous iteration.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

steplength (realtype) scaled norm of the Newton step.

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

KIN_SUCCESS The optional output value has been successfully set.

KIN_MEM_NULL The kin_mem pointer is NULL.

4.5.5.3 KINLS linear solver interface optional output functions

The following optional outputs are available from the KINLS module: workspace requirements, number of calls to the Jacobian routine, number of calls to the system function routine for difference quotient Jacobian or Jacobian-vector approximation, number of linear iterations, number of linear convergence failures, number of calls to the preconditioner setup and solve routines, number of calls to the Jacobian-vector product routine, and last return value from a KINLS function.

KINGetLinWorkSpace

Call flag = KINGetLinWorkSpace(kin_mem, &lenrwLS, &leniwLS);

Description The function KINGetLinWorkSpace returns the KINLS real and integer workspace sizes.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

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

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

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

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 interface has not been initialized.

Notes

The workspace requirements reported by this routine correspond only to memory allocated within this interface and to memory allocated by the SUNLINSOL object attached to it. The template Jacobian matrix allocated by the user outside of KINLS is not included in this report.

In a parallel setting, the above values are global (i.e., summed over all processors).

The previous routines KINDlsGetWorkspace and KINSpilsGetWorkspace 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.

KINGetNumJacEvals

Call flag = KINGetNumJacEvals(kin_mem, &njevals);

Description The function KINGetNumJacEvals returns the cummulative number of calls to the KINLS

Jacobian approximation function.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

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

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

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 interface has not been initialized.

Notes

The previous routine KINDlsGetNumJacEvals 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.

KINGetNumLinFuncEvals

Call flag = KINGetNumLinFuncEvals(kin_mem, &nfevalsLS);

Description The function KINGetNumLinFuncEvals returns the number of calls to the user system

function used to compute the difference quotient approximation to the Jacobian or to

the Jacobian-vector product.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nfevalsLS (long int) the number of calls to the user system function.

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

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 interface has not been initialized.

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

The previous routines KINDlsGetNumFuncEvals and KINSpilsGetNumFuncEvals 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.

KINGetNumLinIters

Call flag = KINGetNumLinIters(kin_mem, &nliters);

Description The function KINGetNumLinIters returns the cumulative number of linear iterations.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nliters (long int) the current number of linear iterations.

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

KINLS_SUCCESS The optional output value has been successfully set.

KINLS_MEM_NULL The kin_mem pointer is NULL.

KINIS_LMEM_NULL The KINLS linear solver interface has not been initialized.

Notes The previous routine KINSpilsGetNumLinIters 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.

KINGetNumLinConvFails

Call flag = KINGetNumLinConvFails(kin_mem, &nlcfails);

Description The function KINGetNumLinConvFails returns the cumulative number of linear conver-

gence failures.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

nlcfails (long int) the current number of linear convergence failures.

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

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 interface has not been initialized.

Notes The previous routine KINSpilsGetNumConvFails 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.

KINGetNumPrecEvals

Call flag = KINGetNumPrecEvals(kin_mem, &npevals);

Description The function KINGetNumPrecEvals returns the cumulative number of preconditioner

evaluations, i.e., the number of calls made to psetup.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

npevals (long int) the current number of calls to psetup.

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

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 interface has not been initialized.

Notes The previous routine KINSpilsGetNumPrecEvals 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.

KINGetNumPrecSolves

Call flag = KINGetNumPrecSolves(kin_mem, &npsolves);

Description The function KINGetNumPrecSolves returns the cumulative number of calls made to

the preconditioner solve function, psolve.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

npsolves (long int) the current number of calls to psolve.

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

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 interface has not been initialized.

Notes The previous routine KINSpilsGetNumPrecSolves 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.

KINGetNumJtimesEvals

Call flag = KINGetNumJtimesEvals(kin_mem, &njvevals);

Description The function KINGetNumJtimesEvals returns the cumulative number made to the Jacobian-

vector product function, jtimes.

kin_mem (void *) pointer to the KINSOL memory block. Arguments

njvevals (long int) the current number of calls to jtimes.

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

The optional output value has been successfully set. KINLS_SUCCESS

KINLS_MEM_NULL The kin_mem pointer is NULL.

KINLS_LMEM_NULL The KINLS linear solver interface has not been initialized.

Notes The previous routine KINSpilsGetNumJtimesEvals 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.

KINGetLastLinFlag

Call flag = KINGetLastLinFlag(kin_mem, &lsflag);

Description The function KINGetLastLinFlag returns the last return value from a KINLS routine.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

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

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

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 interface has not been initialized.

Notes

If the KINLS setup function failed (i.e. KINSolve returned KIN_LSETUP_FAIL) when using the SUNLINSOL_DENSE or SUNLINSOL_BAND modules, then the value of lsflag is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the (dense or banded) Jacobian matrix.

If the KINLS setup function failed when using another SUNLINSOL module, then 1sflag will be SUNLS_PSET_FAIL_UNREC, SUNLS_ASET_FAIL_UNREC, or SUNLS_PACKAGE_FAIL_UNREC.

If the KINLS solve function failed (i.e., KINSol returned KIN_LSOLVE_FAIL), then lsflag contains the error return flag from the SUNLINSOL object, which will be one of the following:

SUNLS_MEM_NULL, indicating that the SUNLINSOL memory is NULL;

SUNLS_ATIMES_FAIL_UNREC, indicating an unrecoverable failure in the Jacobian-times-vector function:

SUNLS_PSOLVE_FAIL_UNREC, indicating that the preconditioner solve function, psolve, failed with an unrecoverable error;

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.

The previous routines KINDlsGetLastFlag and KINSpilsGetLastFlag 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.

KINGetLinReturnFlagName

Call name = KINGetLinReturnFlagName(lsflag);

Description The function KINGetLinReturnFlagName returns the name of the KINLS constant cor-

responding to lsflag.

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

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

Notes The previous routines KINDlsGetReturnFlagName and KINSpilsGetReturnFlagName

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 tran-

sition to the new routine name soon.

4.6 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.

4.6.1 Problem-defining function

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

KINSysFn

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

Purpose This function computes F(u) (or G(u) for fixed-point iteration and Anderson accelera-

tion) for a given value of the vector u.

Arguments u is the current value of the variable vector, u.

fval is the output vector F(u).

user_data is a pointer to user data, the pointer user_data passed to KINSetUserData.

Return value A KINSysFn function should return 0 if successful, a positive value if a recoverable error

occurred (in which case $\tt KINSOL$ will attempt to correct), or a negative value if it failed unrecoverably (in which case the solution process is halted and $\tt KIN_SYSFUNC_FAIL$ is

returned).

Notes Allocation of memory for fval is handled within KINSOL.

4.6.2 Error message handler function

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

KINErrHandlerFn

```
Definition typedef void (*KINErrHandlerFn)(int error_code, const char *module, const char *function, char *msg, void *eh_data);
```

Purpose 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.

msg is the error message.

eh_data is a pointer to user data, the same as the eh_data parameter passed to

KINSetErrHandlerFn.

Return value A KINErrHandlerFn 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.

4.6.3 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:

KINInfoHandlerFn

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

Purpose This function processes informational messages from KINSOL and its sub-modules.

Arguments module is the name of the KINSOL module reporting the information.

function is the name of the function reporting the information.

msg is the message.

ih_data is a pointer to user data, the same as the ih_data parameter passed to

 ${\tt KINSetInfoHandlerFn}.$

Return value A KINInfoHandlerFn function has no return value.

4.6.4 Jacobian construction (matrix-based linear solvers)

If a matrix-based linear solver module is used (i.e., a non-NULL SUNMATRIX object J was supplied to KINSetLinearSolver), the user may provide a function of type KINLsJacFn defined as follows

KINLsJacFn

Definition typedef int (*KINLsJacFn)(N_Vector u, N_Vector fu,

SUNMatrix J, void *user_data,
N_Vector tmp1, N_Vector tmp2);

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

Arguments u

u is the current (unscaled) iterate.

fu is the current value of the vector F(u).

J is the output approximate Jacobian matrix, $J=\partial F/\partial u$, of type SUNMatrix. 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 the KINJacFn function as temporary storage or work space.

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

banded:

A user-supplied banded Jacobian function must load the $\mathbb{N} \times \mathbb{N}$ 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) = $J_{m,n}$. The elements within the band are those with -mupper \leq m-n \leq mlower. Alternatively, SM_COLUMN_B(J, j) returns a pointer to the diagonal element of the j-th column of 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) = $J_{m,n}$. The elements of the j-th column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type SUN-MATRIX_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 §7.4.

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 §7.5.

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.

4.6.5 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 products Jv. If such a function is not supplied, the default is a difference quotient approximation of these products.

KINLsJacTimesVecFn

new_u

Definition typedef int (*KINLsJacTimesVecFn)(N_Vector v, N_Vector Jv, N_Vector u, booleantype *new_u, void *user_data);

Purpose This jtimes 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.

 ${\tt u}$ $\,$ is the current value of the dependent variable vector.

is a flag, input from KINSOL and possibly reset by the user's jtimes function, indicating whether the iterate vector \mathbf{u} has been updated since the last call to jtimes. This is useful if the jtimes function computes and saves Jacobian data that depends on \mathbf{u} for use in computing J(u)v. The input value of $\text{new}_{-}\mathbf{u}$ is SUNTRUE following an update by KINSOL, and in that case any saved Jacobian data depending on \mathbf{u} should be recomputed. The jtimes routine should then set $\text{new}_{-}\mathbf{u}$ to SUNFALSE, so that on subsequent calls to jtimes with the same \mathbf{u} , the saved data can be reused.

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.

The previous function type KINSpilsJacTimesVecFn is identical to KINLsJacTimesVecFn, 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.

4.6.6 Preconditioner solve (iterative linear solvers)

If a user-supplied preconditioner is to be used with a SUNLINSOL solver module, then the user must provide a function to solve the linear system Pz = r where P is the preconditioner matrix, approximating (at least crudely) the system Jacobian $J = \partial F/\partial u$. This function must be of type KINLsPrecSolveFn, defined as follows:

KINLsPrecSolveFn

Definition typedef int (*KINLsPrecSolveFn)(N_Vector u, N_Vector uscale, N_Vector fval, N_Vector fscale, N_Vector v, void *user_data);

Purpose

This function solves the preconditioning system Pz = r.

Arguments

is the current (unscaled) value of the iterate. 11

uscale is a vector containing diagonal elements of the scaling matrix for u.

fval is the vector F(u) evaluated at **u**.

is a vector containing diagonal elements of the scaling matrix for fval. fscale

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 the function KINSetUserData.

Return value The value to be returned by the preconditioner solve function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error, and 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.

The previous function type KINSpilsPrecSolveFn is identical to KINLsPrecSolveFn, 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.

4.6.7 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:

KINLsPrecSetupFn

Definition typedef int (*KINLsPrecSetupFn)(N_Vector u, N_Vector uscale,

N_Vector fval, N_Vector fscale,

void *user_data);

Purpose This function evaluates and/or preprocesses Jacobian-related data needed by the pre-

conditioner solve function.

Arguments u is the current (unscaled) value of the iterate.

uscale is a vector containing diagonal elements of the scaling matrix for 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

the function KINSetUserData.

Return value The value to be returned by the preconditioner setup function is a flag indicating

whether it was successful. This value should be 0 if successful, any other value re-

sulting in halting the KINSOL solver.

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

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

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.

The previous function type KINSpilsPrecSetupFn is identical to KINLsPrecSetupFn, 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.

4.7 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 §6.4.

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 mldq, defined as the number of non-zero diagonals above and below the main diagonal, respectively. However, from the resulting approximate Jacobain 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 mldq 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 KINBBDLocalFn) which approximates the nonlinear system function $G(u) \approx F(u)$ and which is computed locally, and an optional function Gcomm (of type KINBBDCommFn) 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.

KINBBDLocalFn

Definition typedef int (*KINBBDLocalFn)(sunindextype Nlocal, N_Vector u, N_Vector gval, void *user_data);

Purpose 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 A KINBBDLocalFn function should return 0 if successful or a non-zero value if an error occured.

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

Memory for u and gval is handled within the preconditioner module.

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

KINBBDCommFn

Notes

Definition typedef int (*KINBBDCommFn)(sunindextype Nlocal, N_Vector u, void *user_data);

Purpose This Gcomm function performs all interprocess communications necessary for the execu-

tion of the Gloc function above, using the input vector 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 A KINBBDCommFn function should return 0 if successful or a non-zero value if an error occured.

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 system 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 KINBBDPrecInit (see below).

Besides the header files required for the solution of a nonlinear problem (see §4.3), to use the KINBBDPRE module, the main program must include the header file kinbbdpre.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 $\S4.4$ are grayed out.

- 1. Initialize parallel or multi-threaded environment
- 2. Set problem dimensions, etc.
- 3. Set vector with initial guess
- 4. Create KINSOL object
- 5. Allocate internal memory

6. Create linear solver object

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

7. Attach linear solver module

$8. \ \, \textbf{Initialize the} \, \, \textbf{KINBBDPRE} \, \, \textbf{preconditioner} \, \, \textbf{module} \\$

Specify the upper and lower half-bandwidth pairs (mudq, mldq) and (mukeep, mlkeep), and call

to allocate memory for and initialize the internal preconditoner data. The last two arguments of KINBBDPrecInit are the two user-supplied functions described above.

9. Set optional inputs

Note that the user should not overwrite the preconditioner data, setup function, or solve function through calls to KINSetPreconditioner optional input functions.

10. Solve problem

11. Get optional output

Additional optional outputs associated with KINBBDPRE are available by way of two routines described below, KINBBDPrecGetWorkSpace and KINBBDPrecGetNumGfnEvals.

- 12. Deallocate memory for solution vector
- 13. Free solver memory

- 14. Free linear solver memory
- 15. Finalize MPI, if used

The user-callable function that initializes KINBBDPRE (step 8), is described in more detail below.

KINBBDPrecInit

Call flag = KINBBDPrecInit(kin_mem, Nlocal, mudq, mldq,

mukeep, mlkeep, dq_rel_u, Gloc, Gcomm);

Description The function KINBBDPrecInit initializes and allocates memory for the KINBBDPRE pre-

conditioner.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

Nlocal (sunindextype) local vector length.

mudq (sunindextype) upper half-bandwidth to be used in the difference-quotient

Jacobian approximation.

mldq (sunindextype) lower half-bandwidth to be used in the difference-quotient

Jacobian approximation.

mukeep (sunindextype) upper half-bandwidth of the retained banded approximate

Jacobian block.

mlkeep (sunindextype) lower half-bandwidth of the retained banded approximate

Jacobian block.

 dq_rel_u (realtype) the relative increment in components of u used in the difference quotient approximations. The default is $dq_rel_u = \sqrt{unit roundoff}$, which

can be specified by passing $dq_rel_u = 0.0$.

Gloc (KINBBDLocalFn) the C function which computes the approximation $G(u) \approx$

F(u).

Gcomm (KINBBDCommFn) the optional C function which performs all interprocess com-

munication required for the computation of G(u).

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

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 mukeep 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:

KINBBDPrecGetWorkSpace

Call flag = KINBBDPrecGetWorkSpace(kin_mem, &lenrwBBDP, &leniwBBDP);

Description The function KINBBDPrecGetWorkSpace returns the local KINBBDPRE real and integer workspace sizes.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

 ${\tt lenrwBBDP} \ ({\tt long} \ {\tt int}) \ {\tt local} \ {\tt number} \ {\tt of} \ {\tt realtype} \ {\tt values} \ {\tt in} \ {\tt the} \ {\tt KINBBDPRE} \ {\tt workspace}.$

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

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

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 SUNLINSOL object, temporary vectors). These values are local to each process.

The workspaces referred to here exist in addition to those given by the corresponding KINGetLinWorkSpace function.

KINBBDPrecGetNumGfnEvals

Call flag = KINBBDPrecGetNumGfnEvals(kin_mem, &ngevalsBBDP);

Description The function KINBBDPrecGetNumGfnEvals returns the number of calls to the user Gloc

function due to the difference quotient approximation of the Jacobian blocks used within

KINBBDPRE's preconditioner setup function.

Arguments kin_mem (void *) pointer to the KINSOL memory block.

ngevalsBBDP (long int) the number of calls to the user Gloc function.

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

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 Gloc evaluations, the costs associated with KINBBDPRE also include nlinsetups LU factorizations, nlinsetups calls to Gcomm, npsolves banded backsolve calls, and nfevalsLS right-hand side function evaluations, where nlinsetups is an optional KINSOL output and npsolves and nfevalsLS are linear solver optional outputs (see §4.5.5).

Chapter 5

Using KINSOL for Fortran Applications

A Fortran 2003 module (fkinsol_mod) as well as a Fortran 77 style interface (fkinsol) are provided to support the use of kinsol, for the solution of nonlinear systems F(u) = 0, in a mixed Fortran/C setting. While kinsol is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in Fortran.

5.1 KINSOL Fortran 2003 Interface Module

The fkinsol_mod Fortran module defines interfaces to most KINSOL C functions using the intrinsic iso_c_binding module which provides a standardized mechanism for interoperating with C. All interfaced functions are named after the corresponding C function, but with a leading 'F'. For example, the KINSOL function KINCreate is interfaced as FKINCreate. Thus, the steps to use KINSOL and the function calls in Fortran 2003 are identical (ignoring language differences) to those in C. The C functions with Fortran 2003 interfaces indicate this in their description in Chapter 4. The Fortran 2003 KINSOL interface module can be accessed by the use statement, i.e. use fkinsol_mod, and linking to the library libsundials_fkinsol_mod.lib in addition to libsundials_kinsol.lib.

The Fortran 2003 interface modules were generated with SWIG Fortran, a fork of SWIG [22]. Users who are interested in the SWIG code used in the generation process should contact the SUNDIALS development team.

5.1.1 SUNDIALS Fortran 2003 Interface Modules

All of the generic SUNDIALS modules provide Fortran 2003 interface modules. Many of the generic module implementations provide Fortran 2003 interfaces (a complete list of modules with Fortran 2003 interfaces is given in Table 5.1). A module can be accessed with the use statement, e.g. use fnvector_openmp_mod, and linking to the Fortran 2003 library in addition to the C library, e.g. libsundials_fnvecpenmp_mod. lib and libsundials_nvecopenmp.lib.

The Fortran 2003 interfaces leverage the <code>iso_c_binding</code> module and the <code>bind(C)</code> attribute to closely follow the <code>SUNDIALS</code> C API (ignoring language differences). The generic <code>SUNDIALS</code> structures, e.g. <code>N_Vector</code>, are interfaced as Fortran derived types, and function signatures are matched but with an <code>F</code> prepending the name, e.g. <code>FN_VConst</code> instead of <code>N_VConst</code>. Constants are named exactly as they are in the C API. Accordingly, using <code>SUNDIALS</code> via the Fortran 2003 interfaces looks just like using it in C. Some caveats stemming from the language differences are discussed in the section 5.1.3. A discussion on the topic of equivalent data types in C and Fortran 2003 is presented in section 5.1.2.

Further information on the Fortran 2003 interfaces specific to modules is given in the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL alongside the C documentation (chapters 6, 7, 8, and

 $\ref{eq:continuous}$ respectively). For details on where the Fortran 2003 module (.mod) files and libraries are installed see Appendix A.

Table 5.1: Summary of Fortran 2003 interfaces for shared SUNDIALS modules.

Module	Fortran 2003 Module Name
NVECTOR	fsundials_nvector_mod
NVECTOR_SERIAL	fnvector_serial_mod
NVECTOR_PARALLEL	fnvector_parallel_mod
NVECTOR_OPENMP	fnvector_openmp_mod
NVECTOR_PTHREADS	fnvector_pthreads_mod
NVECTOR_PARHYP	Not interfaced
NVECTOR_PETSC	Not interfaced
NVECTOR_CUDA	Not interfaced
NVECTOR_RAJA	Not interfaced
NVECTOR_MANYVECTOR	Not interfaced
NVECTOR_MPIMANYVECTOR	Not interfaced
NVECTOR_MPIPLUSX	Not interfaced
SUNMatrix	fsundials_matrix_mod
SUNMATRIX_BAND	fsunmatrix_band_mod
SUNMATRIX_DENSE	fsunmatrix_dense_mod
SUNMATRIX_SPARSE	fsunmatrix_sparse_mod
SUNLinearSolver	fsundials_linearsolver_mod
SUNLINSOL_BAND	fsunlinsol_band_mod
SUNLINSOL_DENSE	fsunlinsol_dense_mod
SUNLINSOL_LAPACKBAND	Not interfaced
SUNLINSOL_LAPACKDENSE	Not interfaced
SUNLINSOL_KLU	fsunlinsol_klu_mod
SUNLINSOL_SUPERLUMT	Not interfaced
SUNLINSOL_SUPERLUDIST	Not interfaced
SUNLINSOL_SPGMR	fsunlinsol_spgmr_mod
SUNLINSOL_SPFGMR	fsunlinsol_spfgmr_mod
SUNLINSOL_SPBCGS	fsunlinsol_spbcgs_mod
SUNLINSOL_SPTFQMR	fsunlinsol_sptfqmr_mod
SUNLINSOL_PCG	fsunlinsol_pcg_mod
SUNNonlinearSolver	fsundials_nonlinearsolver_mod
SUNNONLINSOL_NEWTON	fsunnonlinsol_newton_mod
SUNNONLINSOL_FIXEDPOINT	fsunnonlinsol_fixedpoint_mod

5.1.2 Data Types

Generally, the Fortran 2003 type that is equivalent to the C type is what one would expect. Primitive types map to the <code>iso_c_binding</code> type equivalent. SUNDIALS generic types 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 5.2 presents a summary of the type equivalencies with the parameter direction in mind.



Currently, the Fortran 2003 interfaces are only compatible with SUNDIALS builds where the realtype is double precision and the sunindextype size is 64-bits.

C type	Parameter Direction	Fortran 2003 type
double	in, inout, out, return	real(c_double)
int	in, inout, out, return	integer(c_int)
long	in, inout, out, return	integer(c_long)
booleantype	in, inout, out, return	integer(c_int)
realtype	in, inout, out, return	real(c_double)
sunindextype	in, inout, out, return	integer(c_long)
double*	in, inout, out	real(c_double), dimension(*)
double*	return	real(c_double), pointer, dimension(:)
int*	in, inout, out	<pre>integer(c_int), dimension(*)</pre>
int*	return	<pre>integer(c_int), pointer, dimension(:)</pre>
long*	in, inout, out	<pre>integer(c_long), dimension(*)</pre>
long*	return	<pre>integer(c_long), pointer, dimension(:)</pre>
realtype*	in, inout, out	real(c_double), dimension(*)
realtype*	return	real(c_double), pointer, dimension(:)
sunindextype*	in, inout, out	<pre>integer(c_long), dimension(*)</pre>
sunindextype*	return	<pre>integer(c_long), pointer, dimension(:)</pre>
realtype[]	in, inout, out	real(c_double), dimension(*)
sunindextype[]	in, inout, out	<pre>integer(c_long), dimension(*)</pre>
N_Vector	in, inout, out	type(N_Vector)
N_Vector	return	type(N_Vector), pointer
SUNMatrix	in, inout, out	type(SUNMatrix)
SUNMatrix	return	type(SUNMatrix), pointer
SUNLinearSolver	in, inout, out	type(SUNLinearSolver)
SUNLinearSolver	return	type(SUNLinearSolver), pointer
SUNNonlinearSolver	in, inout, out	type(SUNNonlinearSolver)
SUNNonlinearSolver	return	type(SUNNonlinearSolver), pointer
FILE*	in, inout, out, return	type(c_ptr)
void*	in, inout, out, return	type(c_ptr)
T**	in, inout, out, return	type(c_ptr)
T***	in, inout, out, return	type(c_ptr)
T****	in, inout, out, return	type(c_ptr)

Table 5.2: C/Fortran 2003 Equivalent Types

5.1.3 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, section 5.1.2 discusses equivalencies of data types in the two languages.

5.1.3.1 Creating generic SUNDIALS objects

In the C API a generic SUNDIALS object, 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. E.g., 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);
Fortran code:
```

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

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

5.1.3.2 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;
x = N_VNew_Serial(N);
/* 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)
                        :: leniw(1), lenrw(1)
integer(c_long)
x => FN_VNew_Serial(x)
! 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)
```

5.1.3.3 Passing procedure pointers and user data

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

Typically when passing user data to a SUNDIALS function, a user may simply cast some custom data structure as a void*. When using the Fortran 2003 interfaces, the same thing can be achieved.

Note, the custom data structure does not have to be bind(C) since it is never accessed on the C side.

```
C code:
MyUserData* udata;
void *cvode_mem;
ierr = CVodeSetUserData(cvode_mem, udata);
Fortran code:
type(MyUserData) :: udata
type(c_ptr) :: cvode_mem
ierr = FCVodeSetUserData(cvode_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.

5.1.3.4 Passing NULL to optional parameters

In the SUNDIALS C API some functions have optional parameters that a caller can pass NULL to. If the optional parameter is of a type that is equivalent to a Fortran type(c_ptr) (see section 5.1.2), 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

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

5.1.3.5 Providing file pointers

Expert SUNDIALS users may notice that there are a few advanced functions in the SUNDIALS C API that take a FILE * argument. Since there is no portable way to convert between a Fortran file descriptor and a C file pointer, a user will need to allocate the FILE * in C. The code example below demonstrates one way of doing this.

C code:

```
void allocate_file_ptr(FILE *fp)
  fp = fopen(...);
int free_file_ptr(FILE *fp)
  return fclose(fp);
}
Fortran code:
subroutine allocate_file_ptr(fp) &
  bind(C,name='allocate_file_ptr')
  use, intrinsic :: iso_c_binding
  type(c_ptr) :: fp
end subroutine
integer(C_INT) function free_file_ptr(fp) &
  bind(C,name='free_file_ptr')
  use, intrinsic :: iso_c_binding
  type(c_ptr) :: fp
end function
program main
  use, intrinsic :: iso_c_binding
  type(c_ptr)
                 :: fp
  integer(C_INT) :: ierr
  call allocate_file_ptr(fp)
  ierr = free_file_ptr(fp)
end program
```

5.1.4 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 used to generate the modules.

5.1.5 FKINSOL, an Interface Module for FORTRAN Applications

The FKINSOL interface module is a package of C functions which support the use of the KINSOL solver, for the solution of nonlinear systems F(u) = 0, in a mixed FORTRAN/C setting. While KINSOL is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in FORTRAN. This package provides the necessary interface to KINSOL for all supplied serial and parallel NVECTOR implementations.

5.2 Important note on portability

In this package, the names of the interface functions, and the names of the FORTRAN user routines called by them, appear as dummy names which are mapped to actual values by a series of definitions

in the header files. By default, those mapping definitions depend in turn on the C macro F77_FUNC defined in the header file sundials_config.h. The mapping defined by F77_FUNC in turn transforms the C interface names to match the name-mangling approach used by the supplied Fortran compiler.

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

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

5.3 Fortran Data Types

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

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

- int32_t equivalent to an INTEGER or INTEGER*4 in FORTRAN
- int64_t equivalent to an INTEGER*8 in FORTRAN

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

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

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

5.3.1 FKINSOL routines

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

- Interface to the NVECTOR modules
 - FNVINITS (defined by NVECTOR_SERIAL) interfaces to N_VNewEmpty_Serial.
 - FNVINITP (defined by NVECTOR_PARALLEL) interfaces to N_VNewEmpty_Parallel.
 - FNVINITOMP (defined by NVECTOR_OPENMP) interfaces to N_VNewEmpty_OpenMP.
 - FNVINITPTS (defined by NVECTOR_PTHREADS) interfaces to N_VNewEmpty_Pthreads.
- Interface to the SUNMATRIX modules

- FSUNBANDMATINIT (defined by SUNMATRIX_BAND) interfaces to SUNBandMatrix.
- FSUNDENSEMATINIT (defined by SUNMATRIX_DENSE) interfaces to SUNDenseMatrix.
- FSUNSPARSEMATINIT (defined by SUNMATRIX_SPARSE) interfaces to SUNSparseMatrix.
- Interface to the SUNLINSOL modules
 - FSUNBANDLINSOLINIT (defined by SUNLINSOL_BAND) interfaces to SUNLinSol_Band.
 - FSUNDENSELINSOLINIT (defined by SUNLINSOL_DENSE) interfaces to SUNLinSol_Dense.
 - FSUNKLUINIT (defined by SUNLINSOL_KLU) interfaces to SUNLinSol_KLU.
 - FSUNKLUREINIT (defined by SUNLINSOL_KLU) interfaces to SUNLinSol_KLUReinit.
 - FSUNLAPACKBANDINIT (defined by SUNLINSOL_LAPACKBAND) interfaces to SUNLinSol_LapackBand.
 - FSUNLAPACKDENSEINIT (defined by SUNLINSOL_LAPACKDENSE) interfaces to SUNLinSol_LapackDense.
 - FSUNPCGINIT (defined by SUNLINSOL_PCG) interfaces to SUNLinSol_PCG.
 - FSUNSPBCGSINIT (defined by SUNLINSOL_SPBCGS) interfaces to SUNLinSol_SPBCGS.
 - FSUNSPFGMRINIT (defined by SUNLINSOL_SPFGMR) interfaces to SUNLinSol_SPFGMR.
 - FSUNSPGMRINIT (defined by SUNLINSOL_SPGMR) interfaces to SUNLinSol_SPGMR.
 - FSUNSPTFQMRINIT (defined by SUNLINSOL_SPTFQMR) interfaces to SUNLinSol_SPTFQMR.
 - FSUNSUPERLUMTINIT (defined by SUNLINSOL_SUPERLUMT) interfaces to SUNLinSol_SuperLUMT.
- Interface to the main kinsol module
 - FKINCREATE interfaces to KINCreate.
 - FKINSETIIN and FKINSETRIN interface to KINSet* functions.
 - FKININIT interfaces to KINInit.
 - FKINSETVIN interfaces to KINSetConstraints.
 - FKINSOL interfaces to KINSol, KINGet* functions, and to the optional output functions for the selected linear solver module.
 - FKINFREE interfaces to KINFree.
- Interface to the KINLS module
 - FKINLSINIT interfaces to KINSetLinearSolver.
 - FKINLSSETJAC interfaces to KINSetJacTimesVecFn.
 - FKINLSSETPREC interfaces to KINSetPreconditioner.
 - FKINDENSESETJAC interfaces to KINSetJacFn.
 - FKINBANDSETJAC interfaces to KINSetJacFn.
 - FKINSPARSESETJAC interfaces to KINSetJacFn.

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

FKINSOL routine	KINSOL function	KINSOL type of
(Fortran, user-supplied)	(C, interface)	interface function
FKFUN	FKINfunc	KINSysFn
FKDJAC	FKINDenseJac	KINLsJacFn
FKBJAC	FKINBandJac	KINLsJacFn
FKINSPJAC	FKINSparseJac	KINLsJacFn
FKPSET	FKINPSet	KINLsPrecSetupFn
FKPSOL	FKINPSol	KINLsPrecSolveFn
FKJTIMES	FKINJtimes	KINLsJacTimesVecFn

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

5.3.2 Usage of the FKINSOL interface module

The usage of FKINSOL requires calls to a few different interface functions, depending on the method options selected, and one or more user-supplied routines which define the problem to be solved. These function calls and user routines are summarized separately below. Some details are omitted, and the user is referred to the description of the corresponding KINSOL functions for information on the arguments of any given user-callable interface routine, or of a given user-supplied function called by an interface function.

1. Nonlinear system function specification

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

```
SUBROUTINE FKFUN (U, FVAL, IER)
DIMENSION U(*), FVAL(*)
```

It must set the FVAL array to F(u), the system function, as a function of U = u. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if it failed unrecoverably (in which case the solution process is halted).

2. NVECTOR module initialization

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

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

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

3. SUNMATRIX module initialization

If using a Newton or Picard iteration with a matrix-based SUNLINSOL linear solver module and one of the SUNMATRIX modules supplied with SUNDIALS, the user must make a call of the form

```
CALL FSUN***MATINIT(...)
```

in which the name and call sequence are as described in the appropriate section of Chapter 7. Note that the dense, band, or sparse matrix options are usable only in a serial or multi-threaded environment.

4. SUNLINSOL module initialization

If using a Newton or Picard iteration with one of the SUNLINSOL linear solver modules supplied with SUNDIALS, the user must make a call of the form

```
CALL FSUNBANDLINSOLINIT(...)

CALL FSUNDENSELINSOLINIT(...)

CALL FSUNKLUINIT(...)

CALL FSUNLAPACKBANDINIT(...)

CALL FSUNLAPACKDENSEINIT(...)

CALL FSUNSPBCGSINIT(...)

CALL FSUNSPFGMRINIT(...)

CALL FSUNSPFGMRINIT(...)

CALL FSUNSPTFQMRINIT(...)

CALL FSUNSPTFQMRINIT(...)
```

in which the call sequence is as described in the appropriate section of Chapter 8. Note that the dense, band, or sparse solvers are usable only in a serial or multi-threaded environment.

Once one of these solvers has been initialized, its solver parameters may be modified using a call to the functions

```
CALL FSUNKLUSETORDERING(...)

CALL FSUNSUPERLUMTSETORDERING(...)

CALL FSUNPCGSETPRECTYPE(...)

CALL FSUNSPBCGSSETPRECTYPE(...)

CALL FSUNSPBCGSSETMAXL(...)

CALL FSUNSPFGMRSETGSTYPE(...)

CALL FSUNSPFGMRSETPRECTYPE(...)

CALL FSUNSPFGMRSETGSTYPE(...)

CALL FSUNSPFGMRSETPRECTYPE(...)

CALL FSUNSPFGMRSETPRECTYPE(...)

CALL FSUNSPTFQMRSETPRECTYPE(...)

CALL FSUNSPTFQMRSETPRECTYPE(...)
```

where again the call sequences are described in the appropriate sections of Chapter 8.

5. Problem specification

To create the main solver memory block, make the following call:

FKINCREATE

Call CALL FKINCREATE (IER)

Description This function creates the KINSOL memory structure.

Arguments None.

Return value IER is the return completion flag. Values are 0 for successful return and -1 other-

wise. See printed message for details in case of failure.

Notes

6. Set optional inputs

Call FKINSETIIN, FKINSETRIN, and/or FKINSETVIN, to set desired optional inputs, if any. See §5.3.3 for details.

7. Solver Initialization

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

FKININIT

Call CALL FKININIT (IOUT, ROUT, IER)

Description This function specifies the optional output arrays, allocates internal memory, and

initializes KINSOL.

Arguments IOUT is an integer array for integer optional outputs.

ROUT is a real array for real optional outputs.

Return value IER is the return completion flag. Values are 0 for successful return and -1 other-

wise. See printed message for details in case of failure.

Notes The user integer data array IOUT must be declared as INTEGER*4 or INTEGER*8

according to the C type long int.

The optional outputs associated with the main KINSOL integrator are listed in Table 5.4.

8. Linear solver interface specification

The Newton and Picard solution methods in KINSOL involve the solution of linear systems related to the Jacobian of the nonlinear system. To attach the linear solver (and optionally the matrix) objects initialized in steps 3 and 4 above, the user of FKINSOL must initialize the KINLS linear solver interface.

To attach any SUNLINSOL object (and optional SUNMATRIX object) to the KINLS interface, then following calls to initialize the SUNLINSOL (and SUNMATRIX) object(s) in steps 3 and 4 above, the user must make the call:

```
CALL FKINLSINIT (IER)
```

where IER is an error return flag which is 0 for success or -1 if a memory allocation failure occurred.

The previous routines FKINDLSINIT and FKINSPILSINIT 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.

KINLS with dense Jacobian matrix

As an option when using the KINLS interface with the SUNLINSOL_DENSE or SUNLINSOL_LAPACKDENSE linear solvers, the user may supply a routine that computes a dense approximation of the system Jacobian $J = \partial F/\partial u$. If supplied, it must have the following form:

```
SUBROUTINE FKDJAC (NEQ, U, FVAL, DJAC, WK1, WK2, IER) DIMENSION U(*), FVAL(*), DJAC(NEQ,*), WK1(*), WK2(*)
```

Typically this routine will use only NEQ, U, and DJAC. It must compute the Jacobian and store it columnwise in DJAC. The input arguments U and FVAL contain the current values of u and F(u), respectively. The vectors WK1 and WK2, of length NEQ, are provided as work space for use in FKDJAC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if FKDJAC failed unrecoverably (in which case the solution process is halted). NOTE: The argument NEQ has a type consistent with C type long int even in the case when the LAPACK dense solver is to be used.

If the FKDJAC routine is provided, then, following the call to FKINLSINIT, the user must make the call:

```
CALL FKINDENSESETJAC (FLAG, IER)
```

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

KINLS with band Jacobian matrix

As an option when using the KINLS interface with the SUNLINSOL_BAND or SUNLINSOL_LAPACKBAND linear solvers, the user may supply a routine that computes a band approximation of the system Jacobian $J = \partial F/\partial u$. If supplied, it must have the following form:

```
SUBROUTINE FKBJAC (NEQ, MU, ML, MDIM, U, FVAL, BJAC, WK1, WK2, IER) DIMENSION U(*), FVAL(*), BJAC(MDIM,*), WK1(*), WK2(*)
```

Typically this routine will use only NEQ, MU, ML, U, and BJAC. It must load the MDIM by N array BJAC with the Jacobian matrix at the current u in band form. Store in BJAC(k, j) the Jacobian element

 $J_{i,j}$ with k=i-j+ MU +1 ($k=1\cdots$ ML + MU + 1) and $j=1\cdots N$. The input arguments U and FVAL contain the current values of u, and F(u), respectively. The vectors WK1 and WK2 of length NEQ are provided as work space for use in FKBJAC. IER is an error return flag, which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if FKBJAC failed unrecoverably (in which case the solution process is halted). NOTE: The arguments NEQ, MU, ML, and MDIM have a type consistent with C type long int even in the case when the LAPACK band solver is to be used.

If the FKBJAC routine is provided, then, following the call to FKINLSINIT, the user must make the call:

```
CALL FKINBANDSETJAC (FLAG, IER)
```

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

KINLS with sparse Jacobian matrix

When using the KINLS interface with either of the SUNLINSOL_KLU or SUNLINSOL_SUPERLUMT linear solvers, the user must supply the FKINSPJAC routine that computes a compressed-sparse-column or compressed-sparse-row approximation of the system Jacobian $J = \partial F/\partial u$. If supplied, it must have the following form:

```
SUBROUTINE FKINSPJAC(Y, FY, N, NNZ, JDATA, JINDEXVALS, & JINDEXPTRS, WK1, WK2, IER)
```

Typically this routine will use only N, NNZ, JDATA, JINDEXVALS and JINDEXPTRS. It must load the N by N compressed sparse column [or compressed sparse row] matrix with storage for NNZ nonzeros, stored in the arrays JDATA (nonzero values), JINDEXVALS (row [or column] indices for each nonzero), JINDEXPTRS (indices for start of each column [or row]), with the Jacobian matrix at the current (y) in CSC [or CSR] form (see sunmatrix_sparse.h for more information). The arguments are Y, an array containing state variables; FY, an array containing residual values; N, the number of matrix rows/columns in the Jacobian; NNZ, allocated length of nonzero storage; JDATA, nonzero values in the Jacobian (of length NNZ); JINDEXVALS, row [or column] indices for each nonzero in Jacobian (of length NNZ); JINDEXPTRS, pointers to each Jacobian column [or row] in the two preceding arrays (of length N+1); WK*, work arrays containing temporary workspace of same size as Y; and IER, error return code (0 if successful, > 0 if a recoverable error occurred, or < 0 if an unrecoverable error occurred.)

To indicate that the FKINSPJAC routine has been provided, then following the call to FKINLSINIT, the following call must be made

```
CALL FKINSPARSESETJAC (IER)
```

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

KINLS with Jacobian-vector product

As an option when using the KINLS linear solver interface, the user may supply a routine that computes the product of the system Jacobian and a given vector. If supplied, it must have the following form:

```
SUBROUTINE FKINJTIMES (V, FJV, NEWU, U, IER) DIMENSION V(*), FJV(*), U(*)
```

Typically this routine will use only U, V, and FJV. It must compute the product vector Jv, where the vector v is stored in V, and store the product in FJV. The input argument U contains the

current value of u. On return, set IER = 0 if FKINJTIMES was successful, and nonzero otherwise. NEWU is a flag to indicate if U has been changed since the last call; if it has, then NEWU = 1, and FKINJTIMES should recompute any saved Jacobian data it uses and reset NEWU to 0. (See §4.6.5.)

To indicate that the FKINJTIMES routine has been provided, then following the call to FKINLSINIT, the following call must be made

```
CALL FKINLSSETJAC (FLAG, IER)
```

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

The previous routine FKINSPILSETJAC 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.

KINLS with preconditioning

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

```
SUBROUTINE FKPSOL (U, USCALE, FVAL, FSCALE, VTEM, IER)
DIMENSION U(*), USCALE(*), FVAL(*), FSCALE(*), VTEM(*)
```

Typically this routine will use only U, FVAL, and VTEM It must solve the preconditioned linear system Pz = r, where r = VTEM is input, and store the solution z in VTEM as well. Here P is the right preconditioner. If scaling is being used, the routine supplied must also account for scaling on either coordinate or function value, as given in the arrays USCALE and FSCALE, respectively.

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

```
SUBROUTINE FKPSET (U, USCALE, FVAL, FSCALE, IER)
DIMENSION U(*), USCALE(*), FVAL(*), FSCALE(*)
```

It must perform any evaluation of Jacobian-related data and preprocessing needed for the solution of the preconditioned linear systems by FKPSOL. The variables U through FSCALE are for use in the preconditioning setup process. Typically, the system function FKFUN is called before any calls to FKPSET, so that FVAL will have been updated. U is the current solution iterate. If scaling is being used, USCALE and FSCALE are available for those operations requiring scaling.

On return, set IER = 0 if FKPSET was successful, or set IER = 1 if an error occurred.

To indicate that the FKINPSET and FKINPSOL routines are supplied, then the user must call

```
CALL FKINLSSETPREC (FLAG, IER)
```

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

The previous routine FKINSPILSETPREC 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.

If the user calls FKINLSSETPREC, the routine FKPSET must be provided, even if it is not needed, and then it should return IER = 0.

!

9. Problem solution

Solving the nonlinear system is accomplished by making the following call:

```
CALL FKINSOL (U, GLOBALSTRAT, USCALE, FSCALE, IER)
```

The arguments are as follows. U is an array containing the initial guess on input, and the solution on return. GLOBALSTRAT is an integer (type INTEGER) defining the global strategy choice (0 specifies Inexact Newton, 1 indicates Newton with line search, 2 indicates Picard iteration, and 3 indicates Fixed Point iteration). USCALE is an array of scaling factors for the U vector. FSCALE is an array of scaling factors for the FVAL vector. IER is an integer completion flag and will have one of the following values: 0 to indicate success, 1 to indicate that the initial guess satisfies F(u) = 0 within tolerances, 2 to indicate apparent stalling (small step), or a negative value to indicate an error or failure. These values correspond to the KINSo1 returns (see §4.5.3 and §B.2). The values of the optional outputs are available in IOPT and ROPT (see Table 5.4).

10. Memory deallocation

To free the internal memory created by calls to FKINCREATE, FKININIT, FNVINIT*, FKINLSINIT, and FSUN***MATINIT, make the call

CALL FKINFREE

5.3.3 FKINSOL optional input and output

In order to keep the number of user-callable FKINSOL interface routines to a minimum, optional inputs to the KINSOL solver are passed through only three routines: FKINSETIIN for integer optional inputs, FKINSETRIN for real optional inputs, and FKINSETVIN for real vector (array) optional inputs. These functions should be called as follows:

```
CALL FKINSETIIN (KEY, IVAL, IER)
CALL FKINSETRIN (KEY, RVAL, IER)
CALL FKINSETVIN (KEY, VVAL, IER)
```

where KEY is a quoted string indicating which optional input is set, IVAL is the integer input value to be used, RVAL is the real input value to be used, and VVAL is the input real array to be used. IER is an integer return flag which is set to 0 on success and a negative value if a failure occurred. For the legal values of KEY in calls to FKINSETIIN and FKINSETRIN, see Table 5.3. The one legal value of KEY for FKINSETVIN is CONSTR_VEC, for providing the array of inequality constraints to be imposed on the solution, if any. The integer IVAL should be declared in a manner consistent with C type long int.

The optional outputs from the KINSOL solver are accessed not through individual functions, but rather through a pair of arrays, IOUT (integer type) of dimension at least 15, and ROUT (real type) of dimension at least 2. These arrays are owned (and allocated) by the user and are passed as arguments to FKININIT. Table 5.4 lists the entries in these two arrays and specifies the optional variable as well as the KINSOL function which is actually called to extract the optional output.

For more details on the optional inputs and outputs, see §4.5.4 and §4.5.5.

5.3.4 Usage of the FKINBBD interface to KINBBDPRE

The FKINBBD interface sub-module is a package of C functions which, as part of the FKINSOL interface module, support the use of the KINSOL solver with the parallel NVECTOR_PARALLEL module and the KINBBDPRE preconditioner module (see §4.7), for the solution of nonlinear problems in a mixed FORTRAN/C setting.

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

- FKINBBDINIT interfaces to KINBBDPrecInit.
- FKINBBDOPT interfaces to KINBBDPRE optional output functions.

Table 5.3: Keys for setting FKINSOL optional inputs

Integer optional inputs FKINSETIIN

Key	Optional input	Default value
PRNT_LEVEL	Verbosity level of output	0
MAA	Number of prior residuals for Anderson Acceleration	0
MAX_NITERS	Maximum no. of nonlinear iterations	200
ETA_FORM	ETA_FORM Form of η coefficient	
MAX_SETUPS	MAX_SETUPS Maximum no. of iterations without prec. setup	
MAX_SP_SETUPS	Maximum no. of iterations without residual check	5
NO_INIT_SETUP	No initial preconditioner setup	SUNFALSE
NO_MIN_EPS	Lower bound on ϵ	SUNFALSE
NO_RES_MON	No residual monitoring	SUNFALSE

Real optional inputs (FKINSETRIN)

Key	Optional input	Default value
FNORM_TOL	Function-norm stopping tolerance	$uround^{1/3}$
SSTEP_TOL	Scaled-step stopping tolerance	$uround^{2/3}$
MAX_STEP	Max. scaled length of Newton step	$1000 D_u u_0 _2$
RERR_FUNC	Relative error for F.D. Jv	$\sqrt{\text{uround}}$
ETA_CONST	Constant value of η	0.1
ETA_PARAMS	Values of γ and α	0.9 and 2.0
RMON_CONST	Constant value of ω	0.9
RMON_PARAMS	Values of ω_{min} and ω_{max}	0.00001 and 0.9

Table 5.4: Description of the FKINSOL optional output arrays IOUT and ROUT

Integer output array IOUT

Integer output array IOUT			
Index	Optional output	KINSOL function	
KINSOL main solver			
1	LENRW	KINGetWorkSpace	
2	LENIW	KINGetWorkSpace	
3	NNI	KINGetNumNonlinSolvIters	
4	NFE	KINGetNumFuncEvals	
5	NBCF	KINGetNumBetaCondFails	
6	NBKTRK	KINGetNumBacktrackOps	
	KINLS linear s	solver interface	
7	LENRWLS	KINGetLinWorkSpace	
8	LENIWLS	KINGetLinWorkSpace	
9	LS_FLAG	KINGetLastLinFlag	
10	NFELS	KINGetNumLinFuncEvals	
11	NJE	KINGetNumJacEvals	
12	NJTV	KINGetNumJtimesEvals	
13	NPE	KINGetNumPrecEvals	
14	NPS	KINGetNumPrecSolves	
15	NLI	KINGetNumLinIters	
16	NCFL	KINGetNumLinConvFails	

Real output array \mathtt{ROUT}

	Index	Optional output	KINSOL function
ĺ	1	FNORM	KINGetFuncNorm
	2	SSTEP	KINGetStepLength

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

FKINBBD routine	KINSOL function	KINSOL type of	
(FORTRAN, user-supplied)	(C, interface)	interface function	
FKLOCFN	FKINgloc	KINBBDLocalFn	
FKCOMMF	FKINgcomm	KINBBDCommFn	
FKJTIMES	FKINJtimes	KINLsJacTimesVecFn	

As with the rest of the FKINSOL routines, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program. Additionally, based on flags discussed above in §5.3.1, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file fkinbbd.h.

The following is a summary of the usage of this module. Steps that are unchanged from the main program described in §5.3.2 are grayed-out.

- 1. Nonlinear system function specification
- 2. NVECTOR module initialization

3. SUNLINSOL module initialization

Initialize one of the iterative SUNLINSOL modules, by calling one of FSUNPCGINIT, FSUNSPBCGSINIT, FSUNSPFGMRINIT, FSUNSPFGMRINIT.

- 4. Problem specification
- 5. Set optional inputs
- 6. Solver Initialization

7. Linear solver interface specification

Initialize the KINLS iterative linear solver interface by calling FKINLSINIT.

To initialize the KINBBDPRE preconditioner, make the following call:

The arguments are as follows. NLOCAL is the local size of vectors for this process. MUDQ and MLDQ are the upper and lower half-bandwidths to be used in the computation of the local Jacobian blocks by difference quotients; these may be smaller than the true half-bandwidths of the Jacobian of the local block of G, when smaller values may provide greater efficiency. MU and ML are the upper and lower half-bandwidths of the band matrix that is retained as an approximation of the local Jacobian block; these may be smaller than MUDQ and MLDQ. IER is a return completion flag. A value of 0 indicates success, while a value of -1 indicates that a memory failure occurred or that an input had an illegal value.

Optionally, to specify that the SPGMR, SPFGMR, SPBCGS, or SPTFQMR solver should use the supplied FKJTIMES, make the call

CALL FKINLSSETJAC (FLAG, IER)

with FLAG $\neq 0$. (See step 8 in §5.3.2).

8. Problem solution

9. KINBBDPRE Optional outputs

Optional outputs specific to the SPGMR, SPFGMR, SPBCGS, or SPTFQMR solver are listed in Table 5.4. To obtain the optional outputs associated with the KINBBDPRE module, make the following call:

```
CALL FKINBBDOPT (LENRBBD, LENIBBD, NGEBBD)
```

The arguments should be consistent with C type long int. Their returned values are as follows: LENRBBD is the length of real preconditioner work space, in realtype words. LENIBBD is the length of integer preconditioner work space, in integer words. These sizes are local to the current process. NGEBBD is the cumulative number of G(u) evaluations (calls to FKLOCFN) so far.

10. Memory deallocation

(The memory allocated for the FKINBBD module is deallocated automatically by FKINFREE.)

11. User-supplied routines

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

```
SUBROUTINE FKLOCFN (NLOC, ULOC, GLOC, IER)
DIMENSION ULOC(*), GLOC(*)
```

This routine is to evaluate the function G(u) approximating F (possibly identical to F), in terms of the array ULOC (of length NLOC), which is the sub-vector of u local to this processor. The resulting (local) sub-vector is to be stored in the array GLOC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if FKLOCFN failed unrecoverably (in which case the solution process is halted).

```
SUBROUTINE FKCOMMFN (NLOC, ULOC, IER)
DIMENSION ULOC(*)
```

This routine is to perform the inter-processor communication necessary for the FKLOCFN routine. Each call to FKCOMMFN is preceded by a call to the system function routine FKFUN with the same argument ULOC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case KINSOL will attempt to correct), or a negative value if FKCOMMFN failed recoverably (in which case the solution process is halted).

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

Optionally, the user can supply a routine FKINJTIMES for the evaluation of Jacobian-vector products, as described above in step 8 in §5.3.2. Note that this routine is required if using Picard iteration.



Chapter 6

Description of the NVECTOR module

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

6.1 The NVECTOR API

The generic NVECTOR API can be broken down into five groups of functions: the core vector operations, the fused vector operations, the vector array operations, the local reduction operations, and finally some utility functions. The first four groups are defined by a particular NVECTOR implementation. The utility functions are defined by the generic NVECTOR itself.

6.1.1 NVECTOR core functions

N_VGetVectorID

Call id = N_VGetVectorID(w);

Description 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.

Arguments w (N_Vector) a NVECTOR object

Return value This function returns an N-Vector_ID. Possible values are given in Table 6.1.

F2003 Name FN_VGetVectorID

 N_{VClone}

Call v = N_VClone(w);

Description 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.

Arguments w (N_Vector) a NVECTOR object

Return value This function returns an N_- Vector object. If an error occurs, then this routine will

return NULL.

 $F2003\ Name\ FN_VClone$

$N_VCloneEmpty$

Call v = N_VCloneEmpty(w);

Description 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 data.

Arguments w (N_Vector) a NVECTOR object

Return value This function returns an N_Vector object. If an error occurs, then this routine will

return NULL.

F2003 Name FN_VCloneEmpty

$N_{-}VDestroy$

Call N_VDestroy(v);

Description Destroys the N_Vector v and frees memory allocated for its internal data.

Arguments v (N_Vector) a NVECTOR object to destroy

Return value None

F2003 Name FN_VDestroy

N_VSpace

Call N_VSpace(v, &lrw, &liw);

Description Returns storage requirements for one N_Vector. 1rw contains the number of realtype

words and 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.

Arguments v (N_Vector) a NVECTOR object

1rw (sunindextype*) out parameter containing the number of realtype words

liw (sunindextype*) out parameter containing the number of integer words

Return value None

F2003 Name FN_VSpace

F2003 Call integer(c_long) :: lrw(1), liw(1)

call FN_VSpace_Serial(v, lrw, liw)

${\tt N_VGetArrayPointer}$

Call vdata = N_VGetArrayPointer(v);

Description Returns a 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. This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, the sparse linear solvers (serial and threaded), and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS.

Arguments v (N_Vector) a NVECTOR object

Return value realtype*

F2003 Name FN_VGetArrayPointer

N_VSetArrayPointer

Call N_VSetArrayPointer(vdata, v);

Description Overwrites the pointer to the data in an N_Vector with a given realtype*. Note that

this assumes that the internal data in 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 for a parallel environment.

Arguments v (N_Vector) a NVECTOR object

Return value None

F2003 Name FN_VSetArrayPointer

N_VGetCommunicator

Call N_VGetCommunicator(v);

Description Returns a pointer to the MPI_Comm object associated with the vector (if applicable). For

MPI-unaware vector implementations, this should return NULL.

Arguments v (N_Vector) a NVECTOR object

Return value A void * pointer to the MPI_Comm object if the vector is MPI-aware, otherwise NULL.

 $F2003 \; \mathrm{Name} \; \; \mathtt{FN_VGetCommunicator}$

N_VGetLength

Call N_VGetLength(v);

Description 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.

Arguments v (N_Vector) a NVECTOR object

Return value sunindextype F2003 Name FN_VGetLength

N_VLinearSum

Call N_VLinearSum(a, x, b, y, z);

Description Performs the operation z = ax + by, where a and b are realtype scalars and x and y

are of type N_Vector: $z_i = ax_i + by_i$, i = 0, ..., n-1.

Arguments a (realtype) constant that scales x

x (N_Vector) a NVECTOR object

b (realtype) constant that scales y

y (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VLinearSum

N_VConst

Call N_VConst(c, z);

Description Sets all components of the N_Vector z to realtype c: $z_i = c, i = 0, \dots, n-1$.

Arguments c (realtype) constant to set all components of z to

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VConst

N_VProd

Call N_VProd(x, y, z);

Description Sets the N_Vector z to be the component-wise product of the N_Vector inputs x and y:

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

Arguments x (N_Vector) a NVECTOR object

y (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VProd

N_VDiv

Call N_VDiv(x, y, z);

Description Sets the N_Vector z to be the component-wise ratio of the N_Vector inputs x and y:

 $z_i = x_i/y_i, i = 0, \dots, n-1$. The y_i may not be tested for 0 values. It should only be

called with a y that is guaranteed to have all nonzero components.

Arguments x (N_Vector) a NVECTOR object

y (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VDiv

N_VScale

Call N_VScale(c, x, z);

Description Scales the N_Vector x by the realtype scalar c and returns the result in z: $z_i = cx_i$, $i = cx_i$

 $0, \ldots, n-1$.

Arguments c (realtype) constant that scales the vector x

x (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VScale

 N_VAbs

Call $N_VAbs(x, z)$;

Description Sets the components of the N_Vector z to be the absolute values of the components of

the N_Vector x: $y_i = |x_i|, i = 0, ..., n - 1.$

Arguments x (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None F2003 Name FN_VAbs

N_VInv

Call N_VInv(x, z);

Description Sets the components of the N_Vector z to be the inverses of the components of the

N-Vector x: $z_i = 1.0/x_i$, i = 0, ..., 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.

Arguments x (N_Vector) a NVECTOR object to

z (N_Vector) a NVECTOR object containing the result

Return value None F2003 Name FN_VInv

N_VAddConst

Call N_VAddConst(x, b, z);

Description Adds the realtype scalar b to all components of x and returns the result in the N_Vector

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

Arguments x (N_Vector) a NVECTOR object

b (realtype) constant added to all components of x

z (N_Vector) a NVECTOR object containing the result

Return value None

 $F2003 \; \mathrm{Name} \; \; \mathtt{FN_VAddConst}$

N_VDotProd

Call d = N_VDotProd(x, y);

Description Returns the value of the ordinary dot product of x and y: $d = \sum_{i=0}^{n-1} x_i y_i$.

Arguments x (N_Vector) a NVECTOR object with y

y (N_Vector) a NVECTOR object with x

Return value realtype

F2003 Name FN_VDotProd

N_VMaxNorm

Call $m = N_VMaxNorm(x);$

Description Returns the maximum norm of the N-Vector x: $m = \max_i |x_i|$.

Arguments x (N_Vector) a NVECTOR object

Return value realtype F2003 Name FN_VMaxNorm

N_VWrmsNorm

Call m = N_VWrmsNorm(x, w)

Description Returns the weighted root-mean-square norm of the N_Vector x with realtype weight

vector w: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i)^2\right)/n}$.

Arguments x (N_Vector) a NVECTOR object

w (N_Vector) a NVECTOR object containing weights

Return value realtype
F2003 Name FN_VWrmsNorm

N_VWrmsNormMask

Description Returns the weighted root mean square norm of the N_Vector x with realtype weight

vector \mathbf{w} built using only the elements of \mathbf{x} corresponding to positive elements of the

N_Vector id: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i H(id_i))^2\right)/n}$, where $H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$

Arguments x (N_Vector) a NVECTOR object

w (N_Vector) a NVECTOR object containing weights

id (N_Vector) mask vector

Return value realtype

F2003 Name FN_VWrmsNormMask

N_{VMin}

Call $m = N_VMin(x);$

Description Returns the smallest element of the N_Vector x: $m = \min_i x_i$.

Arguments x (N_Vector) a NVECTOR object

Return value realtype F2003 Name FN_VMin

N_VWL2Norm

Call m = N_VWL2Norm(x, w);

Description Returns the weighted Euclidean ℓ_2 norm of the N_Vector x with realtype weight vector

w: $m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}$.

Arguments x (N_Vector) a NVECTOR object

w (N_Vector) a NVECTOR object containing weights

Return value realtype F2003 Name FN_VWL2Norm

N_VL1Norm

Call m = N_VL1Norm(x);

Description Returns the ℓ_1 norm of the N_Vector x: $m = \sum_{i=0}^{n-1} |x_i|$. Arguments x (N_Vector) a NVECTOR object to obtain the norm of

Return value realtype F2003 Name FN_VL1Norm

N_VCompare

Call N_VCompare(c, x, z);

Description Compares the components of the N_Vector x to the realtype scalar c and returns an

N_Vector z such that: $z_i = 1.0$ if $|x_i| \ge c$ and $z_i = 0.0$ otherwise.

Arguments c (realtype) constant that each component of x is compared to

x (N_Vector) a NVECTOR object

z (N_Vector) a NVECTOR object containing the result

Return value None

F2003 Name FN_VCompare

N_VInvTest

Call $t = N_VInvTest(x, z);$

Description 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: $z_i = 1.0/x_i$, i = 0, ..., n-1.

Arguments x (N_Vector) a NVECTOR object

z (N_Vector) an output NVECTOR object

Return value Returns a booleantype with value SUNTRUE if all components of x are nonzero (success-

ful inversion) and returns SUNFALSE otherwise.

F2003 Name FN_VInvTest

N_VConstrMask

Call t = N_VConstrMask(c, x, m);

Description Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \ge 0$ if $c_i = 1$, $x_i \le 0$ if

 $c_i = -1$, $x_i < 0$ if $c_i = -2$. There is no constraint on x_i if $c_i = 0$. This routine returns a boolean assigned to SUNFALSE if any element failed the constraint test and assigned to SUNTRUE if all passed. It also sets a mask vector \mathbf{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.

Arguments c (realtype) scalar constraint value

 \mathbf{x} (N_Vector) a NVECTOR object

m (N_Vector) output mask vector

 $Return\ a\ {\tt booleantype}\ with\ value\ {\tt SUNFALSE}\ if\ any\ element\ failed\ the\ constraint\ test,$

and SUNTRUE if all passed.

 $F2003 \; Name \; FN_VConstrMask$

N_VMinQuotient

Call minq = N_VMinQuotient(num, denom);

Description This routine returns the minimum of the quotients obtained by term-wise dividing num_i

by denom_i. A zero element in denom will be skipped. If no such quotients are found, then the large value BIG_REAL (defined in the header file sundials_types.h) is returned.

Arguments num (N_Vector) a NVECTOR object used as the numerator

denom (N_Vector) a NVECTOR object used as the denominator

Return value realtype

F2003 Name FN_VMinQuotient

6.1.2 NVECTOR fused functions

Fused and vector array 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 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.

N_VLinearCombination

Call ier = N_VLinearCombination(nv, c, X, z);

Description This routine computes the linear combination of n_n vectors with n elements:

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

where c is an array of n_v scalars, X is an array of n_v vectors, 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

Arguments

Notes

F2003 Call

nv (int) the number of vectors in the linear combination

c (realtype*) an array of n_v scalars used to scale the corresponding vector in X

X (N_Vector*) an array of n_v NVECTOR objects to be scaled and combined

z (N_Vector) a NVECTOR object containing the result

Return value Returns an int with value 0 for success and a non-zero value otherwise.

vector array.

F2003 Name FN_VLinearCombination

real(c_double) :: c(nv)
type(c_ptr), target :: X(nv)
type(N_Vector), pointer :: z

ierr = FN_VLinearCombination(nv, c, X, z)

N_VScaleAddMulti

Call ier = N_VScaleAddMulti(nv, c, x, Y, Z);

Description This routine scales and adds one vector to n_v vectors with n elements:

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

where c is an array of n_v scalars, x is the vector to be scaled and added to each vector in the vector array of n_v vectors Y, and Z is a vector array of n_v output vectors.

Arguments

nv (int) the number of scalars and vectors in c, Y, and Z

c (realtype*) an array of n_v scalars

x (N_Vector) a NVECTOR object to be scaled and added to each vector in Y

Y (N_Vector*) an array of n_v NVECTOR objects where each vector j will have the vector x scaled by c_j added to it

Z (N_Vector) an output array of n_v NVECTOR objects

Return value Returns an int with value 0 for success and a non-zero value otherwise.

 $F2003 \; \mathrm{Name} \; \mathsf{FN_VScaleAddMulti}$

```
F2003 Call real(c_double) :: c(nv)
type(c_ptr), target :: Y(nv), Z(nv)
type(N_Vector), pointer :: x
ierr = FN_VScaleAddMulti(nv, c, x, Y, Z)
```

N_VDotProdMulti

Call ier = N_VDotProdMulti(nv, x, Y, d);

Description This routine computes the dot product of a vector with n_v other vectors:

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

where d is an array of n_v scalars containing the dot products of the vector x with each of the n_v vectors in the vector array Y.

Arguments nv (int) the number of vectors in Y

x (N_Vector) a NVECTOR object to be used in a dot product with each of the vectors in Y

Y (N_Vector*) an array of n_v NVECTOR objects to use in a dot product with x

d (realtype*) an output array of n_v dot products

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VDotProdMulti

F2003 Call real(c_double) :: d(nv)
type(c_ptr), target :: Y(nv)
type(N_Vector), pointer :: x
ierr = FN_VDotProdMulti(nv, x, Y, d)

6.1.3 NVECTOR vector array functions

$N_{VLinearSumVectorArray}$

Call ier = N_VLinearSumVectorArray(nv, a, X, b, Y, Z);

Description This routine computes the linear sum of two vector arrays containing n_v vectors of n elements:

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

where a and b are scalars and X, Y, and Z are arrays of n_v vectors.

Arguments nv (int) the number of vectors in the vector arrays

a (realtype) constant to scale each vector in X by

X (N_Vector*) an array of n_v NVECTOR objects

Y (N_Vector*) an array of n_v NVECTOR objects

Z (N_Vector*) an output array of n_v NVECTOR objects

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VLinearSumVectorArray

N_VScaleVectorArray

Call ier = N_VScaleVectorArray(nv, c, X, Z);

Description This routine scales each vector of n elements in a vector array of n_v vectors by a potentially different constant:

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

where c is an array of n_v scalars and X and Z are arrays of n_v vectors.

Arguments nv (int) the number of vectors in the vector arrays

 ${\tt c} \pmod{{\tt X}}$ by

X (N_Vector*) an array of n_v NVECTOR objects

Z (N_Vector*) an output array of n_v NVECTOR objects

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VScaleVectorArray

N_VConstVectorArray

Call ier = N_VConstVectorArray(nv, c, X);

Description This routine sets each element in a vector of n elements in a vector array of n_v vectors to the same value:

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

where c is a scalar and X is an array of n_v vectors.

Arguments nv (int) the number of vectors in X

c (realtype) constant to set every element in every vector of X to

X (N_Vector*) an array of n_v NVECTOR objects

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VConstVectorArray

$N_VWrmsNormVectorArray$

Call ier = N_VWrmsNormVectorArray(nv, X, W, m);

Description This routine computes the weighted root mean square norm of n_v vectors with n elements:

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

where m contains the n_v norms of the vectors in the vector array X with corresponding weight vectors W.

Arguments nv (int) the number of vectors in the vector arrays

X (N_Vector*) an array of n_v NVECTOR objects

W (N_Vector*) an array of n_v NVECTOR objects

m (realtype*) an output array of n_v norms

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VWrmsNormVectorArray

N_VWrmsNormMaskVectorArray

Call ier = N_VWrmsNormMaskVectorArray(nv, X, W, id, m);

Description This routine computes the masked weighted root mean square norm of n_v vectors with n elements:

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

 $H(id_i) = 1$ for $id_i > 0$ and is zero otherwise, m contains the n_v norms of the vectors in the vector array X with corresponding weight vectors W and mask vector id.

Arguments nv (int) the number of vectors in the vector arrays

X (N_Vector*) an array of n_v NVECTOR objects

W (N_Vector*) an array of n_v NVECTOR objects

id (N_Vector) the mask vector

m (realtype*) an output array of n_v norms

Return value Returns an int with value 0 for success and a non-zero value otherwise.

F2003 Name FN_VWrmsNormMaskVectorArray

N_VScaleAddMultiVectorArray

Call ier = N_VScaleAddMultiVectorArray(nv, ns, c, X, YY, ZZ);

Description This routine scales and adds a vector in a vector array of n_v vectors to the corresponding vector in n_s vector arrays:

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

where c is an array of n_s scalars, X is a vector array of n_v vectors to be scaled and added to the corresponding vector in each of the n_s vector arrays in the array of vector arrays YY and stored in the output array of vector arrays ZZ.

Arguments nv (int) the number of vectors in the vector arrays

ns (int) the number of scalars in c and vector arrays in YY and ZZ

c (realtype*) an array of n_s scalars

X (N_Vector*) an array of n_v NVECTOR objects

YY (N_Vector**) an array of n_s NVECTOR arrays

ZZ (N_Vector**) an output array of n_s NVECTOR arrays

Return value Returns an int with value 0 for success and a non-zero value otherwise.

N_VLinearCombinationVectorArray

Call ier = N_VLinearCombinationVectorArray(nv, ns, c, XX, Z);

Description This routine computes the linear combination of n_s vector arrays containing n_v vectors with n elements:

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

where c is an array of n_s scalars (type realtype*), XX (type N_Vector**) is an array of n_s vector arrays each containing n_v vectors to be summed into the output vector array of n_v vectors Z (type N_Vector*). If the output vector array Z is one of the vector arrays in XX, then it must be the first vector array in XX.

Arguments nv (int) the number of vectors in the vector arrays

ns (int) the number of scalars in c and vector arrays in YY and ZZ

c (realtype*) an array of n_s scalars

XX (N_Vector**) an array of n_s NVECTOR arrays

Z (N_Vector*) an output array NVECTOR objects

Return value Returns an int with value 0 for success and a non-zero value otherwise.

6.1.4 NVECTOR local reduction functions

Local reduction operations are intended to reduce parallel communication on distributed memory systems, particularly when NVECTOR objects are combined together within a

NVECTOR_MPIMANYVECTOR object (see Section 6.14). If a particular NVECTOR implementation defines a local reduction operation as NULL, the NVECTOR_MPIMANYVECTOR 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 NVECTOR implementations.

N_VDotProdLocal

Call d = N_VDotProdLocal(x, y);

Description 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).

Arguments x (N_Vector) a NVECTOR object

y (N_Vector) a NVECTOR object

Return value realtype

F2003 Name FN_VDotProdLocal

N_VMaxNormLocal

Description This routine computes the MPI task-local portion of the maximum norm of the N_Vector

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

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

Arguments x (N_Vector) a NVECTOR object

Return value realtype

F2003 Name FN_VMaxNormLocal

N_VMinLocal

Call m = N_VMinLocal(x);

Description This routine computes the smallest element of the MPI task-local portion of the N_Vector x:

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

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

Arguments x (N_Vector) a NVECTOR object

Return value realtype
F2003 Name FN_VMinLocal

N_VL1NormLocal

Call n = N_VL1NormLocal(x);

Description 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).

Arguments x (N_Vector) a NVECTOR object

Return value realtype

F2003 Name FN_VL1NormLocal

N_VWSqrSumLocal

Call s = N_VWSqrSumLocal(x,w);

Description This routine computes the MPI task-local portion of the weighted squared sum of the $N_Vector x$ 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).

Arguments x (N_Vector) a NVECTOR object

w (N_Vector) a NVECTOR object containing weights

Return value realtype

F2003 Name FN_VWSgrSumLocal

N_VWSqrSumMaskLocal

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

Description This routine computes the MPI task-local portion of the weighted squared sum of the N_Vector x with weight vector w built using only the elements of x corresponding to positive elements of the N_Vector id:

$$m = \sum_{i=0}^{n_{local}-1} (x_i w_i H(id_i))^2, \text{ where } H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \le 0 \end{cases}$$

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

Arguments x (N_Vector) a NVECTOR object

w (N_Vector) a NVECTOR object containing weights id (N_Vector) a NVECTOR object used as a mask

Return value realtype

F2003 Name FN_VWSqrSumMaskLocal

N_VInvTestLocal

Call t = N_VInvTestLocal(x, z);

Description Sets the MPI task-local components of the N_Vector z to be the inverses of the components of the N_Vector x, with prior testing for zero values:

$$z_i = 1.0/x_i, i = 0, \dots, n_{local} - 1,$$

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

Arguments x (N_Vector) a NVECTOR object

z (N_Vector) an output NVECTOR object

Return value Returns a booleantype with the value SUNTRUE if all task-local components of x are nonzero (successful inversion) and with the value SUNFALSE otherwise.

F2003 Name FN_VInvTestLocal

N_VConstrMaskLocal

Call t = N_VConstrMaskLocal(c,x,m);

Description Performs the following constraint tests:

$$x_i > 0$$
 if $c_i = 2$,
 $x_i \ge 0$ if $c_i = 1$,
 $x_i \le 0$ if $c_i = -1$,
 $x_i < 0$ if $c_i = -2$, and
no test if $c_i = 0$,

for all MPI task-local components of the vectors. It 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.

Arguments c (realtype) scalar constraint value

 ${\tt x}$ (N_Vector) a NVECTOR object

m (N_Vector) output mask vector

Return value Returns a booleantype with the value SUNFALSE if any task-local element failed the constraint test and the value SUNTRUE if all passed.

F2003 Name FN_VConstrMaskLocal

N_VMinQuotientLocal

Call ming = N_VMinQuotientLocal(num,denom);

Description This routine returns the minimum of the quotients obtained by term-wise dividing \mathtt{num}_i by \mathtt{denom}_i , for all MPI task-local components of the vectors. A zero element in \mathtt{denom} will be skipped. If no such quotients are found, then the large value $\mathtt{BIG_REAL}$ (defined in the header file $\mathtt{sundials_types.h}$) is returned.

Arguments num (N_Vector) a NVECTOR object used as the numerator

denom (N_Vector) a NVECTOR object used as the denominator

Return value realtype

 $F2003 \ Name \ FN_VMinQuotientLocal$

6.1.5 NVECTOR utility functions

To aid in the creation of custom NVECTOR modules the generic NVECTOR module provides three utility functions N_VNewEmpty, N_VCopyOps and N_VFreeEmpty. 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 only required operations need to be set and all operations are copied when cloning a vector.

To aid the use of arrays of NVECTOR objects, the generic NVECTOR module also provides the utility functions N_VCloneVectorArray, N_VCloneVectorArrayEmpty, and N_VDestroyVectorArray.

N_{V}

Call v = N_VNewEmpty();

 $Description \quad The \ function \ {\tt N_VNewEmpty} \ allocates \ a \ new \ generic \ {\tt NVECTOR} \ object \ and \ initializes \ its$

content pointer and the function pointers in the operations structure to NULL.

Arguments None

Return value This function returns an N_Vector object. If an error occurs when allocating the object,

then this routine will return NULL.

F2003 Name FN_VNewEmpty

N_VCopyOps

Call retval = N_VCopyOps(w, v);

Description The function N_VCopyOps copies the function pointers in the ops structure of w into the

ops structure of v.

Arguments w (N_Vector) the vector to copy operations from

v (N_Vector) the vector to copy operations to

Return value This returns 0 if successful and a non-zero value if either of the inputs are NULL or the

ops structure of either input is NULL.

F2003 Name FN_VCopyOps

N_VFreeEmpty

Call N_VFreeEmpty(v);

Description 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 (N_Vector)

Return value None

F2003 Name FN_VFreeEmpty

N_VCloneEmptyVectorArray

Call vecarray = N_VCloneEmptyVectorArray(count, w);

Description Creates an array of count variables of type N_Vector, each of the same type as the exist-

ing N_Vector w. It achieves this by calling the implementation-specific N_VCloneEmpty

operation.

Arguments count (int) the size of the vector array

w (N_Vector) the vector to clone

Return value Returns an array of $count N_-Vector$ objects if successful, or NULL if an error occurred

while cloning.

$N_{-}VCloneVectorArray$

Call vecarray = N_VCloneVectorArray(count, w);

Description Creates an array of count variables of type N_Vector, each of the same type as the

existing N_Vector w. It achieves this by calling the implementation-specific N_VClone

operation.

Arguments count (int) the size of the vector array

w (N_Vector) the vector to clone

Return value Returns an array of count N_Vector objects if successful, or NULL if an error occurred

while cloning.

$N_{-}VDestroyVectorArray$

Call N_VDestroyVectorArray(count, w);

Description Destroys (frees) an array of variables of type N_Vector. It depends on the implementation-

specific N_VDestroy operation.

Arguments vs (N_Vector*) the array of vectors to destroy

count (int) the size of the vector array

Return value None

6.1.6 NVECTOR identifiers

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 6.1.

6.1.7 The generic NVECTOR module implementation

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

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

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

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

Vector ID	Vector type	ID Value
SUNDIALS_NVEC_SERIAL	Serial	0
SUNDIALS_NVEC_PARALLEL	Distributed memory parallel (MPI)	1
SUNDIALS_NVEC_OPENMP	OpenMP shared memory parallel	2
SUNDIALS_NVEC_PTHREADS	PThreads shared memory parallel	3
SUNDIALS_NVEC_PARHYP	hypre ParHyp parallel vector	4
SUNDIALS_NVEC_PETSC	PETSc parallel vector	5
SUNDIALS_NVEC_CUDA	CUDA parallel vector	6
SUNDIALS_NVEC_RAJA	RAJA parallel vector	7
SUNDIALS_NVEC_OPENMPDEV	OpenMP parallel vector with device offloading	8
SUNDIALS_NVEC_TRILINOS	Trilinos Tpetra vector	9
SUNDIALS_NVEC_MANYVECTOR	"ManyVector" vector	10
SUNDIALS_NVEC_MPIMANYVECTOR	MPI-enabled "ManyVector" vector	11
SUNDIALS_NVEC_MPIPLUSX	MPI+X vector	12
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	13

```
struct _generic_N_Vector_Ops {
  N_Vector_ID (*nvgetvectorid)(N_Vector);
  N_Vector
               (*nvclone)(N_Vector);
  N_Vector
               (*nvcloneempty)(N_Vector);
  void
               (*nvdestroy)(N_Vector);
  biov
               (*nvspace)(N_Vector, sunindextype *, sunindextype *);
               (*nvgetarraypointer)(N_Vector);
  realtype*
               (*nvsetarraypointer)(realtype *, N_Vector);
  void
  void*
               (*nvgetcommunicator)(N_Vector);
  sunindextype (*nvgetlength)(N_Vector);
  void
               (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
  void
               (*nvconst)(realtype, N_Vector);
               (*nvprod)(N_Vector, N_Vector, N_Vector);
  void
               (*nvdiv)(N_Vector, N_Vector, N_Vector);
  void
  void
               (*nvscale)(realtype, N_Vector, N_Vector);
  void
               (*nvabs)(N_Vector, N_Vector);
  void
               (*nvinv)(N_Vector, N_Vector);
               (*nvaddconst)(N_Vector, realtype, N_Vector);
  void
               (*nvdotprod)(N_Vector, N_Vector);
  realtype
  realtype
               (*nvmaxnorm)(N_Vector);
               (*nvwrmsnorm)(N_Vector, N_Vector);
  realtype
  realtype
               (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
  realtype
               (*nvmin)(N_Vector);
               (*nvwl2norm)(N_Vector, N_Vector);
  realtype
               (*nvl1norm)(N_Vector);
  realtype
               (*nvcompare)(realtype, N_Vector, N_Vector);
  void
  booleantype
               (*nvinvtest)(N_Vector, N_Vector);
               (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
  booleantype
  realtype
               (*nvminquotient)(N_Vector, N_Vector);
  int
               (*nvlinearcombination)(int, realtype*, N_Vector*, N_Vector);
               (*nvscaleaddmulti)(int, realtype*, N_Vector, N_Vector*, N_Vector*);
  int
  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*);
```

```
(*nvconstvectorarray)(int, realtype, N_Vector*);
  int
               (*nvwrmsnomrvectorarray)(int, N_Vector*, N_Vector*, realtype*);
  int
               (*nvwrmsnomrmaskvectorarray)(int, N_Vector*, N_Vector*, N_Vector,
  int
                                             realtype*);
  int
               (*nvscaleaddmultivectorarray)(int, int, realtype*, N_Vector*,
                                              N_Vector**, N_Vector**);
  int
               (*nvlinearcombinationvectorarray)(int, int, realtype*, N_Vector**,
                                                  N_Vector*);
               (*nvdotprodlocal)(N_Vector, N_Vector);
  realtype
  realtype
               (*nvmaxnormlocal)(N_Vector);
               (*nvminlocal)(N_Vector);
  realtype
  realtype
               (*nvl1normlocal)(N_Vector);
               (*nvinvtestlocal)(N_Vector, N_Vector);
  booleantype
  booleantype
               (*nvconstrmasklocal)(N_Vector, N_Vector, N_Vector);
               (*nvminquotientlocal)(N_Vector, N_Vector);
  realtype
  realtype
               (*nvwsqrsumlocal)(N_Vector, N_Vector);
  realtype
               (*nvwsqrsummasklocal(N_Vector, N_Vector, N_Vector);
};
```

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

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

Section 6.1.1 defines a complete list of all standard vector operations defined by the generic NVECTOR module. Sections 6.1.2, 6.1.3 and 6.1.4 list *optional* fused, vector array and local reduction operations, respectively.

The Fortran 2003 interface provides a bind(C) derived-type for the _generic_N_Vector and the _generic_N_Vector_Ops structures. Their definition is given below.

```
type, bind(C), public :: N_Vector
type(C_PTR), public :: content
type(C_PTR), public :: ops
end type N_Vector
type, bind(C), public :: N_Vector_Ops
type(C_FUNPTR), public :: nvgetvectorid
type(C_FUNPTR), public :: nvclone
type(C_FUNPTR), public :: nvcloneempty
type(C_FUNPTR), public :: nvdestroy
type(C_FUNPTR), public :: nvspace
type(C_FUNPTR), public :: nvgetarraypointer
type(C_FUNPTR), public :: nvsetarraypointer
type(C_FUNPTR), public :: nvgetcommunicator
type(C_FUNPTR), public :: nvgetlength
type(C_FUNPTR), public :: nvlinearsum
type(C_FUNPTR), public :: nvconst
type(C_FUNPTR), public :: nvprod
type(C_FUNPTR), public :: nvdiv
```

```
type(C_FUNPTR), public :: nvscale
type(C_FUNPTR), public :: nvabs
type(C_FUNPTR), public :: nvinv
type(C_FUNPTR), public :: nvaddconst
type(C_FUNPTR), public :: nvdotprod
type(C_FUNPTR), public :: nvmaxnorm
type(C_FUNPTR), public :: nvwrmsnorm
type(C_FUNPTR), public :: nvwrmsnormmask
type(C_FUNPTR), public :: nvmin
type(C_FUNPTR), public :: nvwl2norm
type(C_FUNPTR), public :: nvl1norm
type(C_FUNPTR), public :: nvcompare
type(C_FUNPTR), public :: nvinvtest
type(C_FUNPTR), public :: nvconstrmask
type(C_FUNPTR), public :: nvminquotient
type(C_FUNPTR), public :: nvlinearcombination
type(C_FUNPTR), public :: nvscaleaddmulti
type(C_FUNPTR), public :: nvdotprodmulti
type(C_FUNPTR), public :: nvlinearsumvectorarray
type(C_FUNPTR), public :: nvscalevectorarray
type(C_FUNPTR), public :: nvconstvectorarray
type(C_FUNPTR), public :: nvwrmsnormvectorarray
type(C_FUNPTR), public :: nvwrmsnormmaskvectorarray
type(C_FUNPTR), public :: nvscaleaddmultivectorarray
type(C_FUNPTR), public :: nvlinearcombinationvectorarray
type(C_FUNPTR), public :: nvdotprodlocal
type(C_FUNPTR), public :: nvmaxnormlocal
type(C_FUNPTR), public :: nvminlocal
type(C_FUNPTR), public :: nvl1normlocal
type(C_FUNPTR), public :: nvinvtestlocal
type(C_FUNPTR), public :: nvconstrmasklocal
type(C_FUNPTR), public :: nvminquotientlocal
type(C_FUNPTR), public :: nvwsqrsumlocal
type(C_FUNPTR), public :: nvwsqrsummasklocal
end type N_Vector_Ops
```

6.1.8 Implementing a custom NVECTOR

A particular implementation of the NVECTOR module must:

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

It is recommended that a user-supplied NVECTOR implementation returns the SUNDIALS_NVEC_CUSTOM identifier from the N_VGetVectorID function.

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 only required operations need to be set and all operations are copied when cloning a vector.

6.1.8.1 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 Sections 6.1.1-6.1.4 above 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., $m = \min_i \operatorname{real}(x_i)$.
- 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., $z_i = c + 0j$, i = 0, ..., n 1.
- 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 both SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT may be used with any of the IVP solvers (CVODE, CVODES, IDA, IDAS and ARKODE) for complex-valued problems, the Anderson-acceleration feature SUNNONLINSOL_FIXEDPOINT cannot be used due to its reliance on N_VDotProd. By this same logic, the Anderson acceleration feature within KINSOL also will not work with complex-valued vectors.

Similarly, although each package's linear solver interface (e.g., CVLS) may be used on complex-valued problems, none of the built-in SUNMATRIX or SUNLINSOL modules work. Hence a complex-valued user should provide a custom SUNLINSOL (and optionally a custom SUNMATRIX) implementation for solving linear systems, and then attach this module 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 NVECTOR functions used by KINSOL

In Table 6.2 below, we list the vector functions in the NVECTOR module used within 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 solver module, while the remaining five columns show function usage within each of the KINSOL linear solver interfaces, the KINBBDPRE preconditioner module, and the FKINSOL module. Here KINLS stands for the generic linear solver interface in KINSOL.

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.

	KINSOL	KINLS	KINBBDPRE	FKINSOL
$N_{-}VGetVectorID$				
${ t NVGetLength}$		4		
$N_{-}VClone$	√		✓	
$N_{-}VCloneEmpty$				\checkmark
$ exttt{N_VDestroy}$	✓		√	√
N_VSpace	✓	2		
$N_{-}VGetArrayPointer$		1	√	√
$N_{-}VSetArrayPointer$		1		√
${ t NVLinearSum}$	√	√		
$N_{ m VConst}$		√		
N_VProd	√	✓		
$N_{-}VDiv$	√			
N_VScale	√	√	√	
$N_{-}VAbs$	✓			
$N_{-}VInv$	✓			
N_VDotProd	√	√		
$N_{-}VMaxNorm$				
$N_{-}VMin$	✓			
N_VWL2Norm	✓	✓		
N_VL1Norm		3		
N_VConstrMask	√			
${\tt NVMinQuotient}$	✓			
$N_{-}VLinearCombination$	√	√		
$N_{-}VDotProdMulti$	√			

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

Special cases (numbers match markings in table):

- 1. These routines are only required if an internal difference-quotient routine for constructing dense or 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 SUNLINSOL module that does not support the SUNLinSolSetScalingVectors routine is supplied to KINSOL.

Each SUNLINSOL object may require additional NVECTOR routines not listed in the table above. Please see the the relevant descriptions of these modules in Sections 8.5-8.16 for additional detail on their NVECTOR requirements.

The vector functions listed in Table 6.1.1 that are *not* used by KINSOL are N_VAddConst, N_VWrmsNorm, N_VWrmsNormMask, N_VCompare, N_VInvTest, and N_VGetCommunicator. Therefore a user-supplied NVECTOR module for KINSOL could omit these functions.

The optional function N_VLinearCombination is only used when Anderson acceleration is enabled or the SPBCGS, 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 Tables 6.1.2 and 6.1.3 are unused and a user-supplied NVECTOR module for KINSOL could omit these operations.

6.3 The NVECTOR_SERIAL implementation

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

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

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

6.3.1 NVECTOR_SERIAL accessor macros

The following macros are provided to access the content of an NVECTOR_SERIAL vector. The suffix _S in the names denotes the serial version.

• NV_CONTENT_S

This routine gives access to the contents of the serial vector N_Vector.

The assignment $v_cont = NV_CONTENT_S(v)$ sets v_cont to be a pointer to the serial N_Vector content structure.

Implementation:

```
#define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
```

• NV_OWN_DATA_S, NV_DATA_S, NV_LENGTH_S

These macros give individual access to the parts of the content of a serial N_Vector.

The assignment $v_{data} = NV_DATA_S(v)$ sets v_{data} to be a pointer to the first component of the data for the $N_Vector v$. The assignment $NV_DATA_S(v) = v_{data}$ sets the component array of v to be v_{data} by storing the pointer v_{data} .

The assignment $v_len = NV_LENGTH_S(v)$ sets v_len to be the length of v. On the other hand, the call $NV_LENGTH_S(v) = len_v$ sets the length of v to be len_v .

Implementation:

```
#define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )
#define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )
#define NV_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
```

• NV_Ith_S

This macro gives access to the individual components of the data array of an N_Vector.

The assignment $r = NV_{i,i}$ sets r to be the value of the i-th component of v. The assignment $NV_{i,i} = r$ 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])

6.3.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3 and 6.1.4. Their names are obtained from those in these tables by appending the suffix _Serial (e.g. N_VDestroy_Serial). All the standard vector operations listed in 6.1.1 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_VNew_Serial

Prototype N_Vector N_VNew_Serial(sunindextype vec_length);

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

F2003 Name This function is callable as FN_VNew_Serial when using the Fortran 2003 interface module.

N_VNewEmpty_Serial

Prototype N_Vector N_VNewEmpty_Serial(sunindextype vec_length);

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

F2003 Name This function is callable as FN_VNewEmpty_Serial when using the Fortran 2003 interface module.

N_VMake_Serial

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

Description This function creates and allocates memory for a serial vector with user-provided data array.

(This function does *not* allocate memory for v_data itself.)

F2003 Name This function is callable as FN_VMake_Serial when using the Fortran 2003 interface module.

N_VCloneVectorArray_Serial

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

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

F2003 Name This function is callable as FN_VCloneVectorArray_Serial when using the Fortran 2003 interface module.

N_VCloneVectorArrayEmpty_Serial

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

Description This function creates (by cloning) an array of count serial vectors, each with an empty

(NULL) data array.

F2003 Name This function is callable as FN_VCloneVectorArrayEmpty_Serial when using the For-

tran 2003 interface module.

N_VDestroyVectorArray_Serial

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

Description This function frees memory allocated for the array of count variables of type N_Vector

created with N_VCloneVectorArray_Serial or with

N_VCloneVectorArrayEmpty_Serial.

F2003 Name This function is callable as FN_VDestroyVectorArray_Serial when using the Fortran

2003 interface module.

N_VPrint_Serial

Prototype void N_VPrint_Serial(N_Vector v);

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

F2003 Name This function is callable as FN_VPrint_Serial when using the Fortran 2003 interface

module.

N_VPrintFile_Serial

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

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

F2003 Name This function is callable as FN_VPrintFile_Serial when using the Fortran 2003 interface

module.

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 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.

N_VEnableFusedOps_Serial

int N_VEnableFusedOps_Serial(N_Vector v, booleantype tf); Prototype

This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array op-Description

erations in the serial vector. The return value is 0 for success and -1 if the input vector

or its ops structure are NULL.

F2003 Name This function is callable as FN_VEnableFusedOps_Serial when using the Fortran 2003

interface module.

N_VEnableLinearCombination_Serial

Prototype int N_VEnableLinearCombination_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableLinearCombination_Serial when using the Fortran 2003 interface module.

N_VEnableScaleAddMulti_Serial

Prototype int N_VEnableScaleAddMulti_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableScaleAddMulti_Serial when using the Fortran 2003 interface module.

N_VEnableDotProdMulti_Serial

Prototype int N_VEnableDotProdMulti_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableDotProdMulti_Serial when using the Fortran 2003 interface module.

N_VEnableLinearSumVectorArray_Serial

Prototype int N_VEnableLinearSumVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableLinearSumVectorArray_Serial when using the Fortran 2003 interface module.

N_VEnableScaleVectorArray_Serial

Prototype int N_VEnableScaleVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableScaleVectorArray_Serial when using the Fortran 2003 interface module.

N_VEnableConstVectorArray_Serial

Prototype int N_VEnableConstVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableConstVectorArray_Serial when using the Fortran 2003 interface module.

N_VEnableWrmsNormVectorArray_Serial

Prototype int N_VEnableWrmsNormVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormVectorArray_Serial when using the Fortran 2003 interface module.

N_VEnableWrmsNormMaskVectorArray_Serial

Prototype int N_VEnableWrmsNormMaskVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormMaskVectorArray_Serial when using the Fortran 2003 interface module.

N_VEnableScaleAddMultiVectorArray_Serial

Prototype int N_VEnableScaleAddMultiVectorArray_Serial(N_Vector v, booleantype tf);

Description 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.

N_VEnableLinearCombinationVectorArray_Serial

Prototype int N_VEnableLinearCombinationVectorArray_Serial(N_Vector v, booleantype tf);

Description 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) and then access v_data[i] within the loop than it is to use NV_Ith_S(v,i) within the loop.
- N_VNewEmpty_Serial, N_VMake_Serial, and N_VCloneVectorArrayEmpty_Serial set the field $own_data = SUNFALSE$. N_VDestroy_Serial and N_VDestroyVectorArray_Serial will not attempt to free the pointer data for any N_Vector with own_data set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.
- To maximize efficiency, vector operations in the NVECTOR_SERIAL implementation that have more than one N_Vector argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with N_Vector arguments that were all created with the same internal representations.





6.3.3 NVECTOR_SERIAL Fortran interfaces

The NVECTOR_SERIAL module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

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 Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fnvectorserial_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the NVECTOR_SERIAL module also includes a FORTRAN-callable function FNVINITS(code, NEQ, IER), to initialize this NVECTOR_SERIAL module. Here code is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type long int); and IER is an error return flag equal 0 for success and -1 for failure.

6.4 The NVECTOR_PARALLEL implementation

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

```
struct _N_VectorContent_Parallel {
   sunindextype local_length;
   sunindextype global_length;
   booleantype own_data;
   realtype *data;
   MPI_Comm comm;
};
```

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

6.4.1 NVECTOR_PARALLEL accessor macros

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

NV_CONTENT_P

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

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

Implementation:

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

• NV_OWN_DATA_P, NV_DATA_P, NV_LOCLENGTH_P, NV_GLOBLENGTH_P

These macros give individual access to the parts of the content of a parallel N_Vector.

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} .

The assignment v_llen = NV_LOCLENGTH_P(v) sets v_llen to be the length of the local part of v. The call NV_LENGTH_P(v) = $llen_v$ sets the local length of v to be $llen_v$.

The assignment v_glen = NV_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_OWN_DATA_P(v) ( NV_CONTENT_P(v)->own_data )
#define NV_DATA_P(v) ( NV_CONTENT_P(v)->data )
#define NV_LOCLENGTH_P(v) ( NV_CONTENT_P(v)->local_length )
#define NV_GLOBLENGTH_P(v) ( NV_CONTENT_P(v)->global_length )
```

NV_COMM_P

This macro provides access to the MPI communicator used by the NVECTOR_PARALLEL vectors. Implementation:

```
#define NV_COMM_P(v) ( NV_CONTENT_P(v)->comm )
```

• NV Tth P

This macro gives access to the individual components of the local data array of an N_Vector.

The assignment $r = NV_i(v,i)$ sets r to be the value of the i-th component of the local part of v. The assignment $NV_i(v,i) = r$ 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] )
```

6.4.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. Their names are obtained from those in these tables by appending the suffix _Parallel (e.g. N_VDestroy_Parallel). The module NVECTOR_PARALLEL provides the following additional user-callable routines:

N_VNew_Parallel

```
Prototype N_Vector N_VNew_Parallel(MPI_Comm comm, sunindextype local_length, sunindextype global_length);
```

Description This function creates and allocates memory for a parallel vector.

F2003 Name This function is callable as FN_VNew_Parallel when using the Fortran 2003 interface module.

N_VNewEmpty_Parallel

Prototype N_Vector N_VNewEmpty_Parallel(MPI_Comm comm, sunindextype local_length, sunindextype global_length);

Description This function creates a new parallel N_Vector with an empty (NULL) data array.

F2003 Name This function is callable as FN_VNewEmpty_Parallel when using the Fortran 2003 interface module.

N_VMake_Parallel

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

Description 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.

F2003 Name This function is callable as FN_VMake_Parallel when using the Fortran 2003 interface module.

N_VCloneVectorArray_Parallel

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

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

F2003 Name This function is callable as FN_VCloneVectorArray_Parallel when using the Fortran 2003 interface module.

N_VCloneVectorArrayEmpty_Parallel

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

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

F2003 Name This function is callable as FN_VCloneVectorArrayEmpty_Parallel when using the Fortran 2003 interface module.

N_VDestroyVectorArray_Parallel

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

Description This function frees memory allocated for the array of count variables of type N_Vector created with N_VCloneVectorArray_Parallel or with N_VCloneVectorArrayEmpty_Parallel.

F2003 Name This function is callable as FN_VDestroyVectorArray_Parallel when using the Fortran 2003 interface module.

N_VGetLocalLength_Parallel

Prototype sunindextype N_VGetLocalLength_Parallel(N_Vector v);

Description This function returns the local vector length.

F2003 Name This function is callable as FN_VGetLocalLength_Parallel when using the Fortran 2003 interface module.

N_VPrint_Parallel

Prototype void N_VPrint_Parallel(N_Vector v);

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

F2003 Name This function is callable as FN_VPrint_Parallel when using the Fortran 2003 interface

module.

N_VPrintFile_Parallel

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

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

F2003 Name This function is callable as FN_VPrintFile_Parallel when using the Fortran 2003 interface module.

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 with that vector. 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_Parallel will have the default settings for the NVECTOR_PARALLEL module.

N_VEnableFusedOps_Parallel

Prototype int N_VEnableFusedOps_Parallel(N_Vector v, booleantype tf);

Description 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 $\ensuremath{\mathsf{ops}}$ structure are NULL.

F2003 Name This function is callable as FN_VEnableFusedOps_Parallel when using the Fortran 2003 interface module.

N_VEnableLinearCombination_Parallel

Prototype int N_VEnableLinearCombination_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableLinearCombination_Parallel when using the Fortran 2003 interface module.

N_VEnableScaleAddMulti_Parallel

Prototype int N_VEnableScaleAddMulti_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableScaleAddMulti_Parallel when using the Fortran 2003 interface module.

N_VEnableDotProdMulti_Parallel

Prototype int N_VEnableDotProdMulti_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableDotProdMulti_Parallel when using the Fortran 2003 interface module.

N_VEnableLinearSumVectorArray_Parallel

Prototype int N_VEnableLinearSumVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableLinearSumVectorArray_Parallel when using the Fortran 2003 interface module.

N_VEnableScaleVectorArray_Parallel

Prototype int N_VEnableScaleVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableScaleVectorArray_Parallel when using the Fortran 2003 interface module.

N_VEnableConstVectorArray_Parallel

Prototype int N_VEnableConstVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableConstVectorArray_Parallel when using the Fortran 2003 interface module.

| N_VEnableWrmsNormVectorArray_Parallel

Prototype int N_VEnableWrmsNormVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormVectorArray_Parallel when using the Fortran 2003 interface module.

N_VEnableWrmsNormMaskVectorArray_Parallel

Prototype int N_VEnableWrmsNormMaskVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormMaskVectorArray_Parallel when using the Fortran 2003 interface module.

N_VEnableScaleAddMultiVectorArray_Parallel

Prototype int N_VEnableScaleAddMultiVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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.

N_VEnableLinearCombinationVectorArray_Parallel

Prototype int N_VEnableLinearCombinationVectorArray_Parallel(N_Vector v, booleantype tf);

Description 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 = NV_DATA_P(v) and then access v_data[i] within the loop than it is to use NV_Ith_P(v,i) within the loop.
- N_VNewEmpty_Parallel, N_VMake_Parallel, and N_VCloneVectorArrayEmpty_Parallel set the field own_data = SUNFALSE. N_VDestroy_Parallel and N_VDestroyVectorArray_Parallel will not attempt to free the pointer data for any N_Vector with own_data set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.
- To maximize efficiency, vector operations in the NVECTOR_PARALLEL implementation that have more than one N_Vector argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with N_Vector arguments that were all created with the same internal representations.

6.4.3 NVECTOR_PARALLEL Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the NVECTOR_PARALLEL module also includes a FORTRAN-callable function FNVINITP(COMM, code, NLOCAL, NGLOBAL, IER), to initialize this NVECTOR_PARALLEL module. Here COMM is the MPI communicator, code is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NLOCAL and NGLOBAL are the local and global vector sizes, respectively (declared so as to match C type long int); and IER is an error return flag equal 0 for success and -1 for failure. NOTE: If the header file sundials_config.h defines SUNDIALS_MPI_COMM_F2C to be 1 (meaning the MPI implementation used to build SUNDIALS includes the MPI_Comm_f2c function), then COMM can be any valid MPI communicator. Otherwise, MPI_COMM_WORLD will be used, so just pass an integer value as a placeholder.

6.5 The NVECTOR_OPENMP implementation

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





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

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

The header file to include when using this module is nvector_openmp.h. The installed module library to link to is libsundials_nvecopenmp.lib where .lib is typically .so for shared libraries and .a for static libraries. The FORTRAN module file to use when using the FORTRAN 2003 interface to this module is fnvector_openmp_mod.mod.

6.5.1 NVECTOR_OPENMP accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMP vector. The suffix _OMP in the names denotes the OpenMP version.

NV_CONTENT_OMP

This routine gives access to the contents of the OpenMP vector N_Vector.

The assignment $v_cont = NV_CONTENT_OMP(v)$ sets v_cont to be a pointer to the OpenMP N_Vector content structure.

Implementation:

```
#define NV_CONTENT_OMP(v) ( (N_VectorContent_OpenMP)(v->content) )
```

• NV_OWN_DATA_OMP, NV_DATA_OMP, NV_LENGTH_OMP, NV_NUM_THREADS_OMP

These macros give individual access to the parts of the content of a OpenMP N_Vector.

The assignment $v_{data} = NV_DATA_OMP(v)$ sets v_{data} to be a pointer to the first component of the data for the $N_Vector v$. The assignment $NV_DATA_OMP(v) = v_{data}$ sets the component array of v to be v_{data} by storing the pointer v_{data} .

The assignment $v_len = NV_length_OMP(v)$ sets v_len to be the length of v. On the other hand, the call $NV_length_OMP(v) = len_v$ sets the length of v to be len_v .

The assignment v_num_threads = NV_NUM_THREADS_OMP(v) sets v_num_threads to be the number of threads from v. On the other hand, the call NV_NUM_THREADS_OMP(v) = num_threads_v sets the number of threads for v to be num_threads_v.

Implementation:

```
#define NV_OWN_DATA_OMP(v) ( NV_CONTENT_OMP(v)->own_data )
#define NV_DATA_OMP(v) ( NV_CONTENT_OMP(v)->data )
#define NV_LENGTH_OMP(v) ( NV_CONTENT_OMP(v)->length )
#define NV_NUM_THREADS_OMP(v) ( NV_CONTENT_OMP(v)->num_threads )
```

• NV_Ith_OMP

This macro gives access to the individual components of the data array of an N-Vector.

The assignment $r = NV_{int}(v,i)$ sets r to be the value of the i-th component of v. The assignment $NV_{int}(v,i) = r$ 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] )
```

6.5.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. Their names are obtained from those in these tables by appending the suffix _OpenMP (e.g. N_VDestroy_OpenMP). All the standard vector operations listed in 6.1.1 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_VNew_OpenMP

Prototype N_Vector N_VNew_OpenMP(sunindextype vec_length, int num_threads)

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

F2003 Name This function is callable as FN_VNew_OpenMP when using the Fortran 2003 interface module.

N_VNewEmpty_OpenMP

Prototype N_Vector N_VNewEmpty_OpenMP(sunindextype vec_length, int num_threads)

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

F2003 Name This function is callable as FN_VNewEmpty_OpenMP when using the Fortran 2003 interface module.

N_VMake_OpenMP

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

Description This function creates and allocates memory for a OpenMP vector with user-provided data array. This function does *not* allocate memory for v_data itself.

F2003 Name This function is callable as FN_VMake_OpenMP when using the Fortran 2003 interface module.

N_VCloneVectorArray_OpenMP

Prototype N_Vector *N_VCloneVectorArray_OpenMP(int count, N_Vector w)

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

F2003 Name This function is callable as FN_VCloneVectorArray_OpenMP when using the Fortran 2003 interface module.

N_VCloneVectorArrayEmpty_OpenMP

Prototype N_Vector *N_VCloneVectorArrayEmpty_OpenMP(int count, N_Vector w)

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

F2003 Name This function is callable as FN_VCloneVectorArrayEmpty_OpenMP when using the Fortran 2003 interface module.

N_VDestroyVectorArray_OpenMP

Prototype void N_VDestroyVectorArray_OpenMP(N_Vector *vs, int count)

 $created \ with \ {\tt N_VCloneVectorArray_OpenMP} \ or \ with \ {\tt N_VCloneVectorArrayEmpty_OpenMP}.$

F2003 Name This function is callable as FN_VDestroyVectorArray_OpenMP when using the Fortran

2003 interface module.

N_VPrint_OpenMP

Prototype void N_VPrint_OpenMP(N_Vector v)

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

F2003 Name This function is callable as FN_VPrint_OpenMP when using the Fortran 2003 interface

module.

N_VPrintFile_OpenMP

Prototype void N_VPrintFile_OpenMP(N_Vector v, FILE *outfile)

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

 ${\tt F2003~Name~This~function~is~callable~as~FN_VPrintFile_OpenMP~when~using~the~Fortran~2003~interface}$

module.

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.

N_VEnableFusedOps_OpenMP

Prototype int N_VEnableFusedOps_OpenMP(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array op-

erations in the OpenMP vector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

F2003 Name This function is callable as FN_VEnableFusedOps_OpenMP when using the Fortran 2003

interface module.

N_VEnableLinearCombination_OpenMP

Prototype int N_VEnableLinearCombination_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableLinearCombination_OpenMP when using the For-

tran 2003 interface module.

N_VEnableScaleAddMulti_OpenMP

Prototype int N_VEnableScaleAddMulti_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableScaleAddMulti_OpenMP when using the Fortran 2003 interface module.

N_VEnableDotProdMulti_OpenMP

Prototype int N_VEnableDotProdMulti_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableDotProdMulti_OpenMP when using the Fortran 2003 interface module.

N_VEnableLinearSumVectorArray_OpenMP

Prototype int N_VEnableLinearSumVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableLinearSumVectorArray_OpenMP when using the Fortran 2003 interface module.

N_VEnableScaleVectorArray_OpenMP

Prototype int N_VEnableScaleVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableScaleVectorArray_OpenMP when using the Fortran 2003 interface module.

N_VEnableConstVectorArray_OpenMP

 $\label{eq:prototype} Prototype \quad \text{ int N_VEnableConstVectorArray_OpenMP(N_Vector v, booleantype tf)}$

Description 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.

F2003 Name This function is callable as FN_VEnableConstVectorArray_OpenMP when using the Fortran 2003 interface module.

N_VEnableWrmsNormVectorArray_OpenMP

Prototype int N_VEnableWrmsNormVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormVectorArray_OpenMP when using the Fortran 2003 interface module.

N_VEnableWrmsNormMaskVectorArray_OpenMP

Prototype int N_VEnableWrmsNormMaskVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormMaskVectorArray_OpenMP when using the Fortran 2003 interface module.

${\tt N_VEnableScaleAddMultiVectorArray_OpenMP}$

Prototype int N_VEnableScaleAddMultiVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearCombinationVectorArray_OpenMP

Prototype int N_VEnableLinearCombinationVectorArray_OpenMP(N_Vector v, booleantype tf)

Description 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 = NV_DATA_OMP(v) and then access v_data[i] within the loop than it is to use NV_Ith_OMP(v,i) within the loop.
- N_VNewEmpty_OpenMP, N_VMake_OpenMP, and N_VCloneVectorArrayEmpty_OpenMP set the field $own_data = SUNFALSE$. N_VDestroy_OpenMP and N_VDestroyVectorArray_OpenMP will not attempt to free the pointer data for any N_Vector with own_data set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.
- To maximize efficiency, vector operations in the NVECTOR_OPENMP implementation that have more than one N_Vector argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with N_Vector arguments that were all created with the same internal representations.

6.5.3 NVECTOR_OPENMP Fortran interfaces

The NVECTOR_OPENMP module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The nvector_openmp_mod FORTRAN module defines interfaces to most 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 Appendix A.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the NVECTOR_OPENMP module also includes a FORTRAN-callable function FNVINITOMP(code, NEQ, NUMTHREADS, IER), to initialize this module. Here code is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type long int); NUMTHREADS is the number of threads; and IER is an error return flag equal 0 for success and -1 for failure.

6.6 The NVECTOR_PTHREADS implementation

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

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

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

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

6.6.1 NVECTOR PTHREADS accessor macros

The following macros are provided to access the content of an NVECTOR_PTHREADS vector. The suffix _PT in the names denotes the Pthreads version.

NV_CONTENT_PT

This routine gives access to the contents of the Pthreads vector N_Vector.

The assignment $v_cont = NV_CONTENT_PT(v)$ sets v_cont to be a pointer to the Pthreads N_Vector content structure.

Implementation:

```
#define NV_CONTENT_PT(v) ( (N_VectorContent_Pthreads)(v->content) )
```

• NV_OWN_DATA_PT, NV_DATA_PT, NV_LENGTH_PT, NV_NUM_THREADS_PT

These macros give individual access to the parts of the content of a Pthreads N_Vector.

The assignment $v_{data} = NV_DATA_PT(v)$ sets v_{data} to be a pointer to the first component of the data for the $N_Vector v$. The assignment $NV_DATA_PT(v) = v_{data}$ sets the component array of v to be v_{data} by storing the pointer v_{data} .

The assignment $v_len = NV_LENGTH_PT(v)$ sets v_len to be the length of v. On the other hand, the call $NV_LENGTH_PT(v) = len_v$ sets the length of v to be len_v .

The assignment v_num_threads = NV_NUM_THREADS_PT(v) sets v_num_threads to be the number of threads from v. On the other hand, the call NV_NUM_THREADS_PT(v) = num_threads_v sets the number of threads for v to be num_threads_v.

Implementation:

```
#define NV_OWN_DATA_PT(v) ( NV_CONTENT_PT(v)->own_data )
#define NV_DATA_PT(v) ( NV_CONTENT_PT(v)->data )
#define NV_LENGTH_PT(v) ( NV_CONTENT_PT(v)->length )
#define NV_NUM_THREADS_PT(v) ( NV_CONTENT_PT(v)->num_threads )
```

• NV_Ith_PT

This macro gives access to the individual components of the data array of an N-Vector.

The assignment $r = NV_Ith_PT(v,i)$ sets r to be the value of the i-th component of v. The assignment $NV_Ith_PT(v,i) = r$ sets the value of the i-th component of v to be r.

Here i ranges from 0 to n-1 for a vector of length n.

Implementation:

```
#define NV_Ith_PT(v,i) ( NV_DATA_PT(v)[i] )
```

6.6.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. Their names are obtained from those in these tables by appending the suffix _Pthreads (e.g. N_VDestroy_Pthreads). All the standard vector operations listed in 6.1.1 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_VNew_Pthreads

Prototype N_Vector N_VNew_Pthreads(sunindextype vec_length, int num_threads)

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

F2003 Name This function is callable as FN_VNew_Pthreads when using the Fortran 2003 interface module.

N_VNewEmpty_Pthreads

Prototype N_Vector N_VNewEmpty_Pthreads(sunindextype vec_length, int num_threads)

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

F2003 Name This function is callable as FN_VNewEmpty_Pthreads when using the Fortran 2003 interface module.

N_VMake_Pthreads

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

Description This function creates and allocates memory for a Pthreads vector with user-provided data array. This function does *not* allocate memory for v_data itself.

F2003 Name This function is callable as FN_VMake_Pthreads when using the Fortran 2003 interface module.

N_VCloneVectorArray_Pthreads

 $\label{lem:prototype} $$\operatorname{N_Vector} *\operatorname{N_VCloneVectorArray_Pthreads(int\ count,\ N_Vector\ w)}$$

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

F2003 Name This function is callable as FN_VCloneVectorArray_Pthreads when using the Fortran

2003 interface module.

N_VCloneVectorArrayEmpty_Pthreads

Prototype N_Vector *N_VCloneVectorArrayEmpty_Pthreads(int count, N_Vector w)

Description This function creates (by cloning) an array of count Pthreads vectors, each with an

empty (NULL) data array.

F2003 Name This function is callable as FN_VCloneVectorArrayEmpty_Pthreads when using the For-

tran 2003 interface module.

$N_VDestroyVectorArray_Pthreads$

Prototype void N_VDestroyVectorArray_Pthreads(N_Vector *vs, int count)

Description This function frees memory allocated for the array of count variables of type N_Vector

created with N_VCloneVectorArray_Pthreads or with

N_VCloneVectorArrayEmpty_Pthreads.

F2003 Name This function is callable as FN_VDestroyVectorArray_Pthreads when using the Fortran

2003 interface module.

N_VPrint_Pthreads

Prototype void N_VPrint_Pthreads(N_Vector v)

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

F2003 Name This function is callable as FN_VPrint_Pthreads when using the Fortran 2003 interface

module.

N_VPrintFile_Pthreads

Prototype void N_VPrintFile_Pthreads(N_Vector v, FILE *outfile)

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

F2003 Name This function is callable as FN_VPrintFile_Pthreads when using the Fortran 2003 in-

terface module.

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.

N_VEnableFusedOps_Pthreads

Prototype int N_VEnableFusedOps_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableFusedOps_Pthreads when using the Fortran 2003 interface module.

N_VEnableLinearCombination_Pthreads

Prototype int N_VEnableLinearCombination_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableLinearCombination_Pthreads when using the Fortran 2003 interface module.

N_VEnableScaleAddMulti_Pthreads

Prototype int N_VEnableScaleAddMulti_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableScaleAddMulti_Pthreads when using the Fortran 2003 interface module.

N_VEnableDotProdMulti_Pthreads

Prototype int N_VEnableDotProdMulti_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableDotProdMulti_Pthreads when using the Fortran 2003 interface module.

N_VEnableLinearSumVectorArray_Pthreads

Prototype int N_VEnableLinearSumVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableLinearSumVectorArray_Pthreads when using the Fortran 2003 interface module.

N_VEnableScaleVectorArray_Pthreads

Prototype int N_VEnableScaleVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableScaleVectorArray_Pthreads when using the Fortran 2003 interface module.

N_VEnableConstVectorArray_Pthreads

Prototype int N_VEnableConstVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableConstVectorArray_Pthreads when using the Fortran 2003 interface module.

N_VEnableWrmsNormVectorArray_Pthreads

Prototype int N_VEnableWrmsNormVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormVectorArray_Pthreads when using the Fortran 2003 interface module.

${\tt N_VEnableWrmsNormMaskVectorArray_Pthreads}$

Prototype int N_VEnableWrmsNormMaskVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

F2003 Name This function is callable as FN_VEnableWrmsNormMaskVectorArray_Pthreads when using the Fortran 2003 interface module.

N_VEnableScaleAddMultiVectorArray_Pthreads

Prototype int N_VEnableScaleAddMultiVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearCombinationVectorArray_Pthreads

Prototype int N_VEnableLinearCombinationVectorArray_Pthreads(N_Vector v, booleantype tf)

Description 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 = NV_DATA_PT(v) and then access v_data[i] within the loop than it is to use NV_Ith_PT(v,i) within the loop.
- N_VNewEmpty_Pthreads, N_VMake_Pthreads, and N_VCloneVectorArrayEmpty_Pthreads set the field own_data = SUNFALSE. N_VDestroy_Pthreads and N_VDestroyVectorArray_Pthreads will not attempt to free the pointer data for any N_Vector with own_data set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.





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

6.6.3 NVECTOR_PTHREADS Fortran interfaces

The NVECTOR_PTHREADS module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The nvector_pthreads_mod FORTRAN module defines interfaces to most 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 Appendix A.

FORTRAN 77 interface functions

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

6.7 The NVECTOR_PARHYP implementation

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

```
struct _N_VectorContent_ParHyp {
   sunindextype local_length;
   sunindextype global_length;
   booleantype own_parvector;
   MPI_Comm comm;
   HYPRE_ParVector x;
};
```

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

Unlike native SUNDIALS vector types, NVECTOR_PARHYP does not provide macros to access its member variables. Note that NVECTOR_PARHYP requires SUNDIALS to be built with MPI support.

6.7.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 program for CVODE [21] and the ark_diurnal_kry_ph.c example program for ARKODE [29].

The names of parhyp methods are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix Parhyp (e.g. N_VDestroy_Parhyp). The module NVECTOR_PARHYP provides the following additional user-callable routines:

N_{V} NewEmpty_ParHyp

Prototype N_Vector N_VNewEmpty_ParHyp(MPI_Comm comm, sunindextype local_length, sunindextype global_length)

Description This function creates a new parhyp N_Vector with the pointer to the hypre vector set to NULL.

N_VMake_ParHyp

Prototype N_Vector N_VMake_ParHyp(HYPRE_ParVector x)

Description This function creates an N_Vector wrapper around an existing hypre parallel vector. It does not allocate memory for x itself.

N_VGetVector_ParHyp

Prototype HYPRE_ParVector N_VGetVector_ParHyp(N_Vector v)

Description This function returns the underlying hypre vector.

N_VCloneVectorArray_ParHyp

Prototype N_Vector *N_VCloneVectorArray_ParHyp(int count, N_Vector w)

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

N_VCloneVectorArrayEmpty_ParHyp

Prototype N_Vector *N_VCloneVectorArrayEmpty_ParHyp(int count, N_Vector w)

Description This function creates (by cloning) an array of count parallel vectors, each with an empty

(NULL) data array.

N_VDestroyVectorArray_ParHyp

Prototype void N_VDestroyVectorArray_ParHyp(N_Vector *vs, int count)

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

N_VPrint_ParHyp

Prototype void N_VPrint_ParHyp(N_Vector v)

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

N_VPrintFile_ParHyp

Prototype void N_VPrintFile_ParHyp(N_Vector v, FILE *outfile)

Description 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.

N_VEnableFusedOps_ParHyp

Prototype int N_VEnableFusedOps_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearCombination_ParHyp

Prototype int N_VEnableLinearCombination_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleAddMulti_ParHyp

Prototype int N_VEnableScaleAddMulti_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableDotProdMulti_ParHyp

Prototype int N_VEnableDotProdMulti_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearSumVectorArray_ParHyp

Prototype int N_VEnableLinearSumVectorArray_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleVectorArray_ParHyp

Prototype int N_VEnableScaleVectorArray_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableConstVectorArray_ParHyp

Prototype int N_VEnableConstVectorArray_ParHyp(N_Vector v, booleantype tf)

Description 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.

N_VEnableWrmsNormVectorArray_ParHyp

Prototype int N_VEnableWrmsNormVectorArray_ParHyp(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the WRMS norm operation for

vector arrays in the parhyp vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ if the input

vector or its ops structure are NULL.

 ${\tt N_VEnableWrmsNormMaskVectorArray_ParHyp}$

Prototype int N_VEnableWrmsNormMaskVectorArray_ParHyp(N_Vector v, booleantype tf)

 $\begin{tabular}{ll} Description & This function enables ({\tt SUNTRUE}) or disables ({\tt SUNFALSE}) the masked WRMS norm op-$

eration for vector arrays in the parhyp vector. The return value is $\boldsymbol{0}$ for success and $-\boldsymbol{1}$

if the input vector or its ops structure are NULL.

| N_VEnableScaleAddMultiVectorArray_ParHyp

Prototype int N_VEnableScaleAddMultiVectorArray_ParHyp(N_Vector v,

booleantype tf)

Description 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.

 ${\tt N_VEnableLinearCombinationVectorArray_ParHyp}$

Prototype int N_VEnableLinearCombinationVectorArray_ParHyp(N_Vector v,

booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation

for vector arrays in the parhyp vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ 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. 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.

6.8 The NVECTOR_PETSC implementation

The NVECTOR_PETSC module is an NVECTOR wrapper around the PETSc vector. It defines the *content* field of a N_Vector to be a structure containing the global and local lengths of the vector, a pointer to the PETSc vector, an MPI communicator, and a boolean flag *own_data* indicating ownership of the wrapped PETSc vector.

```
struct _N_VectorContent_Petsc {
   sunindextype local_length;
   sunindextype global_length;
   booleantype own_data;
   Vec *pvec;
   MPI_Comm comm;
};
```

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

Unlike native SUNDIALS vector types, NVECTOR_PETSC does not provide macros to access its member variables. Note that NVECTOR_PETSC requires SUNDIALS to be built with MPI support.

6.8.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with SUNDIALS Fortran interfaces. When access to raw vector data is needed, it is recommended to extract the PETSc vector first, and then use PETSc methods to access the data. Usage examples of NVECTOR_PETSC are provided in example programs for IDA [20].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix _Petsc (e.g. N_VDestroy_Petsc). The module NVECTOR_PETSC provides the following additional user-callable routines:

$|N_{V}=0$

Prototype N_Vector N_VNewEmpty_Petsc(MPI_Comm comm, sunindextype local_length, sunindextype global_length)

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped PETSc vector set to (NULL). It is used by the N_VMake_Petsc and N_VClone_Petsc implementations.

N_VMake_Petsc

Prototype N_Vector N_VMake_Petsc(Vec *pvec)

Description This function creates and allocates memory for an NVECTOR_PETSC wrapper around a user-provided PETSc vector. It does *not* allocate memory for the vector **pvec** itself.

N_VGetVector_Petsc

Prototype Vec *N_VGetVector_Petsc(N_Vector v)

Description This function returns a pointer to the underlying PETSc vector.

N_VCloneVectorArray_Petsc

Prototype N_Vector *N_VCloneVectorArray_Petsc(int count, N_Vector w)

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

N_VCloneVectorArrayEmpty_Petsc

Prototype N_Vector *N_VCloneVectorArrayEmpty_Petsc(int count, N_Vector w)

Description This function creates (by cloning) an array of count NVECTOR_PETSC vectors, each with

pointers to Petsc vectors set to (NULL).

N_VDestroyVectorArray_Petsc

Prototype void N_VDestroyVectorArray_Petsc(N_Vector *vs, int count)

Description This function frees memory allocated for the array of count variables of type N_Vector

created with N_VCloneVectorArray_Petsc or with N_VCloneVectorArrayEmpty_Petsc.

N_VPrint_Petsc

Prototype void N_VPrint_Petsc(N_Vector v)

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

N_VPrintFile_Petsc

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

Description 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.

N_VEnableFusedOps_Petsc

Prototype int N_VEnableFusedOps_Petsc(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array oper-

ations in the PETSc vector. The return value is 0 for success and -1 if the input vector

or its ops structure are NULL.

N_VEnableLinearCombination_Petsc

Prototype int N_VEnableLinearCombination_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleAddMulti_Petsc

Prototype int N_VEnableScaleAddMulti_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableDotProdMulti_Petsc

Prototype int N_VEnableDotProdMulti_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearSumVectorArray_Petsc

Prototype int N_VEnableLinearSumVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleVectorArray_Petsc

Prototype int N_VEnableScaleVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableConstVectorArray_Petsc

Prototype int N_VEnableConstVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableWrmsNormVectorArray_Petsc

Prototype int N_VEnableWrmsNormVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableWrmsNormMaskVectorArray_Petsc

Prototype int N_VEnableWrmsNormMaskVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleAddMultiVectorArray_Petsc

Prototype int N_VEnableScaleAddMultiVectorArray_Petsc(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearCombinationVectorArray_Petsc

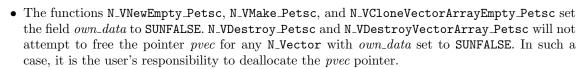
Prototype int N_VEnableLinearCombinationVectorArray_Petsc(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation for vector arrays in the PETSc vector. The return value is 0 for success and -1 if the

input vector or its ops structure are NULL.

Notes

• When there is a need to access components of an N_Vector_Petsc, v, it is recommeded to extract the PETSc vector via x_vec = N_VGetVector_Petsc(v) and then access components using appropriate PETSc functions.



• 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.

6.9 The NVECTOR_CUDA implementation

The NVECTOR_CUDA module is an experimental NVECTOR implementation in the CUDA language. The module allows for SUNDIALS vector kernels to run on GPU devices. It is intended for users who are already familiar with CUDA and GPU programming. Building this vector module requires a CUDA compiler and, by extension, a C++ compiler. The class Vector in the namespace suncudavec manages the vector data layout:

```
template <class T, class I>
class Vector {
    I size_;
    I mem_size_;
    T* h_vec_;
    T* d_vec_;
    ThreadPartitioning<T, I>* partStream_;
    ThreadPartitioning<T, I>* partReduce_;
    bool ownPartitioning_;
    bool ownData_;
    bool managed_mem_;
    ...
};
```

The class members are vector size (length), size of the vector data memory block, pointers to vector data on the host and the device, pointers to ThreadPartitioning implementations that handle thread





partitioning for streaming and reduction vector kernels, a boolean flag that signals if the vector owns the thread partitioning, a boolean flag that signals if the vector owns the data, and a boolean flag that signals if managed memory is used for the data arrays. The class Vector inherits from the empty structure

```
struct _N_VectorContent_Cuda {};
```

to interface the C++ class with the NVECTOR C code. Due to the rapid progress of CUDA development, we expect that the suncudavec::Vector class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the suncudavec::Vector class without requiring changes to the user API.

When instantiated with N_VNew_Cuda, the class Vector will allocate memory 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. Details on each of these constructors are provided below.

To use the NVECTOR_CUDA module, the header file to include is nvector_cuda.h, and the library to link to is libsundials_nveccuda.lib. The extension .lib is typically .so for shared libraries and .a for static libraries.

6.9.1 NVECTOR_CUDA functions

Unlike other native SUNDIALS vector types, NVECTOR_CUDA does not provide macros to access its member variables. Instead, user should use the accessor functions:

N_VGetHostArrayPointer_Cuda

Prototype realtype *N_VGetHostArrayPointer_Cuda(N_Vector v)

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

N_VGetDeviceArrayPointer_Cuda

Prototype realtype *N_VGetDeviceArrayPointer_Cuda(N_Vector v)

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

$N_VIsManagedMemory_Cuda$

Prototype booleantype *N_VIsManagedMemory_Cuda(N_Vector v)

Description This function returns a boolean flag indicating if the vector data is allocated in managed memory or not.

The NVECTOR_CUDA module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3 and 6.1.4, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. Instead, the NVECTOR_CUDA module provides separate functions to access data on the host and on the device. It also provides methods for copying from the host to the device and vice versa. Usage examples of NVECTOR_CUDA are provided in some example programs for CVODE [21].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix _Cuda (e.g. N_VDestroy_Cuda). The module NVECTOR_CUDA provides the following functions:

N_VNew_Cuda

Prototype N_Vector N_VNew_Cuda(sunindextype length)

Description This function creates and allocates memory for a CUDA N_Vector. The vector data array is allocated on both the host and device.

N_VNewManaged_Cuda

Prototype N_Vector N_VNewManaged_Cuda(sunindextype length)

Description This function creates and allocates memory for a CUDA N_Vector. The vector data array

is allocated in managed memory.

N_VNewEmpty_Cuda

Prototype N_Vector N_VNewEmpty_Cuda()

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped CUDA

vector set to NULL. It is used by the N_VNew_Cuda, N_VMake_Cuda, and N_VClone_Cuda

implementations.

N_VMake_Cuda

Prototype N_Vector N_VMake_Cuda(sunindextype length, realtype *h_data, realtype *dev_data)

Description This function creates an NVECTOR_CUDA with user-supplied vector data arrays h_vdata

and d_vdata. This function does not allocate memory for data itself.

N_VMakeManaged_Cuda

Prototype N_Vector N_VMakeManaged_Cuda(sunindextype length, realtype *vdata)

Description This function creates an NVECTOR_CUDA with a user-supplied managed memory data

array. This function does not allocate memory for data itself.

The module NVECTOR_CUDA also provides the following user-callable routines:

N_VSetCudaStream_Cuda

Prototype void N_VSetCudaStream_Cuda(N_Vector v, cudaStream_t *stream)

Description This function sets the CUDA stream that all vector kernels will be launched on. By

default an NVECTOR_CUDA uses the default CUDA stream.

Note: All vectors used in a single instance of a SUNDIALS solver must use the same CUDA stream, and the CUDA stream must be set prior to solver initialization. Additionally, if manually instantiating the stream and reduce ThreadPartitioning of a suncudavec::Vector, ensure that they use the same CUDA stream.

N_VCopyToDevice_Cuda

Prototype void N_VCopyToDevice_Cuda(N_Vector v)

Description This function copies host vector data to the device.

${\tt N_VCopyFromDevice_Cuda}$

Prototype void N_VCopyFromDevice_Cuda(N_Vector v)

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

N_VPrint_Cuda

Prototype void N_VPrint_Cuda(N_Vector v)

Description This function prints the content of a CUDA vector to stdout.

N_VPrintFile_Cuda

Prototype void N_VPrintFile_Cuda(N_Vector v, FILE *outfile)

Description 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.

N_VEnableFusedOps_Cuda

Prototype int N_VEnableFusedOps_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearCombination_Cuda

Prototype int N_VEnableLinearCombination_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleAddMulti_Cuda

Prototype int N_VEnableScaleAddMulti_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableDotProdMulti_Cuda

Prototype int N_VEnableDotProdMulti_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableLinearSumVectorArray_Cuda

Prototype int N_VEnableLinearSumVectorArray_Cuda(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear sum operation for

vector arrays in the CUDA vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ if the input

vector or its ops structure are NULL.

N_VEnableScaleVectorArray_Cuda

Prototype int N_VEnableScaleVectorArray_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableConstVectorArray_Cuda

Prototype int N_VEnableConstVectorArray_Cuda(N_Vector v, booleantype tf)

Description 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.

N_VEnableWrmsNormVectorArray_Cuda

Prototype int N_VEnableWrmsNormVectorArray_Cuda(N_Vector v, booleantype tf)

Description 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.

${\tt N_VEnableWrmsNormMaskVectorArray_Cuda}$

Prototype int N_VEnableWrmsNormMaskVectorArray_Cuda(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm op-

eration for vector arrays in the CUDA vector. The return value is $\bf 0$ for success and $\bf -1$ if

the input vector or its ops structure are NULL.

N_VEnableScaleAddMultiVectorArray_Cuda

Prototype int N_VEnableScaleAddMultiVectorArray_Cuda(N_Vector v, booleantype tf)

 $\label{thm:continuous} Description \quad This function \ enables \ ({\tt SUNTRUE}) \ or \ disables \ ({\tt SUNFALSE}) \ the \ scale \ and \ add \ a \ vector \ array$

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.

N_VEnableLinearCombinationVectorArray_Cuda

Prototype int N_VEnableLinearCombinationVectorArray_Cuda(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation

for vector arrays in the CUDA vector. The return value is 0 for success and -1 if the

input vector or its ops structure are NULL.

Notes

- When there is a need to access components of an N_Vector_Cuda, v, it is recommeded to use functions N_VGetDeviceArrayPointer_Cuda or N_VGetHostArrayPointer_Cuda.
- 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 The NVECTOR_RAJA implementation

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 GPU devices. The module is intended for users who are already familiar with RAJA and GPU programming. Building this vector module requires a C++11 compliant compiler and a CUDA software development toolkit. Besides the CUDA backend, RAJA has other backends such as serial, OpenMP, and OpenACC.



These backends are not used in this SUNDIALS release. Class Vector in namespace sunrajavec manages the vector data layout:

```
template <class T, class I>
class Vector {
    I size_;
    I mem_size_;
    T* h_vec_;
    T* d_vec_;
    ...
};
```

The class members are: vector size (length), size of the vector data memory block, the global vector size (length), a pointer to the vector data on the host, and a pointer to the vector data on the device. The class **Vector** inherits from an empty structure

```
struct _N_VectorContent_Raja { };
```

to interface the C++ class with the NVECTOR C code. When instantiated, the class Vector will allocate memory on both the host and the device. Due to the rapid progress of RAJA development, we expect that the sunrajavec::Vector class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the sunrajavec::Vector class without requiring changes to the user API.

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

6.10.1 NVECTOR_RAJA functions

Unlike other native SUNDIALS vector types, NVECTOR_RAJA does not provide macros to access its member variables. Instead, user should use the accessor functions:

```
N_VGetHostArrayPointer_Raja
```

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

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

```
N_VGetDeviceArrayPointer_Raja
```

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

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

The NVECTOR_RAJA module defines the implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, except for N_VDotProdMulti, N_VWrmsNormVectorArray, and

N_VWrmsNormMaskVectorArray as support for arrays of reduction vectors is not yet supported in RAJA. These function will be added to the NVECTOR_RAJA implementation in the future. Additionally the vector operations N_VGetArrayPointer and N_VSetArrayPointer are not implemented by the RAJA vector. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. The NVECTOR_RAJA module provides separate functions to access data on the host and on the device. It also provides methods for copying data from the host to the device and vice versa. Usage examples of NVECTOR_RAJA are provided in some example programs for CVODE [21].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix _Raja (e.g. N_VDestroy_Raja). The module NVECTOR_RAJA provides the following additional user-callable routines:

N_VNew_Raja

Prototype N_Vector N_VNew_Raja(sunindextype length)

Description This function creates and allocates memory for a CUDA N_Vector. The vector data array

is allocated on both the host and device.

|N_VNewEmpty_Raja

Prototype N_Vector N_VNewEmpty_Raja()

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped RAJA

vector set to NULL. It is used by the N_VNew_Raja, N_VMake_Raja, and N_VClone_Raja

implementations.

N_VMake_Raja

Prototype N_Vector N_VMake_Raja(N_VectorContent_Raja c)

Description This function creates and allocates memory for an NVECTOR_RAJA wrapper around a

user-provided sunrajavec::Vector class. Its only argument is of type

N_VectorContent_Raja, which is the pointer to the class.

$N_VCopyToDevice_Raja$

Prototype realtype *N_VCopyToDevice_Raja(N_Vector v)

Description This function copies host vector data to the device.

N_VCopyFromDevice_Raja

Prototype realtype *N_VCopyFromDevice_Raja(N_Vector v)

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

N_VPrint_Raja

Prototype void N_VPrint_Raja(N_Vector v)

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

N_VPrintFile_Raja

Prototype void N_VPrintFile_Raja(N_Vector v, FILE *outfile)

Description 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.

N_VEnableFusedOps_Raja

Prototype int N_VEnableFusedOps_Raja(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array op-

erations in the RAJA vector. The return value is 0 for success and -1 if the input vector

or its ops structure are NULL.

N_VEnableLinearCombination_Raja

Prototype int N_VEnableLinearCombination_Raja(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination fused

operation in the RAJA vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ if the input

vector or its ops structure are NULL.

N_VEnableScaleAddMulti_Raja

Prototype int N_VEnableScaleAddMulti_Raja(N_Vector v, booleantype tf)

Description 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 ${\tt 0}$ for success

and -1 if the input vector or its ops structure are NULL.

N_VEnableLinearSumVectorArray_Raja

Prototype int N_VEnableLinearSumVectorArray_Raja(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleVectorArray_Raja

Prototype int N_VEnableScaleVectorArray_Raja(N_Vector v, booleantype tf)

Description 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.

N_VEnableConstVectorArray_Raja

Prototype int N_VEnableConstVectorArray_Raja(N_Vector v, booleantype tf)

Description 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.

${\tt N_VEnableScaleAddMultiVectorArray_Raja}$

Prototype int N_VEnableScaleAddMultiVectorArray_Raja(N_Vector v, booleantype tf)

Description 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.

```
N_VEnableLinearCombinationVectorArray_Raja
```

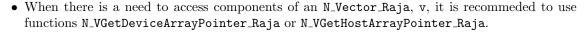
```
Prototype int N_VEnableLinearCombinationVectorArray_Raja(N_Vector v, booleantype tf)
```

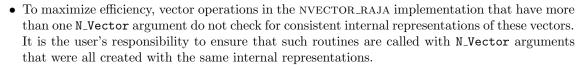
Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation

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





6.11 The NVECTOR_OPENMPDEV implementation

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.

6.11.1 NVECTOR_OPENMPDEV accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMPDEV vector.

NV_CONTENT_OMPDEV

This routine gives access to the contents of the NVECTOR_OPENMPDEV vector N_Vector.

The assignment v_cont = NV_CONTENT_OMPDEV(v) sets v_cont to be a pointer to the NVECTOR_OPENMPDEV N_Vector content structure.

Implementation:

```
#define NV_CONTENT_OMPDEV(v) ( (N_VectorContent_OpenMPDEV)(v->content) )
```

NV_OWN_DATA_OMPDEV, NV_DATA_HOST_OMPDEV, NV_DATA_DEV_OMPDEV, NV_LENGTH_OMPDEV

These macros give individual access to the parts of the content of an $NVECTOR_OPENMPDEV$ N_Vector .

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. 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.



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 .

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 .

Implementation:

```
#define NV_OWN_DATA_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->own_data )
#define NV_DATA_HOST_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->host_data )
#define NV_DATA_DEV_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->dev_data )
#define NV_LENGTH_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->length )
```

6.11.2 NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor 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 vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix <code>_OpenMPDEV</code> (e.g. <code>N_VDestroy_OpenMPDEV</code>). The module <code>NVECTOR_OPENMPDEV</code> provides the following additional user-callable routines:

N_VNew_OpenMPDEV

Prototype N_Vector N_VNew_OpenMPDEV(sunindextype vec_length)

Description This function creates and allocates memory for an NVECTOR_OPENMPDEV N_Vector.

N_VNewEmpty_OpenMPDEV

Prototype N_Vector N_VNewEmpty_OpenMPDEV(sunindextype vec_length)

Description This function creates a new NVECTOR_OPENMPDEV N_Vector with an empty (NULL) host and device data arrays.

N_VMake_OpenMPDEV

Prototype N_Vector N_VMake_OpenMPDEV(sunindextype vec_length, realtype *h_vdata, realtype *d_vdata)

Description 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.

N_VCloneVectorArray_OpenMPDEV

Prototype N_Vector *N_VCloneVectorArray_OpenMPDEV(int count, N_Vector w)

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

N_VCloneVectorArrayEmpty_OpenMPDEV

Prototype N_Vector *N_VCloneVectorArrayEmpty_OpenMPDEV(int count, N_Vector w)

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

N_VDestroyVectorArray_OpenMPDEV

Prototype void N_VDestroyVectorArray_OpenMPDEV(N_Vector *vs, int count)

Description This function frees memory allocated for the array of count variables of type N_Vector

created with N_VCloneVectorArray_OpenMPDEV or with

N_VCloneVectorArrayEmpty_OpenMPDEV.

N_VGetHostArrayPointer_OpenMPDEV

Prototype realtype *N_VGetHostArrayPointer_OpenMPDEV(N_Vector v)

Description This function returns a pointer to the host data array.

| N_VGetDeviceArrayPointer_OpenMPDEV

Prototype realtype *N_VGetDeviceArrayPointer_OpenMPDEV(N_Vector v)

Description This function returns a pointer to the device data array.

N_VPrint_OpenMPDEV

Prototype void N_VPrint_OpenMPDEV(N_Vector v)

Description This function prints the content of an NVECTOR_OPENMPDEV vector to stdout.

N_VPrintFile_OpenMPDEV

Prototype void N_VPrintFile_OpenMPDEV(N_Vector v, FILE *outfile)

Description This function prints the content of an NVECTOR_OPENMPDEV vector to outfile.

N_VCopyToDevice_OpenMPDEV

Prototype void N_VCopyToDevice_OpenMPDEV(N_Vector v)

Description This function copies the content of an NVECTOR_OPENMPDEV vector's host data array

to the device data array.

| N_VCopyFromDevice_OpenMPDEV

Prototype void N_VCopyFromDevice_OpenMPDEV(N_Vector v)

Description 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.

N_VEnableFusedOps_OpenMPDEV

Prototype int N_VEnableFusedOps_OpenMPDEV(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array op-

erations in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1

if the input vector or its ops structure are NULL.

N_VEnableLinearCombination_OpenMPDEV

Prototype int N_VEnableLinearCombination_OpenMPDEV(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleAddMulti_OpenMPDEV

Prototype int N_VEnableScaleAddMulti_OpenMPDEV(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale and add a vector to

multiple vectors fused operation in the ${\tt NVECTOR_OPENMPDEV}$ vector. The return value

is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableDotProdMulti_OpenMPDEV

Prototype int N_VEnableDotProdMulti_OpenMPDEV(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the multiple dot products fused

operation in the ${\tt NVECTOR_OPENMPDEV}$ vector. The return value is 0 for success and

-1 if the input vector or its ops structure are NULL.

N_VEnableLinearSumVectorArray_OpenMPDEV

Prototype int N_VEnableLinearSumVectorArray_OpenMPDEV(N_Vector v, booleantype tf)

Description 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.

N_VEnableScaleVectorArray_OpenMPDEV

Prototype int N_VEnableScaleVectorArray_OpenMPDEV(N_Vector v, booleantype tf)

Description 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.

N_VEnableConstVectorArray_OpenMPDEV

Prototype int N_VEnableConstVectorArray_OpenMPDEV(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the const operation for vector

arrays in the ${\tt NVECTOR_OPENMPDEV}$ vector. The return value is 0 for success and -1 if

the input vector or its ops structure are NULL.

N_VEnableWrmsNormVectorArray_OpenMPDEV

Prototype int N_VEnableWrmsNormVectorArray_OpenMPDEV(N_Vector v, booleantype tf)

Description 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.

N_VEnableWrmsNormMaskVectorArray_OpenMPDEV

Prototype int N_VEnableWrmsNormMaskVectorArray_OpenMPDEV(N_Vector v,

booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm op-

eration for vector arrays in the ${\tt NVECTOR_OPENMPDEV}$ vector. The return value is 0 for

success and -1 if the input vector or its ops structure are NULL.

N_VEnableScaleAddMultiVectorArray_OpenMPDEV

Prototype int N_VEnableScaleAddMultiVectorArray_OpenMPDEV(N_Vector v,

booleantype tf)

Description 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.

N_VEnableLinearCombinationVectorArray_OpenMPDEV

 $\label{linearCombinationVectorArray_OpenMPDEV(N_Vector \ v, \ \ \ \ \)} Prototype \qquad \text{int N_VEnableLinearCombinationVectorArray_OpenMPDEV(N_Vector v, \ \ \ \ \ \)}$

booleantype tf)

Description 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 = NV_DATA_HOST_OMPDEV(v) for the host array or d_data = NV_DATA_DEV_OMPDEV(v) for the device array and then access h_data[i] or d_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
- to date.

 N VNewEmpty OpenMPDEV N VMake OpenMPDEV and N VCloneVectorArrayEmpty OpenMPDEV set
- N_VNewEmpty_OpenMPDEV, N_VMake_OpenMPDEV, and N_VCloneVectorArrayEmpty_OpenMPDEV set the field own_data = SUNFALSE. 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 pointer.
- 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 internal representations.

6.12 The NVECTOR_TRILINOS implementation

The NVECTOR_TRILINOS module is an NVECTOR wrapper around the Trilinos Tpetra vector. The interface to Tpetra is implemented in the Sundials::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::TpetraVectorInterface class is defined as:

```
typedef Tpetra::Vector<realtype, sunindextype, sunindextype> vector_type;
```

The Tpetra vector will use the SUNDIALS-specified realtype as its scalar type, and it will use sunindextype as the global and the local ordinal types. This type definition will use Tpetra's default node type. Available Kokkos node types in 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.

6.12.1 NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.4, and 6.1.4, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor 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 [20].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.4, and 6.1.4 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::TpetraVector, located in the file SundialsTpetraVectorKernels.hpp. The module NVECTOR_TRILINOS provides the following additional user-callable functions:

• N_VGetVector_Trilinos

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.

```
Teuchos::RCP<vector_type> N_VGetVector_Trilinos(N_Vector v);
```

N_VMake_Trilinos

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.

```
N_Vector N_VMake_Trilinos(Teuchos::RCP<vector_type> v);
```

Notes

- The template parameter vector_type should be set as:
 typedef Sundials::TpetraVectorInterface::vector_type vector_type
 This will ensure that data types used in Tpetra vector match those in SUNDIALS.
- When there is a need to access components of an N_Vector_Trilinos, v, it is recommeded to extract the Trilinos vector object via x_vec = N_VGetVector_Trilinos(v) and then access components using the appropriate Trilinos functions.
- The functions N_VDestroy_Trilinos and N_VDestroyVectorArray_Trilinos only delete the N_Vector wrapper. The underlying Tpetra vector object will exist for as long as there is at least one reference to it.

6.13 The NVECTOR_MANYVECTOR implementation

The NVECTOR_MANYVECTOR implementation of the NVECTOR module provided with SUNDIALS is designed to facilitate problems with an inherent data partitioning for the solution vector within a computational node. 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. We envision two generic use cases for this implementation:

- A. Heterogeneous computational architectures: for users who wish to partition data on a node between different computing resources, they may create architecture-specific subvectors for each partition. For example, a user could create one serial component based on NVECTOR_SERIAL, another component for GPU accelerators based on NVECTOR_CUDA, and another threaded component based on NVECTOR_OPENMP.
- B. Structure of arrays (SOA) data layouts: for users who wish to create separate subvectors for each solution component, e.g., in a Navier-Stokes simulation they could have separate subvectors for density, velocities and pressure, which are combined together into a single NVECTOR_MANYVECTOR for the overall "solution".

We note that the above use cases are not 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 required set of operations. Additionally, NVECTOR_MANYVECTOR sets no limit on the number of subvectors that may be attached (aside from the limitations of using sunindextype for indexing, and standard per-node memory limitations). However, while this ostensibly supports subvectors with one entry each (i.e., one subvector for each solution entry), we anticipate that this extreme situation will hinder performance due to non-stride-one memory accesses and increased function call overhead. We therefore recommend a relatively coarse partitioning of the problem, although actual performance will likely be problem-dependent.

As a final note, in the coming years we plan to introduce additional algebraic solvers and time integration modules that will leverage the problem partitioning enabled by NVECTOR_MANYVECTOR. However, even at present we anticipate that users will be able to leverage such data partitioning in their problem-defining ODE right-hand side, DAE residual, or nonlinear solver residual functions.

6.13.1 NVECTOR_MANYVECTOR structure

The NVECTOR_MANYVECTOR implementation defines the *content* field of N_Vector to be a structure containing the number of subvectors comprising the ManyVector, the global length of the ManyVector (including all subvectors), a pointer to the beginning of the array of subvectors, and a boolean flag own_data indicating ownership of the subvectors that populate subvec_array.

```
struct _N_VectorContent_ManyVector {
  sunindextype num_subvectors; /* number of vectors attached */
  sunindextype global_length; /* overall manyvector length */
  N_Vector* subvec_array; /* pointer to N_Vector array */
  booleantype own_data; /* flag indicating data ownership */
};
```

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

6.13.2 NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, except for N_VGetArrayPointer, N_VSetArrayPointer, N_VScaleAddMultiVectorArray,

and N_VLinearCombinationVectorArray. As such, this vector cannot be used with the SUNDIALS Fortran-77 interfaces, nor 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 Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix _ManyVector (e.g. N_VDestroy_ManyVector). The module NVECTOR_MANYVECTOR provides the following additional user-callable routines:

N_VNew_ManyVector

Prototype N_Vector N_VNew_ManyVector(sunindextype num_subvectors, N_Vector *vec_array);

Description 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).

$N_VGetSubvector_ManyVector$

Prototype N_Vector N_VGetSubvector_ManyVector(N_Vector v, sunindextype vec_num);

Description This function returns the vec_num subvector from the NVECTOR array.

N_VGetSubvectorArrayPointer_ManyVector

Prototype realtype *N_VGetSubvectorArrayPointer_ManyVector(N_Vector v, sunindextype vec_num);

Description This function returns the data array pointer for the vec_num subvector from the NVEC-TOR array.

If the input vec_num is invalid, or if the subvector does not support the N_VGetArrayPointer operation, then NULL is returned.

${\tt N_VSetSubvectorArrayPointer_ManyVector}$

Prototype int N_VSetSubvectorArrayPointer_ManyVector(realtype *v_data, N_Vector v, sunindextype vec_num);

Description This function sets the data array pointer for the vec_num subvector from the NVECTOR

If the input vec_num is invalid, or if the subvector does not support the N_VSetArrayPointer operation, then this routine returns -1; otherwise it returns 0.

$N_VGetNumSubvectors_ManyVector$

Prototype sunindextype N_VGetNumSubvectors_ManyVector(N_Vector v);

Description 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 or N_VMake_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 and N_VMake_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 or N_VMake_ManyVector.

N_VEnableFusedOps_ManyVector

Prototype int N_VEnableFusedOps_ManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array operations in the ManyVector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableLinearCombination_ManyVector

Prototype int N_VEnableLinearCombination_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableScaleAddMulti_ManyVector

Prototype int N_VEnableScaleAddMulti_ManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale and add a vector to multiple vectors fused operation in the ManyVector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

${\tt N_VEnableDotProdMulti_ManyVector}$

Prototype int N_VEnableDotProdMulti_ManyVector(N_Vector v, booleantype tf);

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

${\tt N_VEnableLinearSumVectorArray_ManyVector}$

Prototype int N_VEnableLinearSumVectorArray_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableScaleVectorArray_ManyVector

Prototype int N_VEnableScaleVectorArray_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableConstVectorArray_ManyVector

Prototype int N_VEnableConstVectorArray_ManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the const operation for vector arrays in the ManyVector. The return value is 0 for success and -1 if the input vector

or its ops structure are NULL.

N_VEnableWrmsNormVectorArray_ManyVector

Prototype int N_VEnableWrmsNormVectorArray_ManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the WRMS norm operation for vector arrays in the ManyVector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

N_VEnableWrmsNormMaskVectorArray_ManyVector

Prototype int N_VEnableWrmsNormMaskVectorArray_ManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm op-

eration for vector arrays in the ManyVector. 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.

6.14 The NVECTOR_MPIMANYVECTOR implementation

The NVECTOR_MPIMANYVECTOR implementation of the NVECTOR module provided with SUNDIALS is designed to facilitate problems with an inherent data partitioning for the solution vector, and when using distributed-memory parallel architectures. As such, the MPIManyVector implementation supports all use cases allowed by the MPI-unaware ManyVector implementation, as well as partitioning data between nodes in a parallel environment. These data partitions are entirely user-defined, through construction of distinct NVECTOR modules for each component, that are then combined together to form the NVECTOR_MPIMANYVECTOR. We envision three generic use cases for this implementation:

- A. Heterogeneous computational architectures (single-node or multi-node): for users who wish to partition data on a node between different computing resources, they may create architecture-specific subvectors for each partition. For example, a user could create one MPI-parallel component based on NVECTOR_PARALLEL, another single-node component for GPU accelerators based on NVECTOR_CUDA, and another threaded single-node component based on NVECTOR_OPENMP.
- B. Process-based multiphysics decompositions (multi-node): for users who wish to combine separate simulations together, e.g., where one subvector resides on one subset of MPI processes, while another subvector resides on a different subset of MPI processes, and where the user has created a MPI intercommunicator to connect these distinct process sets together.





C. Structure of arrays (SOA) data layouts (single-node or multi-node): for users who wish to create separate subvectors for each solution component, e.g., in a Navier-Stokes simulation they could have separate subvectors for density, velocities and pressure, which are combined together into a single NVECTOR_MPIMANYVECTOR for the overall "solution".

We note that the above use cases are not mutually exclusive, and the NVECTOR_MPIMANYVECTOR implementation should support arbitrary combinations of these cases.

The NVECTOR_MPIMANYVECTOR implementation is designed to work with any NVECTOR subvectors that implement the minimum required set of operations, however significant performance benefits may be obtained when subvectors additionally implement the optional local reduction operations listed in Table 6.1.4.

Additionally, NVECTOR_MPIMANYVECTOR sets no limit on the number of subvectors that may be attached (aside from the limitations of using sunindextype for indexing, and standard per-node memory limitations). However, while this ostensibly supports subvectors with one entry each (i.e., one subvector for each solution entry), we anticipate that this extreme situation will hinder performance due to non-stride-one memory accesses and increased function call overhead. We therefore recommend a relatively coarse partitioning of the problem, although actual performance will likely be problem-dependent.

As a final note, in the coming years we plan to introduce additional algebraic solvers and time integration modules that will leverage the problem partitioning enabled by NVECTOR_MPIMANYVECTOR. However, even at present we anticipate that users will be able to leverage such data partitioning in their problem-defining ODE right-hand side, DAE residual, or nonlinear solver residual functions.

6.14.1 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 tasks), 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
                                                                      */
                                 /* number of vectors attached
  sunindextype
                num_subvectors;
  sunindextype
                                  /* overall mpimanyvector length
                global_length;
                                  /* pointer to N_Vector array
  N_Vector*
                subvec_array;
  booleantype
                own_data;
                                  /* flag indicating data ownership
};
```

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

Note: If SUNDIALS is configured with MPI disabled, then the MPIManyVector library will not be built. Furthermore, any user codes that include nvector_mpimanyvector.h *must* be compiled using an MPI-aware compiler (whether the specific user code utilizes MPI or not). We note that the NVECTOR_MANYVECTOR implementation is designed for ManyVector use cases in an MPI-unaware environment.

6.14.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, except for N_VGetArrayPointer, N_VSetArrayPointer, N_VScaleAddMultiVectorArray, and N_VLinearCombinationVectorArray. As such, this vector cannot be used with the SUNDIALS Fortran-77 interfaces, nor 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 Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix _MPIManyVector (e.g. N_VDestroy_MPIManyVector). The module NVECTOR_MPIMANYVECTOR provides the following additional user-callable routines:

$N_VNew_MPIManyVector$

Prototype N_Vector N_VNew_MPIManyVector(sunindextype num_subvectors, N_Vector *vec_array);

Description

This function creates an 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).

$N_VMake_MPIManyVector$

Description

This function creates an 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 the memory reference to this user-created MPI communicator. We note that since many MPI implementations <code>#define MPI_COMM_WORLD</code> to be a specific integer <code>value</code> (that has no memory reference), users who wish to supply <code>MPI_COMM_WORLD</code> to this routine should first set a specific <code>MPI_Comm</code> variable to <code>MPI_COMM_WORLD</code> before passing in the reference, e.g.

```
MPI_Comm comm;
comm = MPI_COMM_WORLD;
N_Vector x;
x = N_VMake_MPIManyVector(&comm, ...);
```

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 NULL, although in this case, it would be simpler to call N_VNew_MPIManyVector instead.

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_VGetSubvector_MPIManyVector

Prototype N_Vector N_VGetSubvector_MPIManyVector(N_Vector v, sunindextype vec_num);

Description This function returns the vec_num subvector from the NVECTOR array.

N_VGetSubvectorArrayPointer_MPIManyVector

 $\label{eq:prototype} Prototype \quad \textit{realtype *N_VGetSubvectorArrayPointer_MPIManyVector(N_Vector v, sunindextype)} \\$

vec_num);

Description This function returns the data array pointer for the vec_num subvector from the NVEC-

TOR array.

If the input $\mathtt{vec_num}$ is invalid, or if the subvector does not support the $\mathtt{N_VGetArrayPointer}$

operation, then NULL is returned.

${\tt N_VSetSubvectorArrayPointer_MPIManyVector}$

Prototype int N_VSetSubvectorArrayPointer_MPIManyVector(realtype *v_data, N_Vector v,

sunindextype vec_num);

Description This function sets the data array pointer for the vec_num subvector from the NVECTOR

array.

 $If the input \verb|vec_num| is invalid|, or if the subvector does not support the \verb|N_VSetArrayPointer| is invalid|, or if the subvector does not support the \verb|N_VSetArrayPointer| is invalid|, or if the subvector does not support the \verb|N_VSetArrayPointer| is invalid|, or if the subvector does not support the \verb|N_VSetArrayPointer| is invalid|, or if the subvector does not support the Subvector does not$

operation, then this routine returns -1; otherwise it returns 0.

N_VGetNumSubvectors_MPIManyVector

Prototype sunindextype N_VGetNumSubvectors_MPIManyVector(N_Vector v);

Description 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.

N_VEnableFusedOps_MPIManyVector

Prototype int N_VEnableFusedOps_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) all fused and vector array operations in the MPIManyVector. The return value is 0 for success and -1 if the input

erations in the MPIManyVector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

N_VEnableLinearCombination_MPIManyVector

Prototype int N_VEnableLinearCombination_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination fused operation in the MPIManyVector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

N_VEnableScaleAddMulti_MPIManyVector

Prototype int N_VEnableScaleAddMulti_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale and add a vector to multiple vectors fused operation in the MPIManyVector. The return value is 0 for

success and -1 if the input vector or its ops structure are NULL.

N_VEnableDotProdMulti_MPIManyVector

Prototype int N_VEnableDotProdMulti_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the multiple dot products fused

operation in the MPIMany Vector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

N_VEnableLinearSumVectorArray_MPIManyVector

Prototype int N_VEnableLinearSumVectorArray_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear sum operation for

vector arrays in the MPIMany Vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ if the

input vector or its ops structure are NULL.

N_VEnableScaleVectorArray_MPIManyVector

Prototype int N_VEnableScaleVectorArray_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale operation for vector

arrays in the MPIMany Vector. The return value is ${\tt 0}$ for success and ${\tt -1}$ if the input

vector or its ops structure are NULL.

N_VEnableConstVectorArray_MPIManyVector

Prototype int N_VEnableConstVectorArray_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the const operation for vector

arrays in the MPIMany Vector. The return value is 0 for success and -1 if the input

vector or its ops structure are NULL.

N_VEnableWrmsNormVectorArray_MPIManyVector

Prototype int N_VEnableWrmsNormVectorArray_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the WRMS norm operation for

vector arrays in the MPIMany Vector. The return value is 0 for success and -1 if the

input vector or its ops structure are NULL.

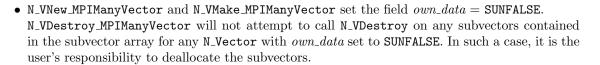
N_VEnableWrmsNormMaskVectorArray_MPIManyVector

Prototype int N_VEnableWrmsNormMaskVectorArray_MPIManyVector(N_Vector v, booleantype tf);

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm operation for vector arrays in the MPIManyVector. The return value is 0 for success and

-1 if the input vector or its ops structure are NULL.

Notes







• 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.

6.15 The NVECTOR_MPIPLUSX implementation

The NVECTOR_MPIPLUSX implementation of the NVECTOR module provided with SUNDIALS 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 required set of operations. 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.

6.15.1 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 Section 6.14.1.

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.

6.15.2 NVECTOR MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, from the NVECTOR_MPIMANYVECTOR (see section 6.14.2) except for N_VGetArrayPointer and N_VSetArrayPointer; the module provides its own implementation of these functions that call the local vector implementations. Therefore, the NVECTOR_MPIPLUSX module implements all of the operations listed in the referenced sections except for N_VScaleAddMultiVectorArray, and N_VLinearCombinationVectorArray Accordingly, it's compatibility with the SUNDIALS Fortran-77 interface, and 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_VMake_MPIPlusX

Prototype N_Vector N_VMake_MPIPlusX(MPI_Comm *comm,

N_Vector *local_vector);

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

The input comm should be the memory reference to this user-created MPI communicator. We note that since many MPI implementations #define MPI_COMM_WORLD to be a specific integer value (that has no memory reference), users who wish to supply MPI_COMM_WORLD

to this routine should first set a specific MPI_Comm variable to MPI_COMM_WORLD before passing in the reference, e.g.

```
MPI_Comm comm;
comm = MPI_COMM_WORLD;
N_Vector x;
x = N_VMake_MPIPlusX(&comm, ...);
```

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 N_Vector 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_VGetLocalVector_MPIPlusX

Prototype N_Vector N_VGetLocalVector_MPIPlusX(N_Vector v);

Description This function returns the local vector underneath the MPIPlusX NVECTOR.

N_VGetArrayPointer_MPIPlusX

Prototype realtype* N_VGetLocalVector_MPIPlusX(N_Vector v);

Description This function returns the data array pointer for the local vector if the local vector implements the N_VGetArrayPointer operation; otherwise it returns NULL.

N_VSetArrayPointer_MPIPlusX

Prototype void N_VSetArrayPointer_MPIPlusX(realtype *data, N_Vector v);

Description 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 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 local vector representations.

6.16 NVECTOR Examples

There are NVector examples that may be installed for the implementations provided with SUNDIALS. Each implementation makes use of the functions in test_nvector.c. These example functions show simple usage of the NVector family of functions. The input to the examples are the vector length, number of threads (if threaded implementation), and a print timing flag.

The following is a list of the example functions in test_nvector.c:

• Test_N_VClone: Creates clone of vector and checks validity of clone.





- Test_N_VCloneEmpty: Creates clone of empty vector and checks validity of clone.
- Test_N_VCloneVectorArray: Creates clone of vector array and checks validity of cloned array.
- Test_N_VCloneVectorArray: Creates clone of empty vector array and checks validity of cloned array.
- Test_N_VGetArrayPointer: Get array pointer.
- Test_N_VSetArrayPointer: Allocate new vector, set pointer to new vector array, and check values.
- Test_N_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_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
- ullet Test_N_VLinearCombination Case 1b: Test $z=a\ x$
- Test_N_VLinearCombination Case 2a: Test x = a x + b y
- ullet 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 2a: Y[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 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]
- ullet Test_N_VScaleVectorArray Case 1a: z=c
- Test_N_VScaleVectorArray Case 1b: Z[i] = c
- Test_N_VWrmsNormVectorArray Case 1a: Create a vector of know values, find and validate the
 weighted root mean square norm.
- Test_N_VWrmsNormVectorArray Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each.
- Test_N_VWrmsNormMaskVectorArray Case 1a: Create a vector of know values, find and validate the weighted root mean square norm using all elements except one.
- Test_N_VWrmsNormMaskVectorArray Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each using all elements except one.
- Test_N_VScaleAddMultiVectorArray Case 1a: y = a x + y
- Test_N_VScaleAddMultiVectorArray Case 1b: z = a x + y
- Test_N_VScaleAddMultiVectorArray Case 2a: Y[j][0] = a[j] X[0] + Y[j][0]
- Test_N_VScaleAddMultiVectorArray Case 2b: Z[j][0] = a[j] X[0] + Y[j][0]
- Test_N_VScaleAddMultiVectorArray Case 3a: Y[0][i] = a[0] X[i] + Y[0][i]
- Test_N_VScaleAddMultiVectorArray Case 3b: Z[0][i] = a[0] X[i] + Y[0][i]
- Test_N_VScaleAddMultiVectorArray Case 4b: Z[j][i] = a[j] X[i] + Y[j][i]
- ullet 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]
- $\bullet \ \, \mathsf{Test_N_VLinearCombinationVectorArray} \ \, \mathsf{Case} \ \, 6a: \ \, \mathsf{X}[0][i] = \mathsf{X}[0][i] + \mathsf{c}[1] \ \, \mathsf{X}[1][i] + \mathsf{c}[2] \ \, \mathsf{X}[2][i]$
- 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.

Chapter 7

Description of the SUNMatrix module

For problems that involve direct methods for solving linear systems, the SUNDIALS solvers not only operate on generic vectors, but also on generic matrices (of type SUNMatrix), through a set of operations defined by the particular SUNMATRIX implementation. Users can provide their own specific implementation of the SUNMATRIX module, particularly in cases where they provide their own NVECTOR and/or linear solver modules, and require matrices that are compatible with those implementations. Alternately, we provide three SUNMATRIX implementations: dense, banded, and sparse. The generic operations are described below, and descriptions of the implementations provided with SUNDIALS follow.

7.1 The SUNMatrix API

The SUNMATRIX API can be grouped into two sets of functions: the core matrix operations, and utility functions. Section 7.1.1 lists the core operations, while Section 7.1.2 lists the utility functions.

7.1.1 SUNMatrix core functions

The generic SUNMatrix object defines the following set of core operations:

SUNMatGetID

Call id = SUNMatGetID(A);

Description Returns the type identifier for the matrix A. It is used to determine the matrix imple-

mentation type (e.g. dense, banded, sparse,...) from the abstract SUNMatrix interface. This is used to assess compatibility with SUNDIALS-provided linear solver implementa-

tions.

Arguments A (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX_ID, possible values are given in the Table 7.2.

F2003 Name FSUNMatGetID

SUNMatClone

Call B = SUNMatClone(A);

Description Creates a new SUNMatrix of the same type as an existing matrix A and sets the ops

field. It does not copy the matrix, but rather allocates storage for the new matrix.

Arguments A (SUNMatrix) a SUNMATRIX object

Return value SUNMatrix
F2003 Name FSUNMatClone
F2003 Call type(SUNMatrix), pointer :: B
B => FSUNMatClone(A)

SUNMatDestroy

Call SUNMatDestroy(A);

Description Destroys A and frees memory allocated for its internal data.

Arguments A (SUNMatrix) a SUNMATRIX object

Return value None

F2003 Name FSUNMatDestroy

SUNMatSpace

Call ier = SUNMatSpace(A, &lrw, &liw);

Description Returns the storage requirements for the matrix A. lrw is a long int containing the

number of realtype words and liw is a long int containing the number of integer words.

Arguments A (SUNMatrix) a SUNMATRIX object

lrw (sunindextype*) the number of realtype words
liw (sunindextype*) the number of integer words

Return value None

Notes 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.

F2003 Name FSUNMatSpace

F2003 Call integer(c_long) :: lrw(1), liw(1) ier = FSUNMatSpace(A, lrw, liw)

SUNMatZero

Call ier = SUNMatZero(A);

Description Performs the operation $A_{ij} = 0$ for all entries of the matrix A.

Arguments A (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX return code of type int denoting success/failure

 $F2003 \; \mathrm{Name} \; \; \mathtt{FSUNMatZero}$

SUNMatCopy

Call ier = SUNMatCopy(A,B);

Description Performs the operation $B_{ij} = A_{i,j}$ for all entries of the matrices A and B.

Arguments A (SUNMatrix) a SUNMATRIX object

B (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX return code of type int denoting success/failure

F2003 Name FSUNMatCopy

SUNMatScaleAdd

Call ier = SUNMatScaleAdd(c, A, B);

Description Performs the operation A = cA + B.

Arguments c (realtype) constant that scales A

A (SUNMatrix) a SUNMATRIX object

B (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX return code of type int denoting success/failure

 $F2003 \; \mathrm{Name} \; \; \mathtt{FSUNMatScaleAdd}$

SUNMatScaleAddI

Call ier = SUNMatScaleAddI(c, A);

Description Performs the operation A = cA + I.

Arguments c (realtype) constant that scales A

A (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX return code of type int denoting success/failure

F2003 Name FSUNMatScaleAddI

SUNMatMatvecSetup

Call ier = SUNMatMatvecSetup(A);

Description Performs any setup necessary to perform a matrix-vector product. It is useful for

SUNMatrix implementations which need to prepare the matrix itself, or communication

structures before performing the matrix-vector product.

Arguments A (SUNMatrix) a SUNMATRIX object

Return value A SUNMATRIX return code of type int denoting success/failure

F2003 Name FSUNMatMatvecSetup

SUNMatMatvec

Call ier = SUNMatMatvec(A, x, y);

Description Performs the matrix-vector product operation, y = Ax. It should only be called with

vectors x and y that are compatible with the matrix A - both in storage type and

dimensions.

Arguments A (SUNMatrix) a SUNMATRIX object

x (N_Vector) a NVECTOR object

y (N_Vector) an output NVECTOR object

Return value A SUNMATRIX return code of type int denoting success/failure

F2003 Name FSUNMatMatvec

7.1.2 SUNMatrix utility functions

To aid in the creation of custom SUNMATRIX modules the generic SUNMATRIX module provides two utility functions SUNMatNewEmpty and SUNMatVCopyOps.

SUNMatNewEmpty

Call A = SUNMatNewEmpty();

Description The function SUNMatNewEmpty allocates a new generic SUNMATRIX object and initializes

its content pointer and the function pointers in the operations structure to NULL.

Arguments None

Return value This function returns a SUNMatrix object. If an error occurs when allocating the object,

then this routine will return NULL.

F2003 Name FSUNMatNewEmpty

SUNMatFreeEmpty

Call SUNMatFreeEmpty(A);

Description 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 (SUNMatrix) a SUNMatrix object

Return value None

F2003 Name FSUNMatFreeEmpty

SUNMatCopyOps

Call retval = SUNMatCopyOps(A, B);

Description The function SUNMatCopyOps copies the function pointers in the ops structure of A into

the ops structure of B.

Arguments A (SUNMatrix) the matrix to copy operations from

B (SUNMatrix) the matrix to copy operations to

Return value This returns 0 if successful and a non-zero value if either of the inputs are NULL or the

ops structure of either input is NULL.

 $F2003 \ \mathrm{Name} \ FSUNMatCopyOps$

7.1.3 SUNMatrix return codes

The functions provided to SUNMATRIX modules within the SUNDIALS-provided SUNMATRIX implementations utilize a common set of return codes, shown in Table 7.1. These adhere to a common pattern: 0 indicates success, and a negative value indicates a failure. The actual values of each return code are primarily to provide additional information to the user in case of a failure.

Table 7.1: Description of the SUNMatrix return codes

Name	Value	Description
SUNMAT_SUCCESS	0	successful call or converged solve
		continued on next page

Matrix ID	Matrix type	ID Value
SUNMATRIX_DENSE	Dense $M \times N$ matrix	0
SUNMATRIX_BAND	Band $M \times M$ matrix	1
SUNMATRIX_SPARSE	Sparse (CSR or CSC) $M \times N$ matrix	2
SUNMATRIX_SLUNRLOC	Adapter for the SuperLU_DIST SuperMatrix	3
SUNMATRIX_CUSTOM	User-provided custom matrix	4

Table 7.2: Identifiers associated with matrix kernels supplied with SUNDIALS.

Name	Value	Description
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 -		the SUNMatMatvecSetup routine needs to be called be-
		fore calling SUNMatMatvec

7.1.4 SUNMatrix identifiers

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 7.2. It is recommended that a user-supplied SUNMATRIX implementation use the SUNMATRIX_CUSTOM identifier.

7.1.5 Compatibility of SUNMatrix modules

We note that not all SUNMATRIX types are compatible with all NVECTOR types provided with SUNDIALS. This is primarily due to the need for compatibility within the SUNMatMatvec routine; however, compatibility between SUNMATRIX and NVECTOR implementations is more crucial when considering their interaction within SUNLINSOL objects, as will be described in more detail in Chapter 8. More specifically, in Table 7.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Matrix	Serial	Parallel	OpenMP	pThreads	hypre	PETSC	CUDA	RAJA	User
Interface		(MPI)			Vec.	Vec.			Suppl.
Dense	✓		✓	✓					✓
Band	✓		✓	✓					✓
Sparse	✓		✓	✓					✓
SLUNRloc	✓	\checkmark	\checkmark	✓	✓	✓			✓
User supplied	✓	✓	✓	✓	✓	✓	✓	✓	✓

Table 7.3: SUNDIALS matrix interfaces and vector implementations that can be used for each.

7.1.6 The generic SUNMatrix module implementation

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

typedef struct _generic_SUNMatrix *SUNMatrix;

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

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

```
struct _generic_SUNMatrix_Ops {
  SUNMatrix_ID (*getid)(SUNMatrix);
               (*clone)(SUNMatrix);
  SUNMatrix
  void
               (*destroy)(SUNMatrix);
               (*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
  int
               (*space)(SUNMatrix, long int*, long int*);
};
```

The generic SUNMATRIX module defines and implements the matrix operations acting on SUNMatrix objects. These routines are nothing but wrappers for the matrix operations defined by a particular SUNMATRIX implementation, which are accessed through the *ops* field of the SUNMatrix structure. To 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));
}
```

Section 7.1.1 contains a complete list of all matrix operations defined by the generic Sunmatrix module

The Fortran 2003 interface provides a bind(C) derived-type for the _generic_SUNMatrix and the _generic_SUNMatrix_Ops structures. Their definition is given below.

```
type, bind(C), public :: SUNMatrix
type(C_PTR), public :: content
type(C_PTR), public :: ops
end type SUNMatrix
type, bind(C), public :: SUNMatrix_Ops
type(C_FUNPTR), public :: getid
type(C_FUNPTR), public :: clone
type(C_FUNPTR), public :: destroy
type(C_FUNPTR), public :: zero
type(C_FUNPTR), public :: copy
type(C_FUNPTR), public :: scaleadd
type(C_FUNPTR), public :: scaleaddi
type(C_FUNPTR), public :: matvecsetup
type(C_FUNPTR), public :: matvec
type(C_FUNPTR), public :: space
end type SUNMatrix_Ops
```

7.1.7 Implementing a custom SUNMatrix

A particular implementation of the Sunmatrix module must:

- Specify the *content* field of the SUNMatrix object.
- Define and implement a minimal subset of the matrix operations. See the documentation for each SUNDIALS solver to determine which SUNMATRIX operations they require.
 - Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNMATRIX module (each with different SUNMatrix internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free a SUNMatrix with the new *content* field and with *ops* pointing to the new matrix operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined SUNMatrix (e.g., a routine to print the content for debugging purposes).
- Optionally, provide accessor macros or functions as needed for that particular implementation to access different parts of the *content* field of the newly defined SUNMatrix.

It is recommended that a user-supplied SUNMATRIX implementation use the ${\tt SUNMATRIX_CUSTOM}$ identifier.

To aid in the creation of custom SUNMATRIX modules the generic SUNMATRIX module provides two utility functions SUNMatNewEmpty and SUNMatVCopyOps. 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. These functions are described in Section 7.1.2.

7.2 SUNMatrix functions used by KINSOL

In Table 7.4 below, 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 interface and the KINBBDPRE preconditioner module. 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.

SUNMatGetID
SUNMatDestroy
SUNMatZero
SUNMatSpace

SUNMatSpace

Table 7.4: List of matrix functions usage by KINSOL code modules

The matrix functions listed in Section 7.1.1 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 Section 7.1.1 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.

7.3 The SUNMatrix_Dense implementation

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

```
struct _SUNMatrixContent_Dense {
  sunindextype M;
  sunindextype N;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
These entries of the content field contain the following information:
      - number of rows
      - number of columns
data - pointer to a contiguous block of realtype variables. The elements of the dense matrix are
       stored columnwise, i.e. the (i,j)-th element of a dense Sunmatrix A (with 0 \le i < M and 0 \le i < M).
       j < N) may be accessed via data[j*M+i].
ldata - length of the data array (= M \cdot N).
cols - array of pointers. cols[j] points to the first element of the j-th column of the matrix in the
       array data. The (i,j)-th element of a dense Sunmatrix A (with 0 \le i < M and 0 \le j < N)
       may be accessed via cols[j][i].
```

The header file to include when using this module is sunmatrix/sunmatrix_dense.h. The SUNMATRIX_DENSE module is accessible from all SUNDIALS solvers without linking to the libsundials_sunmatrixdense module library.

7.3.1 SUNMatrix Dense accessor macros

The following macros are provided to access the content of a SUNMATRIX_DENSE matrix. The prefix SM_{-} in the names denotes that these macros are for SUNMatrix implementations, and the suffix $_{-}D$ denotes that these are specific to the dense version.

SM_CONTENT_D

This macro gives access to the contents of the dense SUNMatrix.

The assignment A_cont = SM_CONTENT_D(A) sets A_cont to be a pointer to the dense SUNMatrix content structure.

Implementation:

```
#define SM_CONTENT_D(A) ( (SUNMatrixContent_Dense)(A->content) )
```

• SM_ROWS_D, SM_COLUMNS_D, and SM_LDATA_D

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

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

Implementation:

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

• SM_DATA_D and SM_COLS_D

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

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

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

Implementation:

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

SM COLUMN D and SM ELEMENT D

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

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

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

Implementation:

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

7.3.2 SUNMatrix_Dense functions

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix _Dense (e.g. SUNMatCopy_Dense). All the standard matrix operations listed in Section 7.1.1 with the suffix _Dense appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Dense).

The module SUNMATRIX_DENSE provides the following additional user-callable routines:

SUNDenseMatrix

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

Description 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.

F2003 Name This function is callable as FSUNDenseMatrix when using the Fortran 2003 interface module.

SUNDenseMatrix_Print

Prototype void SUNDenseMatrix_Print(SUNMatrix A, FILE* outfile)

Description 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.

SUNDenseMatrix_Rows

Prototype sunindextype SUNDenseMatrix_Rows(SUNMatrix A)

Description This function returns the number of rows in the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix.Rows when using the Fortran 2003 inter-

face module.

SUNDenseMatrix_Columns

Prototype sunindextype SUNDenseMatrix_Columns(SUNMatrix A)

Description This function returns the number of columns in the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix_Columns when using the Fortran 2003

interface module.

SUNDenseMatrix_LData

Prototype sunindextype SUNDenseMatrix_LData(SUNMatrix A)

Description This function returns the length of the data array for the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix_LData when using the Fortran 2003 inter-

face module.

SUNDenseMatrix_Data

Prototype realtype* SUNDenseMatrix_Data(SUNMatrix A)

Description This function returns a pointer to the data array for the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix_Data when using the Fortran 2003 inter-

face module.

SUNDenseMatrix_Cols

Prototype realtype** SUNDenseMatrix_Cols(SUNMatrix A)

Description This function returns a pointer to the cols array for the dense SUNMatrix.

SUNDenseMatrix_Column

Prototype realtype* SUNDenseMatrix_Column(SUNMatrix A, sunindextype j)

Description This function returns a pointer to the first entry of the jth column of the dense SUNMatrix.

The resulting pointer should be indexed over the range 0 to M-1.

F2003 Name This function is callable as FSUNDenseMatrix_Column when using the Fortran 2003 in-

terface module.

Notes

- When looping over the components of a dense SUNMatrix A, the most efficient approaches are to:
 - First obtain the component array via A_data = SM_DATA_D(A) or A_data = SUNDenseMatrix_Data(A) and then access A_data[i] within the loop.
 - First obtain the array of column pointers via A_cols = SM_COLS_D(A) or
 A_cols = SUNDenseMatrix_Cols(A), and then access A_cols[j][i] within the loop.
 - Within a loop over the columns, access the column pointer via
 A_colj = SUNDenseMatrix_Column(A,j) and then to access the entries within that column using A_colj[i] within the loop.

All three of these are more efficient than using SM_ELEMENT_D(A,i,j) within a double loop.

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



7.3.3 SUNMatrix_Dense Fortran interfaces

The SUNMATRIX_DENSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunmatrix_dense_mod FORTRAN module defines interfaces to most SUNMATRIX_DENSE 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 SUNDenseMatrix is interfaced as FSUNDenseMatrix.

The Fortran 2003 Sunmatrix_dense_mod, and linking to the library libsundials_fsunmatrix_dense_mod. lib in addition to the C library. For details on where the library and module file fsunmatrix_dense_mod.mod are installed see Appendix A. We note that the module is accessible from the Fortran 2003 Sundials integrators without separately linking to the libsundials_fsunmatrixdense_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the SUNMATRIX_DENSE module also includes the FORTRAN-callable function FSUNDenseMatInit(code, M, N, ier) to initialize this SUNMATRIX_DENSE module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); M and N are the corresponding dense matrix construction arguments (declared to match C type long int); and ier is an error return flag equal to 0 for success and -1 for failure. Both code and ier are declared to match C type int. Additionally, when using ARKODE with a non-identity mass matrix, the FORTRAN-callable function FSUNDenseMassMatInit(M, N, ier) initializes this SUNMATRIX_DENSE module for storing the mass matrix.

7.4 The SUNMatrix_Band implementation

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

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

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

```
M - number of rows
```

```
N - number of columns (N = M)
```

 $\mathtt{mu} \quad \text{- upper half-bandwidth, } 0 \leq \mathtt{mu} < \mathtt{N}$

ml - lower half-bandwidth, $0 \le ml < N$

s_mu - storage upper bandwidth, mu ≤ s_mu < N. The LU decomposition routines in the associated SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(N-1,mu+ml) because of partial pivoting. The s_mu field holds the upper half-bandwidth allocated for A.

```
ldim - leading dimension (ldim \geq s_mu+ml+1)
```

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

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

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

The header file to include when using this module is sunmatrix/sunmatrix_band.h. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers without linking to the libsundials_sunmatrixband module library.

7.4.1 SUNMatrix_Band accessor macros

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

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

The assignment $A_cont = SM_CONTENT_B(A)$ sets A_cont to be a pointer to the banded SUNMatrix content structure.

Implementation:

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



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

• SM_ROWS_B, SM_COLUMNS_B, SM_UBAND_B, SM_LBAND_B, SM_SUBAND_B, SM_LDIM_B, and SM_LDATA_B

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

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

Implementation:

```
#define SM_ROWS_B(A) ( SM_CONTENT_B(A)->M )
#define SM_COLUMNS_B(A) ( SM_CONTENT_B(A)->N )
#define SM_UBAND_B(A) ( SM_CONTENT_B(A)->mu )
#define SM_LBAND_B(A) ( SM_CONTENT_B(A)->ml )
#define SM_SUBAND_B(A) ( SM_CONTENT_B(A)->s_mu )
#define SM_LDIM_B(A) ( SM_CONTENT_B(A)->ldim )
#define SM_LDATA_B(A) ( SM_CONTENT_B(A)->ldata )
```

SM_DATA_B and SM_COLS_B

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

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

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

Implementation:

```
#define SM_DATA_B(A) ( SM_CONTENT_B(A)->data )
#define SM_COLS_B(A) ( SM_CONTENT_B(A)->cols )
```

• SM_COLUMN_B, SM_COLUMN_ELEMENT_B, and SM_ELEMENT_B

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

The assignments SM_ELEMENT_B(A,i,j) = a_ij and a_ij = SM_ELEMENT_B(A,i,j) reference the (i,j)-th element of the N × N band matrix A, where $0 \le i, j \le N-1$. The location (i,j) should further satisfy $j-mu \le i \le j+ml$.

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 × N band matrix A, $0 \le j \le N-1$. The type of the expression $SM_COLUMN_B(A,j)$ is realtype *. The pointer returned by the call $SM_COLUMN_B(A,j)$ can be treated as an array which is indexed from -mu to ml.

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 $j-mu \le i \le j+ml$.

Implementation:

7.4.2 SUNMatrix Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix _Band (e.g. SUNMatCopy_Band). All the standard matrix operations listed in Section 7.1.1 with the suffix _Band appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Band).

The module SUNMATRIX_BAND provides the following additional user-callable routines:

SUNBandMatrix

Prototype SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu, sunindextype ml)

Description 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_LAPACKBAND modules.

F2003 Name This function is callable as FSUNBandMatrix when using the Fortran 2003 interface module.

SUNBandMatrixStorage

Prototype SUNMatrix SUNBandMatrixStorage(sunindextype N, sunindextype mu, sunindextype ml, sunindextype smu)

Description 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.

SUNBandMatrix_Print

Prototype void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile)

Description 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.

SUNBandMatrix_Rows

Prototype sunindextype SUNBandMatrix_Rows(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_Rows when using the Fortran 2003 interface module.

SUNBandMatrix_Columns

Prototype sunindextype SUNBandMatrix_Columns(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_Columns when using the Fortran 2003 in-

terface module.

SUNBandMatrix_LowerBandwidth

Prototype sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_LowerBandwidth when using the Fortran

2003 interface module.

SUNBandMatrix_UpperBandwidth

Prototype sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_UpperBandwidth when using the Fortran

2003 interface module.

SUNBandMatrix_StoredUpperBandwidth

Prototype sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_StoredUpperBandwidth when using the

Fortran 2003 interface module.

SUNBandMatrix_LDim

Prototype sunindextype SUNBandMatrix_LDim(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_LDim when using the Fortran 2003 interface

module.

SUNBandMatrix_Data

Prototype realtype* SUNBandMatrix_Data(SUNMatrix A)

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

F2003 Name This function is callable as FSUNBandMatrix_Data when using the Fortran 2003 interface

module.

SUNBandMatrix_Cols

Prototype realtype** SUNBandMatrix_Cols(SUNMatrix A)

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

SUNBandMatrix_Column

Prototype realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j)

Description 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.

F2003 Name This function is callable as FSUNBandMatrix_Column when using the Fortran 2003 interface module.

Notes

- When looping over the components of a banded SUNMatrix A, the most efficient approaches are to:
 - First obtain the component array via A_data = SM_DATA_B(A) or A_data = SUNBandMatrix_Data(A) and then access A_data[i] within the loop.
 - First obtain the array of column pointers via A_cols = SM_COLS_B(A) or A_cols = SUNBandMatrix_Cols(A), and then access A_cols[j][i] within the loop.
 - Within a loop over the columns, access the column pointer via
 A_colj = SUNBandMatrix_Column(A,j) and then to access the entries within that column using SM_COLUMN_ELEMENT_B(A_colj,i,j).

All three of these are more efficient than using SM_ELEMENT_B(A,i,j) within a double loop.

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

7.4.3 SUNMatrix Band Fortran interfaces

The SUNMATRIX_BAND module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunmatrix_band_mod FORTRAN module defines interfaces to most SUNMATRIX_BAND 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 SUNBandMatrix is interfaced as FSUNBandMatrix.

The Fortran 2003 Sunmatrix_band interface module can be accessed with the use statement, i.e. use fsunmatrix_band_mod, and linking to the library libsundials_fsunmatrixband_mod.lib in addition to the C library. For details on where the library and module file fsunmatrix_band_mod.mod are installed see Appendix A. We note that the module is accessible from the Fortran 2003 Sundials integrators without separately linking to the libsundials_fsunmatrixband_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the SUNMATRIX_BAND module also includes the FORTRAN-callable function FSUNBandMatInit(code, N, mu, ml, ier) to initialize this SUNMATRIX_BAND module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); N, mu, and ml are the corresponding band matrix construction arguments (declared to match C type long int); and ier is an error return flag equal to 0 for success and -1 for failure. Both code and ier are declared to match C type int. Additionally, when using ARKODE with a non-identity mass matrix, the FORTRAN-callable function FSUNBandMassMatInit(N, mu, ml, ier) initializes this SUNMATRIX_BAND module for storing the mass matrix.



7.5 The SUNMatrix_Sparse implementation

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

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

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

```
M - number of rows
N - number of columns
```

NP

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

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

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

sparsetype - type of the sparse matrix (CSC_MAT or CSR_MAT)

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

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

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

```
rowvals - pointer to indexvals when sparsetype is CSC_MAT, otherwise set to NULL. colptrs - pointer to indexptrs when sparsetype is CSC_MAT, otherwise set to NULL. colvals - pointer to indexvals when sparsetype is CSR_MAT, otherwise set to NULL. rowptrs - pointer to indexptrs when sparsetype is CSR_MAT, otherwise set to NULL.
```

For example, the 5×4 CSC matrix

$$\left[\begin{array}{cccc} 0 & 3 & 1 & 0 \\ 3 & 0 & 0 & 2 \\ 0 & 7 & 0 & 0 \\ 1 & 0 & 0 & 9 \\ 0 & 0 & 0 & 5 \end{array}\right]$$

could be stored in this structure as either

```
M = 5;
 N = 4;
 NNZ = 8;
  NP = N;
  data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0};
  sparsetype = CSC_MAT;
  indexvals = {1, 3, 0, 2, 0, 1, 3, 4};
  indexptrs = \{0, 2, 4, 5, 8\};
or
 M = 5;
 N = 4;
  NNZ = 10;
  NP = N;
  data = \{3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0, *, *\};
  sparsetype = CSC_MAT;
  indexvals = \{1, 3, 0, 2, 0, 1, 3, 4, *, *\};
  indexptrs = \{0, 2, 4, 5, 8\};
```

where the first has no unused space, and the second has additional storage (the entries marked with * may contain any values). Note in both cases that the final value in indexptrs is 8, indicating the total number of nonzero entries in the matrix.

Similarly, in CSR format, the same matrix could be stored as

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 2.0, 7.0, 1.0, 9.0, 5.0};
sparsetype = CSR_MAT;
indexvals = {1, 2, 0, 3, 1, 0, 3, 3};
indexptrs = {0, 2, 4, 5, 7, 8};
```

The header file to include when using this module is sunmatrix/sunmatrix_sparse.h. The SUNMATRIX_SPARSE module is accessible from all SUNDIALS solvers without linking to the libsundials_sunmatrixsparse module library.

7.5.1 SUNMatrix_Sparse accessor macros

The following macros are provided to access the content of a SUNMATRIX_SPARSE matrix. The prefix SM_{-} in the names denotes that these macros are for SUNMatrix implementations, and the suffix $_{-}S$ denotes that these are specific to the sparse version.

• SM_CONTENT_S

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

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

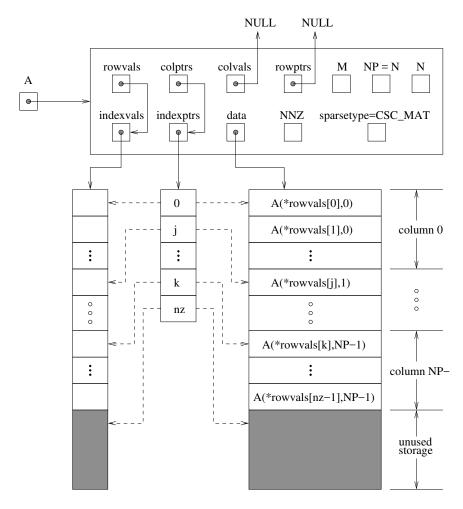


Figure 7.2: Diagram of the storage for a compressed-sparse-column matrix. Here A is an $M \times N$ sparse matrix with storage for up to NNZ nonzero entries (the allocated length of both data and indexvals). The entries in indexvals may assume values from 0 to M-1, corresponding to the row index (zero-based) of each nonzero value. The entries in data contain the values of the nonzero entries, with the row i, column j entry of A (again, zero-based) denoted as A(i,j). The indexptrs array contains N+1 entries; the first N denote the starting index of each column within the indexvals and data arrays, while the final entry points one past the final nonzero entry. Here, although NNZ values are allocated, only nz are actually filled in; the greyed-out portions of data and indexvals indicate extra allocated space.

Implementation:

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

• SM_ROWS_S, SM_COLUMNS_S, SM_NNZ_S, SM_NP_S, and SM_SPARSETYPE_S

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

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

Implementation:

• SM_DATA_S, SM_INDEXVALS_S, and SM_INDEXPTRS_S

These macros give access to the data and index arrays for the matrix entries.

The assignment $A_{data} = SM_DATA_S(A)$ sets A_{data} to be a pointer to the first component of the data array for the sparse SUNMatrix A. The assignment $SM_DATA_S(A) = A_{data}$ sets the data array of A to be A_{data} by storing the pointer A_{data} .

Similarly, the assignment A_indexvals = SM_INDEXVALS_S(A) sets A_indexvals to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix A. The assignment A_indexptrs = SM_INDEXPTRS_S(A) sets A_indexptrs to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).

Implementation:

```
#define SM_DATA_S(A) ( SM_CONTENT_S(A)->data )
#define SM_INDEXVALS_S(A) ( SM_CONTENT_S(A)->indexvals )
#define SM_INDEXPTRS_S(A) ( SM_CONTENT_S(A)->indexptrs )
```

7.5.2 SUNMatrix_Sparse functions

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). All the standard matrix operations listed in Section 7.1.1 with the suffix _Sparse appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Sparse).

The module SUNMATRIX_SPARSE provides the following additional user-callable routines:

SUNSparseMatrix

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

Description This function creates and allocates memory for a sparse SUNMatrix. Its arguments are the number of rows and columns of the matrix, M and N, the maximum number of nonzeros to be stored in the matrix, NNZ, and a flag sparsetype indicating whether to use CSR or CSC format (valid arguments are CSR_MAT or CSC_MAT).

F2003 Name This function is callable as FSUNSparseMatrix when using the Fortran 2003 interface module.

SUNSparseFromDenseMatrix

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

Description This function creates a new sparse matrix from an existing dense matrix by copying all values with magnitude larger than droptol into the sparse matrix structure.

Requirements:

- A must have type SUNMATRIX_DENSE;
- droptol must be non-negative;
- sparsetype must be either CSC_MAT or CSR_MAT.

The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

F2003 Name This function is callable as FSUNSparseFromDenseMatrix when using the Fortran 2003 interface module.

SUNSparseFromBandMatrix

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

Description This function creates a new sparse matrix from an existing band matrix by copying all values with magnitude larger than droptol into the sparse matrix structure.

Requirements:

- A must have type SUNMATRIX_BAND;
- droptol must be non-negative;
- sparsetype must be either CSC_MAT or CSR_MAT.

The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

F2003 Name This function is callable as FSUNSparseFromBandMatrix when using the Fortran 2003 interface module.

SUNSparseMatrix_Realloc

Prototype int SUNSparseMatrix_Realloc(SUNMatrix A)

Description 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).

F2003 Name This function is callable as FSUNSparseMatrix_Realloc when using the Fortran 2003 interface module.

SUNSparseMatrix_Reallocate

Prototype int SUNSparseMatrix_Reallocate(SUNMatrix A, sunindextype NNZ)

Description This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has storage for a specified number of nonzeros. Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse or if NNZ is negative).

F2003 Name This function is callable as $FSUNSparseMatrix_Reallocate$ when using the Fortran 2003 interface module.

SUNSparseMatrix_Print

Prototype void SUNSparseMatrix_Print(SUNMatrix A, FILE* outfile)

Description 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.

SUNSparseMatrix_Rows

Prototype sunindextype SUNSparseMatrix_Rows(SUNMatrix A)

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

F2003 Name This function is callable as FSUNSparseMatrix_Rows when using the Fortran 2003 inter-

face module.

SUNSparseMatrix_Columns

Prototype sunindextype SUNSparseMatrix_Columns(SUNMatrix A)

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

F2003 Name This function is callable as FSUNSparseMatrix_Columns when using the Fortran 2003

interface module.

SUNSparseMatrix_NNZ

Prototype sunindextype SUNSparseMatrix_NNZ(SUNMatrix A)

Description This function returns the number of entries allocated for nonzero storage for the sparse

matrix SUNMatrix.

F2003 Name This function is callable as FSUNSparseMatrix_NNZ when using the Fortran 2003 inter-

face module.

SUNSparseMatrix_NP

Prototype sunindextype SUNSparseMatrix_NP(SUNMatrix A)

Description This function returns the number of columns/rows for the sparse SUNMatrix, depending

on whether the matrix uses CSC/CSR format, respectively. The indexptrs array has

NP+1 entries.

F2003 Name This function is callable as FSUNSparseMatrix_NP when using the Fortran 2003 interface

module.

${\tt SUNSparseMatrix_SparseType}$

Prototype int SUNSparseMatrix_SparseType(SUNMatrix A)

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

F2003 Name This function is callable as FSUNSparseMatrix_SparseType when using the Fortran 2003

interface module.

SUNSparseMatrix_Data

Prototype realtype* SUNSparseMatrix_Data(SUNMatrix A)

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

F2003 Name This function is callable as FSUNSparseMatrix_Data when using the Fortran 2003 inter-

face module.

SUNSparseMatrix_IndexValues

Prototype sunindextype* SUNSparseMatrix_IndexValues(SUNMatrix A)

Description 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.

F2003 Name This function is callable as FSUNSparseMatrix_IndexValues when using the Fortran

2003 interface module.

${\tt SUNSparseMatrix_IndexPointers}$

Prototype sunindextype* SUNSparseMatrix_IndexPointers(SUNMatrix A)

Description 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.

F2003 Name This function is callable as $FSUNSparseMatrix_IndexPointers$ when using the Fortran

2003 interface module.

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

7.5.3 SUNMatrix_Sparse Fortran interfaces

The SUNMATRIX_SPARSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunmatrix_sparse_mod FORTRAN module defines interfaces to most SUNMATRIX_SPARSE 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 SUNSparseMatrix is interfaced as FSUNSparseMatrix.

The Fortran 2003 Sunmatrix_sparse interface module can be accessed with the use statement, i.e. use fsunmatrix_sparse_mod, and linking to the library libsundials_fsunmatrixsparse_mod.lib in addition to the C library. For details on where the library and module file fsunmatrix_sparse_mod.mod are installed see Appendix A. We note that the module is accessible from the Fortran 2003 sundials integrators without separately linking to the libsundials_fsunmatrixsparse_mod library.

FORTRAN 77 interface functions

For solvers that include a Fortran interface module, the SUNMATRIX_SPARSE module also includes the Fortran-callable function FSUNSparseMatInit(code, M, N, NNZ, sparsetype, ier) to initialize this SUNMATRIX_SPARSE module for a given SUNDIALS solver. Here code is an integer input for the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); M, N and NNZ are the corresponding sparse matrix construction arguments (declared to match C type long int); sparsetype is an integer flag indicating the sparse storage type (0 for CSC, 1 for CSR); and ier is an error return flag equal to 0 for success and -1 for failure. Each of code, sparsetype and ier are declared so as to match C type int. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function FSUNSparseMassMatInit(M, N, NNZ, sparsetype, ier) initializes this SUNMATRIX_SPARSE module for storing the mass matrix.



7.6 The SUNMatrix_SLUNRloc implementation

The SUNMATRIX_SLUNRLOC implementation of the SUNMATRIX module provided with SUNDIALS is an adapter for the SuperMatrix structure provided by the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li [2, 17, 25, 26]. It is designed to be used with the SUNLINSOL_SUPERLUDIST linear solver discussed in Section 8.10. 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.

7.6.1 SUNMatrix_SLUNRloc functions

The module SUNMATRIX_SLUNRLOC provides the following user-callable routines:

```
Call A = SUNMatrix_SLUNRloc(Asuper, grid);

Description The function SUNMatrix_SLUNRloc creates and allocates memory for a SUNMATRIX_SLUNRLOC object.

Arguments Asuper (SuperMatrix*) a fully-allocated SuperLU_DIST SuperMatrix that the SUN-Matrix will wrap; must have Stype = SLU_NR_loc, Dtype = SLU_D, Mtype = SLU_GE to be compatible grid (gridinfo_t*) the initialized SuperLU_DIST 2D process grid structure

Return value a SUNMatrix object if Asuper is compatible else NULL
```

Notes

SUNMatrix_SLUNRloc_Print

Call SUNMatrix_SLUNRloc_Print(A, fp);

Description The function SUNMatrix_SLUNRloc_Print prints the underlying SuperMatrix content.

Arguments A (SUNMatrix) the matrix to print

fp (FILE) the file pointer used for printing

Return value void

Notes

SUNMatrix_SLUNRloc_SuperMatrix

Call Asuper = SUNMatrix_SLUNRloc_SuperMatrix(A);

Description The function SUNMatrix_SLUNRloc_SuperMatrix provides access to the underlying Su-

perLU_DIST SuperMatrix of A.

Arguments A (SUNMatrix) the matrix to access

Return value SuperMatrix*

Notes

SUNMatrix_SLUNRloc_ProcessGrid

Call grid = SUNMatrix_SLUNRloc_ProcessGrid(A);

Description The function SUNMatrix_SLUNRloc_ProcessGrid provides access to the SuperLU_DIST

gridinfo_t structure associated with A.

Arguments A (SUNMatrix) the matrix to access

Return value gridinfo_t*

Notes

SUNMatrix_SLUNRloc_OwnData

Call does_own_data = SUNMatrix_SLUNRloc_OwnData(A);

Description The function SUNMatrix_SLUNRloc_OwnData returns true if the SUNMatrix object is

responsible for freeing A_super, otherwise it returns false.

Arguments A (SUNMatrix) the matrix to access

Return value booleantype

Notes

The SUNMATRIX_SLUNRLOC module defines implementations of all generic SUNMatrix operations listed in Section 7.1.1:

- 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, but A and B must have the same sparsity pattern
- SUNMatScaleAddI_SLUNRloc performs A = cA + I, but 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

The SUNMATRIX_SLUNRLOC module requires that the complete diagonal, i.e. nonzeros and zeros, is present in order to use the SUNMatScaleAddI operation.



Chapter 8

Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS packages operate using generic linear solver modules defined through the 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_linearsolver.h.

The implementations provided with SUNDIALS work in coordination with the SUNDIALS generic NVECTOR and SUNMATRIX modules to provide a set of compatible data structures and solvers for the solution of linear systems using direct or iterative (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 NVECTOR 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

$$\tilde{A} = S_1 P_1^{-1} A P_2^{-1} S_2^{-1},$$

$$\tilde{b} = S_1 P_1^{-1} b,$$

$$\tilde{x} = S_2 P_2 x,$$
(8.2)

and where

- P_1 is the left preconditioner,
- P_2 is the right preconditioner,
- S_1 is a diagonal matrix of scale factors for $P_1^{-1}b$,
- S_2 is a diagonal matrix of scale factors for P_2x .

The scaling matrices are chosen so that $S_1P_1^{-1}b$ and S_2P_2x have dimensionless components. If preconditioning is done on the left only $(P_2 = I)$, by a matrix P, then S_2 must be a scaling for x, while S_1 is a scaling for $P^{-1}b$, and so may also be taken as a scaling for x. Similarly, if preconditioning is done on the right only $(P_1 = I \text{ and } P_2 = P)$, then S_1 must be a scaling for b, while S_2 is a scaling for Px, and may also be taken as a scaling for b.

SUNDIALS packages request that iterative linear solvers stop based on the 2-norm of the scaled preconditioned residual meeting a prescribed tolerance

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

When provided an iterative SUNLINSOL implementation that does not support the scaling matrices S_1 and S_2 , SUNDIALS' packages will adjust the value of tol accordingly (see §8.4.2 for more details). In this case, they instead request that iterative linear solvers stop based on the criteria

$$||P_1^{-1}b - P_1^{-1}Ax||_2 < \text{tol.}$$

We note that the corresponding adjustments to tol in this case are non-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 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 sections 8.1.1 – 8.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 8.1.4. A table of linear solver return codes is given in section 8.1.5. The SUNLinearSolver type and the generic SUNLINSOL module are defined in section 8.1.6. The section 8.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 8.3 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 SUNLINSOL functions required by this SUNDIALS package as well as other package specific details are given in section 8.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

8.1 The SUNLinear Solver API

The SUNLINSOL API defines several linear solver operations that enable SUNDIALS packages to utilize any SUNLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group of functions consists of set routines to supply the linear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving linear solver statistics. All of these functions are defined in the header file sundials/sundials_linearsolver.h.

8.1.1 SUNLinearSolver core functions

The core linear solver functions consist of two required functions to get the linear solver type (SUNLinSolGetType) and solve the linear system Ax = b (SUNLinSolSolve). The remaining three functions for initializing the linear solver object once all solver-specific options have been set (SUNLinSolInitialize), setting up the linear solver object to utilize an updated matrix A (SUNLinSolSetup), and for destroying the linear solver object (SUNLinSolFree) are optional.

SUNLinSolGetType

Call type = SUNLinSolGetType(LS);

Description The required function SUNLinSolGetType returns the type identifier for the linear solver LS. It is used to determine the solver type (direct, iterative, or matrix-iterative) from

the abstract SUNLinearSolver interface.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

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

- 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.

Notes See section 8.3.1 for more information on intended use cases corresponding to the linear

solver type.

F2003 Name FSUNLinSolGetType

SUNLinSolInitialize

Call retval = SUNLinSolInitialize(LS);

Description The optional function SUNLinSolInitialize performs linear solver initialization (as-

suming that all solver-specific options have been set).

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value This should return zero for a successful call, and a negative value for a failure, ideally

returning one of the generic error codes listed in Table 8.1.

F2003 Name FSUNLinSolInitialize

${\tt SUNLinSolSetup}$

Call retval = SUNLinSolSetup(LS, A);

Description The *optional* function SUNLinSolSetup 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.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

A (SUNMatrix) a SUNMATRIX object.

Return value This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 8.1.

F2003 Name FSUNLinSolSetup

SUNLinSolSolve

Call retval = SUNLinSolSolve(LS, A, x, b, tol);

Description The required function SUNLinSolSolve solves a linear system Ax = b.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

A (SUNMatrix) a SUNMATRIX object.

x (N_Vector) a NVECTOR object containing the initial guess for the solution of the linear system, and the solution to the linear system upon return.

b (N_Vector) a NVECTOR object containing the linear system right-hand side.

tol (realtype) the desired linear solver tolerance.

Return value This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 8.1.

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 instead 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.

F2003 Name FSUNLinSolSolve

SUNLinSolFree

Call retval = SUNLinSolFree(LS);

Description The optional function SUNLinSolFree frees memory allocated by the linear solver.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value This should return zero for a successful call and a negative value for a failure.

F2003 Name FSUNLinSolFree

8.1.2 SUNLinearSolver set functions

The following set functions are used to supply linear solver modules with functions defined by the SUNDIALS packages and to modify solver parameters. Only the routine for setting the matrix-vector product routine is required, and that is only 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.

SUNLinSolSetATimes

Call retval = SUNLinSolSetATimes(LS, A_data, ATimes);

Description The function SUNLinSolSetATimes is required for matrix-free linear solvers; otherwise it is optional.

This routine provides an ATimesFn function pointer, as well as a void* pointer to a data structure used by this routine, to a linear solver object. SUNDIALS packages will call this function to set the matrix-vector product function to either a solver-provided difference-quotient via vector operations or a user-supplied solver-specific routine.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

A_data (void*) data structure passed to ATimes.

ATimes (ATimesFn) function pointer implementing the matrix-vector product routine.

Return value This routine should return zero for a successful call, and a negative value for a failure,

ideally returning one of the generic error codes listed in Table 8.1.

F2003 Name FSUNLinSolSetATimes

SUNLinSolSetPreconditioner

Call retval = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);

Description The optional function SUNLinSolSetPreconditioner provides PSetupFn and PSolveFn

function pointers that implement the preconditioner solves P_1^{-1} and P_2^{-1} from equations (8.1)-(8.2). This routine will be called by a SUNDIALS package, which will provide translation between the generic Pset and Psol calls and the package- or user-supplied

routines.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Pdata (void*) data structure passed to both Pset and Psol.

Pset (PSetupFn) function pointer implementing the preconditioner setup.
Psol (PSolveFn) function pointer implementing the preconditioner solve.

Return value This routine should return zero for a successful call, and a negative value for a failure,

ideally returning one of the generic error codes listed in Table 8.1.

F2003 Name FSUNLinSolSetPreconditioner

SUNLinSolSetScalingVectors

Call retval = SUNLinSolSetScalingVectors(LS, s1, s2);

Description The optional function SUNLinSolSetScalingVectors provides left/right scaling vectors

for the linear system solve. Here, $\tt s1$ and $\tt s2$ are NVECTOR of positive scale factors containing the diagonal of the matrices S_1 and S_2 from equations (8.1)-(8.2), respectively. Neither of these vectors need to be tested for positivity, and a NULL argument for either

indicates that the corresponding scaling matrix is the identity.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

 ${\tt s1}$ (N_Vector) diagonal of the matrix S_1

s2 (N_Vector) diagonal of the matrix S_2

Return value This routine should return zero for a successful call, and a negative value for a failure,

ideally returning one of the generic error codes listed in Table 8.1.

 $F2003\ \mathrm{Name}\ FSUNLinSolSetScalingVectors$

8.1.3 SUNLinearSolver get functions

The following get functions allow SUNDIALS packages to retrieve results from a linear solve. All routines are optional.

SUNLinSolNumIters

Call its = SUNLinSolNumIters(LS);

Description The optional function SUNLinSolNumIters should return the number of linear iterations

performed in the last 'solve' call.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value int containing the number of iterations

 $F2003\ \mathrm{Name}\ FSUNLinSolNumIters$

SUNLinSolResNorm

Call rnorm = SUNLinSolResNorm(LS);

Description The optional function SUNLinSolResNorm should return the final residual norm from

the last 'solve' call.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value realtype containing the final residual norm

F2003 Name FSUNLinSolResNorm

SUNLinSolResid

Call rvec = SUNLinSolResid(LS);

Description 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 NVECTOR containing the

preconditioned initial residual vector.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value N_Vector containing the final residual vector

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.

F2003 Name FSUNLinSolResid

SUNLinSolLastFlag

Call lflag = SUNLinSolLastFlag(LS);

Description The optional function SUNLinSollastFlag should return the last error flag encountered

within the linear solver. This is not called by the SUNDIALS packages directly; it allows

the user to investigate linear solver issues after a failed solve.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

Return value long int containing the most recent error flag

 $F2003 \ Name \ FSUNLinSolLastFlag$

SUNLinSolSpace

Call retval = SUNLinSolSpace(LS, &lrw, &liw);

Description The optional function SUNLinSolSpace should return the storage requirements for the

linear solver LS.

Arguments LS (SUNLinearSolver) a SUNLINSOL object.

lrw (long int*) the number of realtype words stored by the linear solver.

liw (long int*) the number of integer words stored by the linear solver.

Return value This should return zero for a successful call, and a negative value for a failure, ideally

returning one of the generic error codes listed in Table 8.1.

Notes This function is advisory only, for use in determining a user's total space requirements.

F2003 Name FSUNLinSolSpace

8.1.4 Functions provided by SUNDIALS packages

To interface with the 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 interfaces to the linear systems of equations that result in their solution. The types for functions provided to a SUNLINSOL module are defined in the header file sundials_iterative.h, and are described below.

ATimesFn

Definition typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);

Purpose These functions compute the action of a matrix on a vector, performing the operation z = Av. Memory for z should already be allocted prior to calling this function. The

vector v should be left unchanged.

Arguments A_data is a pointer to client data, the same as that supplied to SUNLinSolSetATimes.

v is the input vector to multiply.

z is the output vector computed.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

${\tt PSetupFn}$

Definition typedef int (*PSetupFn)(void *P_data)

Purpose These functions set up any requisite problem data in preparation for calls to the corre-

sponding PSolveFn.

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

 ${\tt SUNLinSolSetPreconditioner}.$

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

PSolveFn

Definition typedef int (*PSolveFn)(void *P_data, N_Vector r, N_Vector z, realtype tol, int lr)

Purpose

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

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

where the weight vector for the WRMS norm may be accessed from the main package memory structure. The vector ${\tt r}$ should not be modified by the PSolveFn.

Arguments

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

r is the right-hand side vector for the preconditioner system.

z is the solution vector for the preconditioner system.

tol is the desired tolerance for an iterative preconditioner.

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

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

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, shown in Table 8.1. These adhere to a common pattern: 0 indicates success, a postitive 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 are primarily to provide additional information to the user in case of a linear solver failure.

Table 8.1: Description of the SUNLinearSolver error codes

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

Name	Value	Description
SUNLS_QRFACT_FAIL	7	a singular matrix was encountered during a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_LUFACT_FAIL	8	a singular matrix was encountered during a LU factorization (SUNLINSOL_DENSE/SUNLINSOL_BAND)

8.1.6 The generic SUNLinearSolver module

SUNDIALS packages interact with specific SUNLINSOL implementations through the generic SUNLINSOL module on which all other SUNLINSOL iplementations are built. The SUNLinearSolver type is a pointer to a structure containing an implementation-dependent *content* field, and an *ops* field. The type SUNLinearSolver is defined as

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

The generic SUNLINSOL module defines and implements the linear solver operations defined in Sections 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 generic SUNLINSOL module, namely SUNLinSolInitialize, which initializes a SUNLINSOL object for use after it has been created and configured, and returns a flag denoting a successful/failed operation:

```
int SUNLinSolInitialize(SUNLinearSolver S)
{
  return ((int) S->ops->initialize(S));
}
```

The Fortran 2003 interface provides a bind(C) derived-type for the _generic_SUNLinearSolver and the _generic_SUNLinearSolver_Ops structures. Their definition is given below.

```
type, bind(C), public :: SUNLinearSolver
type(C_PTR), public :: content
type(C_PTR), public :: ops
end type SUNLinearSolver
type, bind(C), public :: SUNLinearSolver_Ops
type(C_FUNPTR), public :: gettype
type(C_FUNPTR), public :: setatimes
type(C_FUNPTR), public :: setpreconditioner
type(C_FUNPTR), public :: setscalingvectors
type(C_FUNPTR), public :: initialize
type(C_FUNPTR), public :: setup
type(C_FUNPTR), public :: solve
type(C_FUNPTR), public :: numiters
type(C_FUNPTR), public :: resnorm
type(C_FUNPTR), public :: lastflag
type(C_FUNPTR), public :: space
type(C_FUNPTR), public :: resid
type(C_FUNPTR), public :: free
end type SUNLinearSolver_Ops
```

8.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 8.2 we show the matrix-based linear solvers available as SUNLINSOL modules, and the compatible matrix implementations. Recall that Table 4.1 shows the compatibility between all SUNLINSOL modules and vector implementations.

Table 8.2:	SUNDIALS	matrix-based	linear	solvers	and	matrix	implementations	that	can	be	used	for
each.												

Linear Solver	Dense	Banded	Sparse	SLUNRloc	User
Interface	Matrix	Matrix	Matrix	Matrix	Supplied
Dense	✓				✓
Band		√			✓
LapackDense	√				✓
LapackBand		√			✓
KLU			√		✓
SuperLU_DIST				✓	✓
SUPERLUMT			✓		√
User supplied	✓	√	√	✓	✓

8.3 Implementing a custom SUNLinearSolver module

A particular implementation of the Sunlinsol module must:

- Specify the *content* field of the SUNLinearSolver object.
- Define and implement a minimal subset of the linear solver operations. See the section 8.4 to determine which SUNLINSOL operations are required for this SUNDIALS package.

Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNLINSOL module (each with different SUNLinearSolver internal data representations) in the same code.

 Define and implement user-callable constructor and destructor routines to create and free a SUNLinearSolver with the new content field and with ops pointing to the new linear solver operations.

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 that the associated functionality is not supported.

To aid in the creation of custom SUNLINSOL modules the generic SUNLINSOL module provides the utility functions SUNLinSolNewEmpty and SUNLinSolFreeEmpty. When used in custom SUNLINSOL constructors the function SUNLinSolNewEmpty will ease the introduction of any new optional linear solver operations to the SUNLINSOL API by ensuring only required operations need to be set.

SUNLinSolNewEmpty

Call LS = SUNLinSolNewEmpty();

Description The function SUNLinSolNewEmpty allocates a new generic SUNLINSOL object and initial-

izes its content pointer and the function pointers in the operations structure to NULL.

Arguments None

Return value This function returns a SUNLinearSolver object. If an error occurs when allocating

the object, then this routine will return NULL.

F2003 Name FSUNLinSolNewEmpty

SUNLinSolFreeEmpty

Call SUNLinSolFreeEmpty(LS);

Description This routine frees the generic SUNLinSolFreeEmpty 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 (SUNLinearSolver)

Return value None

F2003 Name FSUNLinSolFreeEmpty

Additionally, a SUNLINSOL 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 to a particular problem.
- Provide additional user-callable "get" routines acting on the SUNLinearSolver object, e.g., for returning various solve statistics.

8.3.1 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. External solvers provide similar routines with the necessary functionality and thus will require minimal effort to wrap within custom SUNMATRIX and SUNLINSOL implementations. Sections 7.2 and 8.4 include a list of the required set of routines that compatible SUNMATRIX and SUNLINSOL implementations must provide. As SUNDIALS packages utilize generic SUNLINSOL modules allowing for user-supplied SUNLinearSolver implementations, there exists 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 following sections.

Direct linear solvers

Direct linear solver modules require a matrix and compute an 'exact' solution to the linear system defined by the matrix. Multiple matrix formats and associated direct linear solvers are supplied with SUNDIALS through different SUNMATRIX and SUNLINSOL implementations. SUNDIALS packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations. As a result, each package's linear solver interface recomputes Jacobian 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 Chapters 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 compute an inexact solution to the linear system defined by the package-supplied ATimes routine. SUNDIALS supplies multiple scaled, preconditioned iterative linear solver (spils) SUNLINSOL modules that support scaling to allow users to handle non-dimensionalization (as best as possible) within each SUNDIALS package and retain variables and define equations as desired in their applications. For linear solvers that do not support left/right scaling, the tolerance supplied to the linear solver is adjusted to compensate (see section 8.4.2 for more details); however, this use case may be non-optimal and cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single problem.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, Sundials a user must implement a custom sunlinear solver for the linear solver following the API described in Chapter 8. This user-supplied sunlinear solver must then self-identify as having Sunlinear solver_iterative type.

Matrix-based iterative linear solvers (reusing A)

Matrix-based iterative linear solver modules require a matrix and compute an inexact solution to the linear system defined by the matrix. This matrix will be updated infrequently and resued across multiple solves to amortize cost of matrix construction. As in the direct linear solver case, only wrappers for the matrix and linear solver in Sunmatrix and Sunlinsol implementations need to be created to utilize a new linear solver. This user-supplied Sunlinsol module must then self-identify as having Sunlinear Solver Matrix_Iterative type.

At present, SUNDIALS has one example problem that uses this approach for wrapping a structured-grid matrix, linear solver, and preconditioner from the *hypre* library that may be used as a template for other customized implementations (see examples/arkode/CXX_parhyp/ark_heat2D_hypre.cpp).

Matrix-based iterative linear solvers (current A)

For users who wish to utilize a matrix-based iterative linear solver module 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 spils SUNLINSOL implementations (SUNLINSOL_SPGMR, SUNLINSOL_SPFGMR, SUNLINSOL_SPFGMR, OR SUNLINSOL_SPTFQMR, or SUNLINSOL_PCG) as the outer solver. The creation and storage of the preconditioner matrix, and interfacing with the corresponding linear solver, can be handled through a package's preconditioner 'setup' and 'solve' functionality (see $\S4.5.4.2$) without creating SUNMATRIX and SUNLINSOL implementations. This usage mode is recommended primarily because the SUNDIALS-provided spils modules support the 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 ATimesFn routine.

8.4 KINSOL SUNLinearSolver interface

Table 8.3 below lists the SUNLINSOL 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 \checkmark to indicate that they are required, or with \dagger to indicate that they are only called if they are non-NULL in the SUNLINSOL 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 SUNLINSOL module, then KINLS will consider all solves as requiring zero iterations.
- 2. Although SUNLinSolResNorm is optional, if it is not implemented by the SUNLINSOL then KINLS will consider all solves a 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.

SUNLinSolSpace

Table 8.3: List of linear solver function usage in the KINLS interface

Since there are a wide range of potential SUNLINSOL use cases, the following subsections describe some details of the KINLS interface, in the case that interested users wish to develop custom SUNLINSOL modules.

8.4.1 Lagged matrix information

If the SUNLINSOL object self-identifies as having type SUNLINEARSOLVER_DIRECT or SUNLINEARSOLVER_MATRIX_ITERATIVE, then the SUNLINSOL object solves a linear system *defined* by a SUNMATRIX object. As a result, KINSOL can perform its optional residual monitoring scheme, described in §2.

8.4.2 Iterative linear solver tolerance

If the SUNLINSOL 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 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. 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) should satisfy the assumption

$$(D_F)_{i,i} \approx D_{Fmean}$$
, for $i = 0, \ldots, n-1$.

2. The SUNLINSOL 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 converted as follows (using the notation from equations (8.1)-(8.2)):

$$\begin{split} &\left\|\tilde{b} - \tilde{A}\tilde{x}\right\|_{2} < \text{tol} \\ \Leftrightarrow &\left\|D_{F}P_{1}^{-1}b - D_{F}P_{1}^{-1}Ax\right\|_{2} < \text{tol} \\ \Leftrightarrow &\left[\left(D_{F}\right)_{i,i}\left(P_{1}^{-1}(b - Ax)\right)_{i}\right]^{2} < \text{tol}^{2} \\ \Leftrightarrow &\left[\left(P_{F,mean}^{2}\sum_{i=0}^{n-1}\left[\left(P_{1}^{-1}(b - Ax)\right)_{i}\right]^{2} < \text{tol}^{2} \right] \\ \Leftrightarrow &\left[\left(P_{1}^{-1}(b - Ax)\right)_{i}\right]^{2} < \left(\frac{\text{tol}}{D_{F,mean}}\right)^{2} \\ \Leftrightarrow &\left\|P_{1}^{-1}(b - Ax)\right\|_{2} < \frac{\text{tol}}{D_{F,mean}} \end{split}$$

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 $delta = tol/D_{F,mean}$ is supplied to the SUNLINSOL object.

8.5 The SUNLinearSolver_Dense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems. The SUNLINSOL_DENSE module is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_DENSE module, include the header file sunlinsol/sunlinsol_dense.h. We note that the SUNLINSOL_DENSE module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsoldense module library.

8.5.1 SUNLinearSolver_Dense description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting $(\mathcal{O}(N^3) \cos t)$, 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 $(\mathcal{O}(N^2) \text{ cost})$.

8.5.2 SUNLinearSolver_Dense functions

The SUNLINSOL_DENSE module provides the following user-callable constructor for creating a SUNLinearSolver object.

Call LS = SUNLinSol_Dense(y, A);

Description The function SUNLinSol Dense creates and allocates memory for a dense

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

A (SUNMatrix) a SUNMATRIX_DENSE matrix template for cloning matrices needed

within the solver

Return value This returns 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 con-

sistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this

compatibility check.

Deprecated Name For backward compatibility, the wrapper function SUNDenseLinearSolver with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_Dense

The SUNLINSOL_DENSE module defines implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- 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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

8.5.3 SUNLinearSolver_Dense Fortran interfaces

The SUNLINSOL_DENSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_dense_mod FORTRAN module defines interfaces to all SUNLINSOL_DENSE 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 SUNLinSol_Dense is interfaced as FSUNLinSol_Dense.

The FORTRAN 2003 SUNLINSOL_DENSE interface module can be accessed with the use statement, i.e. use fsunlinsol_dense_mod, and linking to the library libsundials_fsunlinsoldense_mod.lib in addition to the C library. For details on where the library and module file fsunlinsol_dense_mod.mod are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fsunlinsoldense_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_DENSE module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNDENSELINSOLINIT

Call FSUNDENSELINSOLINIT(code, ier)

Description The function FSUNDENSELINSOLINIT can be called for Fortran programs to create a

dense SUNLinearSolver object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_DENSE module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSDENSELINSOLINIT

Call FSUNMASSDENSELINSOLINIT(ier)

Description The function FSUNMASSDENSELINSOLINIT can be called for Fortran programs to create

a dense SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes

This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

8.5.4 SUNLinearSolver_Dense content

The SUNLINSOL_DENSE module defines the *content* field of a SUNLinearSolver as the following structure:

8.6 The SUNLinearSolver_Band implementation

This section describes the SUNLINSOL implementation for solving banded linear systems. The SUNLINSOL_BAND module is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_BAND module, include the header file sunlinsol/sunlinsol_band.h. We note that the SUNLINSOL_BAND module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolband module library.

8.6.1 SUNLinearSolver_Band description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, PA = LU, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the pivots array.
- The "solve" call performs pivoting and forward and backward substitution using the stored pivots array and the *LU* factors held in the SUNMATRIX_BAND object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth mu and lower bandwidth ml, then the upper triangular factor U can have upper bandwidth as big as smu = MIN(N-1,mu+ml). The lower triangular factor L has lower bandwidth ml.



8.6.2 SUNLinearSolver_Band functions

The SUNLINSOL_BAND module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_Band

Call LS = SUNLinSol_Band(y, A);

Description The function SUNLinSol_Band creates and allocates memory for a band

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

A (SUNMatrix) a ${\tt SUNMATRIX_BAND}$ matrix template for cloning matrices needed

within the solver

Return value This returns 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 con-

sistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this

compatibility check.

Additionally, this routine will verify that the input matrix A is allocated with

appropriate upper bandwidth storage for the LU factorization.

Deprecated Name For backward compatibility, the wrapper function SUNBandLinearSolver with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_Band

The SUNLINSOL_BAND module defines band implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_Band
- SUNLinSolInitialize_Band this does nothing, since all consistency checks are performed at solver creation.
- ullet 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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

8.6.3 SUNLinearSolver_Band Fortran interfaces

The SUNLINSOL_BAND module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_band_mod FORTRAN module defines interfaces to all SUNLINSOL_BAND 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 SUNLinSol_Band is interfaced as FSUNLinSol_Band.

The FORTRAN 2003 SUNLINSOL_BAND interface module can be accessed with the use statement, i.e. use fsunlinsol_band_mod, and linking to the library libsundials_fsunlinsolband_mod.lib in addition to the C library. For details on where the library and module file fsunlinsol_band_mod.mod are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fsunlinsolband_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_BAND module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNBANDLINSOLINIT

Call FSUNBANDLINSOLINIT(code, ier)

Description The function FSUNBANDLINSOLINIT can be called for Fortran programs to create a band

SUNLinearSolver object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been

initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_BAND module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSBANDLINSOLINIT

Call FSUNMASSBANDLINSOLINIT(ier)

Description The function FSUNMASSBANDLINSOLINIT can be called for Fortran programs to create a

band SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called after both the NVECTOR and SUNMATRIX mass-matrix

objects have been initialized.

8.6.4 SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a SUNLinearSolver as the following structure:

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

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

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

8.7 The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LA-PACK. The SUNLINSOL_LAPACKDENSE module is designed to be used with the corresponding SUNMA-TRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKDENSE module, include the header file sunlinsol/sunlinsol_lapackdense.h. The installed module library to link to is libsundials_sunlinsollapackdense.lib where .lib is typically .so for shared libraries and .a for static libraries.

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



8.7.1 SUNLinearSolver_LapackDense description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting $(\mathcal{O}(N^3) \cos t)$, 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 $(\mathcal{O}(N^2) \text{ cost})$.

8.7.2 SUNLinearSolver_LapackDense functions

compatibility check.

The SUNLINSOL_LAPACKDENSE module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_LapackDense	
Call	LS = SUNLinSol_LapackDense(y, A);
Description	The function SUNLinSol_LapackDense creates and allocates memory for a LAPACK based, dense SUNLinearSolver object.
Arguments	<pre>y (N_Vector) a template for cloning vectors needed within the solver A (SUNMatrix) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver</pre>
Return value	This returns a ${\tt SUNLinearSolver}$ object. If either A or y are incompatible then this routine will return ${\tt NULL}$.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to

the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this

Deprecated Name For backward compatibility, the wrapper function SUNLapackDense with idential input and output arguments is also provided.

The SUNLINSOL_LAPACKDENSE module defines dense implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_LapackDense
- SUNLinSolInitialize_LapackDense this does nothing, since all consistency checks are performed at solver creation.
- ullet 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

8.7.3 SUNLinearSolver_LapackDense Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKDENSE module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNLAPACKDENSEINIT

Call FSUNLAPACKDENSEINIT(code, ier)

Description The function FSUNLAPACKDENSEINIT can be called for Fortran programs to create a LAPACK-based dense SUNLinearSolver object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKDENSE module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSLAPACKDENSEINIT

Call FSUNMASSLAPACKDENSEINIT(ier)

Description The function FSUNMASSLAPACKDENSEINIT can be called for Fortran programs to create a LAPACK-based, dense SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

8.7.4 SUNLinearSolver_LapackDense content

The SUNLINSOL_LAPACKDENSE module defines the *content* field of a SUNLinearSolver as the following structure:

8.8 The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LA-PACK. The SUNLINSOL_LAPACKBAND module is designed to be used with the corresponding SUNMA-TRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKBAND module, include the header file $sunlinsol/sunlinsol_lapackband.h$. The installed module library to link to is $libsundials_sunlinsollapackband.lib$ where .lib is typically .so for shared libraries and .a for static libraries.

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



8.8.1 SUNLinearSolver_LapackBand description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, PA = LU, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the pivots array.
- The "solve" call performs pivoting and forward and backward substitution using the stored pivots array and the LU factors held in the SUNMATRIX_BAND object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth mu and lower bandwidth ml, then the upper triangular factor U can have upper bandwidth as big as smu = MIN(N-1,mu+ml). The lower triangular factor L has lower bandwidth ml.



8.8.2 SUNLinearSolver_LapackBand functions

The SUNLINSOL_LAPACKBAND module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_LapackBand

Call LS = SUNLinSol_LapackBand(y, A);

Description The function SUNLinSol_LapackBand creates and allocates memory for a LAPACK-

based, band SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

A (SUNMatrix) a SUNMATRIX_BAND matrix template for cloning matrices needed

within the solver

Return value This returns 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 con-

sistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this

compatibility check.

Additionally, this routine will verify that the input matrix A is allocated with

appropriate upper bandwidth storage for the LU factorization.

Deprecated Name For backward compatibility, the wrapper function SUNLapackBand with idential

input and output arguments is also provided.

The SUNLINSOL_LAPACKBAND module defines band implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- 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.
- $\bullet \ {\tt SUNLinSolFree_LapackBand}$

8.8.3 SUNLinearSolver_LapackBand Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKBAND module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNLAPACKDENSEINIT

Call FSUNLAPACKBANDINIT(code, ier)

Description The function FSUNLAPACKBANDINIT can be called for Fortran programs to create a

LAPACK-based band SUNLinearSolver object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been

initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKBAND module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSLAPACKBANDINIT

Call FSUNMASSLAPACKBANDINIT(ier)

Description The function FSUNMASSLAPACKBANDINIT can be called for Fortran programs to create a

LAPACK-based, band SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called after both the NVECTOR and SUNMATRIX mass-matrix

objects have been initialized.

8.8.4 SUNLinearSolver_LapackBand content

The SUNLINSOL_LAPACKBAND module defines the *content* field of a SUNLinearSolver as the following structure:

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

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

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

8.9 The SUNLinearSolver_KLU implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with KLU. The SUNLINSOL_KLU module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

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

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 10]. In order to use the SUNLINSOL_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have realtype set to either extended or single (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available sunindextype options.



8.9.1 SUNLinearSolver_KLU description

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

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

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

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.
- On subsequent calls to the "setup" routine, it calls the appropriate KLU "refactor" routine, followed by estimates of the numerical conditioning using the relevant "rcond", and if necessary "condest", routine(s). If these estimates of the condition number are larger than $\varepsilon^{-2/3}$ (where ε is the double-precision unit roundoff), then a new factorization is performed.
- The module includes the routine SUNKLUReInit, that can be called by the user to force a full or partial refactorization at the next "setup" call.
- The "solve" call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.9.2 SUNLinearSolver_KLU functions

The SUNLINSOL_KLU module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_KLU

Call LS = SUNLinSol_KLU(y, A);

Description The function SUNLinSol_KLU creates and allocates memory for a KLU-based

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

A (SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver

Return value This returns 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 con-

sistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to

SUNDIALS, these will be included within this compatibility check.

Deprecated Name For backward compatibility, the wrapper function SUNKLU with idential input and

output arguments is also provided.

F2003 Name FSUNLinSol_KLU

The SUNLINSOL_KLU module defines implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- 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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_KLU module also defines the following additional user-callable functions.

SUNLinSol_KLUReInit

Call retval = SUNLinSol_KLUReInit(LS, A, nnz, reinit_type);

Description The function SUNLinSol_KLUReInit reinitializes memory and flags for a new fac-

torization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed or if the structure of the linear system has changed which would require a new symbolic

(and numeric factorization).

Arguments LS (SUNLinearSolver) a template for cloning vectors needed within the

solver

A (SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning ma-

trices needed within the solver

nnz (sunindextype) the new number of nonzeros in the matrix

reinit_type (int) flag governing the level of reinitialization. The allowed values

• SUNKLU_REINIT_FULL – The Jacobian matrix will be destroyed and a new one will be allocated based on the nnz value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.

• SUNKLU_REINIT_PARTIAL - Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of nnz given in the sparse matrix provided to the original constructor routine (or the previous SUNLinSol_KLUReInit call).

Return value The return values from this function are SUNLS_MEM_NULL (either S or A are NULL),

SUNLS_ILL_INPUT (A does not have type SUNMATRIX_SPARSE or reinit_type is invalid), SUNLS_MEM_FAIL (reallocation of the sparse matrix failed) or SUNLS_SUCCESS.

Notes This routine will perform consistency checks to ensure that it is called with con-

sistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to

SUNDIALS, these will be included within this compatibility check.

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

Deprecated Name For backward compatibility, the wrapper function SUNKLUReInit with idential in-

put and output arguments is also provided.

F2003 Name FSUNLinSol_KLUReInit

SUNLinSol_KLUSetOrdering

Call retval = SUNLinSol_KLUSetOrdering(LS, ordering);

Description This function sets the ordering used by KLU for reducing fill in the linear solve.

Arguments LS (SUNLinearSolver) the SUNLINSOL_KLU object

ordering (int) flag indicating the reordering algorithm to use, the options are:

0 AMD,

1 COLAMD, and

2 the natural ordering.

The default is 1 for COLAMD.

Return value The return values from this function are SUNLS_MEM_NULL (S is NULL),

SUNLS_ILL_INPUT (invalid ordering choice), or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNKLUSetOrdering with iden-

tial input and output arguments is also provided.

F2003 Name FSUNLinSol_KLUSetOrdering

8.9.3 SUNLinearSolver_KLU Fortran interfaces

The SUNLINSOL_KLU module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_klu_mod FORTRAN module defines interfaces to all SUNLINSOL_KLU 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 SUNLinSol_klu is interfaced as FSUNLinSol_klu.

The FORTRAN 2003 SUNLINSOL_KLU interface module can be accessed with the use statement, i.e. use fsunlinsol_klu_mod, and linking to the library libsundials_fsunlinsolklu_mod.lib in addition to the C library. For details on where the library and module file fsunlinsol_klu_mod.mod are installed see Appendix A.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_KLU module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNKLUINIT

Call FSUNKLUINIT(code, ier)

Description The function FSUNKLUINIT can be called for Fortran programs to create a SUNLIN-

SOL_KLU object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been

initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_KLU module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSKLUINIT

Call FSUNMASSKLUINIT(ier)

Description The function FSUNMASSKLUINIT can be called for Fortran programs to create a KLU-

based SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called after both the NVECTOR and SUNMATRIX mass-matrix

objects have been initialized.

The SUNLinSol_KLUReInit and SUNLinSol_KLUSetOrdering routines also support FORTRAN interfaces for the system and mass matrix solvers:

FSUNKLUREINIT

Call FSUNKLUREINIT(code, nnz, reinit_type, ier)

Description The function FSUNKLUREINIT can be called for Fortran programs to re-initialize a SUN-

LINSOL_KLU object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA,

3 for KINSOL, and 4 for ARKODE).

nnz (sunindextype*) the new number of nonzeros in the matrix

reinit_type (int*) flag governing 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 SUNLinSol_KLUReInit call).

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_KLUReInit for complete further documentation of this routine.

FSUNMASSKLUREINIT

Call FSUNMASSKLUREINIT(nnz, reinit_type, ier)

Description The function FSUNMASSKLUREINIT can be called for Fortran programs to re-initialize a

SUNLINSOL_KLU object for mass matrix linear systems.

Arguments The arguments are identical to FSUNKLUREINIT above, except that code is not needed

since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_KLUReInit for complete further documentation of this routine.

FSUNKLUSETORDERING

Call FSUNKLUSETORDERING(code, ordering, ier)

Description The function FSUNKLUSETORDERING can be called for Fortran programs to change the

reordering algorithm used by KLU.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

ordering (int*) flag indication the reordering algorithm to use. Options include:

0 AMD.

1 COLAMD, and

2 the natural ordering.

The default is 1 for COLAMD.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_KLUSetOrdering for complete further documentation of this routine.

FSUNMASSKLUSETORDERING

Call FSUNMASSKLUSETORDERING(ier)

Description The function FSUNMASSKLUSETORDERING can be called for Fortran programs to change

the reordering algorithm used by KLU for mass matrix linear systems.

Arguments The arguments are identical to FSUNKLUSETORDERING above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_KLUSetOrdering for complete further documentation of this routine.

8.9.4 SUNLinearSolver_KLU content

The SUNLINSOL_KLU module defines the content field of a SUNLinearSolver as the following structure:

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

first_factorize - flag indicating whether the factorization has ever been performed,

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

common - storage structure for common KLU solver components,

klu_solver - pointer to the appropriate KLU solver function (depending on whether it is using

a CSR or CSC sparse matrix).

8.10 The SUNLinearSolver_SuperLUDIST implementation

The SuperLU_DIST implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SUPERLUDIST, is designed to be used with the corresponding SUNMATRIX_SLUNRLOC matrix type, and one of the serial, threaded or parallel NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, NVECTOR_PTHREADS, NVECTOR_PARALLEL, or NVECTOR_PARHYP).

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

8.10.1 SUNLinearSolver_SuperLUDIST description

The SUNLINSOL_SUPERLUDIST module is a SUNLINSOL adapter for the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li [2, 17, 25, 26]. The package uses a SPMD parallel programming model and multithreading to enhance efficiency in distributed-memory parallel environments with multicore nodes and possibly GPU accelerators. It uses MPI for communication, OpenMP for threading, and CUDA for GPU support. In order to use the SUNLINSOL_SUPERLUDIST interface to SuperLU_DIST, it is assumed that SuperLU_DIST has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SuperLU_DIST (see Appendix A for details). Additionally, the adapter 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 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.

8.10.2 SUNLinearSolver_SuperLUDIST functions

The SUNLINSOL_SUPERLUDIST module defines implementations of all "direct" linear solver operations listed in Sections 8.1.1-8.1.3:

- 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
- SUNLinSolve_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

SUNLinSol_SuperLUDIST

In addition, the module SUNLINSOL_SUPERLUDIST provides the following user-callable routines:

```
Call
            LS = SUNLinSol_SuperLUDIST(y, A, grid, lu, scaleperm, solve, stat, options);
            The function SUNLinSol_SuperLUDIST creates and allocates memory for a SUNLIN-
Description
            SOL_SUPERLUDIST object.
Arguments
                     (N_Vector) a template for cloning vectors needed within the solver
            У
                     (SUNMatrix) a SUNMATRIX_SLUNRLOC matrix template for cloning matrices
            Α
                     needed within the solver
                     (gridinfo_t*)
            grid
                     (LUstruct_t*)
            scaleperm (ScalePermstruct_t*)
            solve
                     (SOLVEstruct_t*)
                     (SuperLUStat_t*)
            stat
```

Return value This returns a SUNLinearSolver object. If either A or y are incompatible then this routine will return NULL.

options (superlu_dist_options_t*)

Notes This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SuperLU_DIST library.

This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SLUNRLOC matrix type and the NVECTOR_SERIAL, NVECTOR_PARALLEL,

NVECTOR_PARHYP, 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 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 SUNLIN-SOL_SUPERLUDIST solver. Specifically the member Fact, is modified in the setup and solve routines.

SUNLinSol_SuperLUDIST_GetBerr

Call realtype berr = SUNLinSol_SuperLUDIST_GetBerr(LS);

Description The function SUNLinSol_SuperLUDIST_GetBerr returns the componentwise relative back-

ward error of the computed solution.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value realtype

Notes

SUNLinSol_SuperLUDIST_GetGridinfo

Call gridinfo_t *grid = SUNLinSol_SuperLUDIST_GetGridinfo(LS);

Description The function SUNLinSol_SuperLUDIST_GetGridinfo returns the SuperLU_DIST struc-

ture that contains the 2D process grid.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value gridinfo_t*

Notes

SUNLinSol_SuperLUDIST_GetLUstruct

Call LUstruct_t *lu = SUNLinSol_SuperLUDIST_GetLUstruct(LS);

Description The function SUNLinSol_SuperLUDIST_GetLUstruct returns the SuperLU_DIST struc-

ture that contains the distributed L and U factors.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value LUstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSuperLUOptions

Call superlu_dist_options_t *opts = SUNLinSol_SuperLUDIST_GetSuperLUOptions(LS);

Description The function SUNLinSol_SuperLUDIST_GetSuperLUOptions returns the SuperLU_DIST

structure that contains the options which control how the linear system is factorized

and solved.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value superlu_dist_options_t*

Notes

SUNLinSol_SuperLUDIST_GetScalePermstruct

```
Call ScalePermstruct_t *sp = SUNLinSol_SuperLUDIST_GetScalePermstruct(LS);
```

structure that contains the vectors that describe the transformations done to the matrix,

A.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value ScalePermstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSOLVEstruct

```
Call SOLVEstruct_t *solve = SUNLinSol_SuperLUDIST_GetSOLVEstruct(LS);
```

Description The function SUNLinSol_SuperLUDIST_GetSOLVEstruct returns the SuperLU_DIST struc-

ture that contains information for communication during the solution phase.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value SOLVEstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSuperLUStat

```
Call SuperLUStat_t *stat = SUNLinSol_SuperLUDIST_GetSuperLUStat(LS);
```

Description The function SUNLinSol_SuperLUDIST_GetSuperLUStat returns the SuperLU_DIST struc-

ture that stores information about runtime and flop count.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value SuperLUStat_t*

Notes

8.10.3 SUNLinearSolver_SuperLUDIST content

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

```
struct _SUNLinearSolverContent_SuperLUDIST {
  booleantype
                          first_factorize;
  long int
                          last_flag;
  realtype
                          berr;
  gridinfo_t
                          *grid;
  LUstruct_t
                          *lu;
  superlu_dist_options_t *options;
  ScalePermstruct_t
                          *scaleperm;
  SOLVEstruct_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,

 ${\bf last_flag}$ - last error return flag from calls to internal routines,

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,

options - pointer to SuperLU_DIST options structure,

scaleperm - pointer to the SuperLU_DIST structure that stores vectors describing the transformations done to the matrix, A,

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

8.11 The SUNLinearSolver_SuperLUMT implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with SuperLU_MT. The SUPERLUMT module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). While these are compatible, it is not recommended to use a threaded vector module with SUNLINSOL_SUPERLUMT unless it is the NVECTOR_OPENMP module and the SUPERLUMT library has also been compiled with OpenMP.

The header file to include 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 SUNLINSOL_SUPERLUMT module is a SUNLINSOL wrapper for the SUPERLUMT sparse matrix factorization and solver library written by X. Sherry Li [3, 24, 12]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step. In order to use the SUNLINSOL_SUPERLUMT interface to SUPERLUMT, it is assumed that SUPERLUMT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SUPERLUMT (see Appendix A for details). Additionally, this wrapper only supports single- and double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have realtype set to extended (see Section 4.2). Moreover, since the SUPERLUMT library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SUPERLUMT library is installed using the same integer precision as the SUNDIALS sunindextype option.



8.11.1 SUNLinearSolver_SuperLUMT description

The SUPERLUMT library has a symbolic factorization routine that computes the permutation of the linear system matrix to reduce fill-in on subsequent LU factorizations (using COLAMD, minimal degree ordering on $A^T * A$, minimal degree ordering on $A^T + A$, or natural ordering). Of these ordering choices, the default value in the SUNLINSOL_SUPERLUMT module is the COLAMD ordering.

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

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.
- On subsequent calls to the "setup" routine, it skips the symbolic factorization, and only refactors the input matrix.
- The "solve" call performs pivoting and forward and backward substitution using the stored SUPERLUMT data structures. We note that in this solve SUPERLUMT operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.11.2 SUNLinearSolver_SuperLUMT functions

The module SUNLINSOL_SUPERLUMT provides the following user-callable constructor for creating a SUNLinearSolver object.

|SUNLinSol_SuperLUMT

Call LS = SUNLinSol_SuperLUMT(y, A, num_threads);

Description The function SUNLinSol_SuperLUMT creates and allocates memory for a

SuperLU_MT-based SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

A (SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning ma-

trices needed within the solver

num_threads (int) desired number of threads (OpenMP or Pthreads, depending

on how SUPERLUMT was installed) to use during the factorization

steps

Return value This returns a SUNLinearSolver object. If either A or y are incompatible then 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 SUPERLUMT library.

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

The num_threads argument is not checked and is passed directly to SUPERLUMT routines.

Deprecated Name For backward compatibility, the wrapper function SUNSuperLUMT with idential input and output arguments is also provided.

The SUNLINSOL_SUPERLUMT module defines implementations of all "direct" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_SuperLUMT
- SUNLinSolInitialize_SuperLUMT this sets the first_factorize flag to 1 and resets the internal SUPERLUMT statistics variables.
- SUNLinSolSetup_SuperLUMT this performs either a *LU* factorization or refactorization of the input matrix.
- SUNLinSolSolve_SuperLUMT this calls the appropriate SUPERLUMT solve routine to utilize the *LU* factors to solve the linear system.
- SUNLinSolLastFlag_SuperLUMT
- SUNLinSolSpace_SuperLUMT this only returns information for the storage within the solver *interface*, i.e. storage for the integers last_flag and first_factorize. For additional space requirements, see the SUPERLUMT documentation.
- SUNLinSolFree_SuperLUMT

The SUNLINSOL_SUPERLUMT module also defines the following additional user-callable function.

SUNLinSol_SuperLUMTSetOrdering

Call retval = SUNLinSol_SuperLUMTSetOrdering(LS, ordering);

Description This function sets the ordering used by SUPERLUMT for reducing fill in the linear

solve.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SUPERLUMT object

ordering (int) a flag indicating the ordering algorithm to use, the options are:

0 natural ordering

1 minimal degree ordering on $A^T A$ 2 minimal degree ordering on $A^T + A$

3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

Return value The return values from this function are SUNLS_MEM_NULL (S is NULL),

SUNLS_ILL_INPUT (invalid ordering choice), or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSuperLUMTSetOrdering with

idential input and output arguments is also provided.

8.11.3 SUNLinearSolver_SuperLUMT Fortran interfaces

For solvers that include a Fortran interface module, the SUNLINSOL_SUPERLUMT module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNSUPERLUMTINIT

Call FSUNSUPERLUMTINIT(code, num_threads, ier)

Description The function FSUNSUPERLUMTINIT can be called for Fortran programs to create a SUN-

LINSOL_KLU object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA,

3 for KINSOL, and 4 for ARKODE).

 $\verb"num_threads" (int*) desired number of threads (OpenMP or Pthreads, depending on$

how SUPERLUMT was installed) to use during the factorization steps

Return value \mathtt{ier} is a return completion flag equal to 0 for a success return and $\mathtt{-1}$ otherwise. See

printed message for details in case of failure.

Notes This routine must be called after both the NVECTOR and SUNMATRIX objects have been

initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SUPERLUMT module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSSUPERLUMTINIT

Call FSUNMASSSUPERLUMTINIT(num_threads, ier)

Description The function FSUNMASSSUPERLUMTINIT can be called for Fortran programs to create a

SuperLU_MT-based SUNLinearSolver object for mass matrix linear systems.

Arguments num_threads (int*) desired number of threads (OpenMP or Pthreads, depending on

how superlumt was installed) to use during the factorization steps.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called after both the NVECTOR and SUNMATRIX mass-matrix

objects have been initialized.

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

FSUNSUPERLUMTSETORDERING

Call FSUNSUPERLUMTSETORDERING(code, ordering, ier)

 $\label{thm:constraint} \textbf{Description} \quad \text{The function } \textbf{FSUNSUPERLUMTSETORDERING} \ \text{can be called for Fortran programs to update}$

the ordering algorithm in a SUNLINSOL_SUPERLUMT object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

ordering (int*) a flag indicating the ordering algorithm, options are:

0 natural ordering

1 minimal degree ordering on A^TA

2 minimal degree ordering on $A^T + A$

3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SuperLUMTSetOrdering for complete further documentation of this rou-

tine.

FSUNMASSUPERLUMTSETORDERING

Call FSUNMASSUPERLUMTSETORDERING(ordering, ier)

Description The function FSUNMASSUPERLUMTSETORDERING can be called for Fortran programs to

 $update\ the\ ordering\ algorithm\ in\ a\ {\tt SUNLINSOL_SUPERLUMT}\ object\ for\ mass\ matrix\ linear$

systems.

Arguments ordering (int*) a flag indicating the ordering algorithm, options are:

0 natural ordering

1 minimal degree ordering on A^TA

2 minimal degree ordering on $A^T + A$

3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SuperLUMTSetOrdering for complete further documentation of this rou-

tine.

8.11.4 SUNLinearSolver_SuperLUMT content

The SUNLINSOL_SUPERLUMT module defines the *content* field of a SUNLinearSolver as the following structure:

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

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

last_flag - last error return flag from internal function evaluations,

first_factorize - flag indicating whether the factorization has ever been performed,

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

Gstat - GStat_t object used in solve,

perm_r, perm_c - permutation arrays used in solve,

N - size of the linear system,

num_threads - number of OpenMP/Pthreads threads to use,

diag_pivot_thresh - threshold on diagonal pivoting,

ordering - flag for which reordering algorithm to use,
options - pointer to SUPERLUMT options structure.

8.12 The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [31]) iterative linear solver. The SUNLINSOL_SPGMR module is designed to be compatible with any NVECTOR 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). When using Classical Gram-Schmidt, the optional function N_VDotProdMulti may be supplied for increased efficiency.

To access the SUNLINSOL_SPGMR module, include the header file sunlinsol/sunlinsol_spgmr.h. We note that the SUNLINSOL_SPGMR module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolspgmr module library.

8.12.1 SUNLinearSolver_SPGMR description

This solver is constructed to perform the following operations:

- During construction, the xcor and vtemp arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPGMR to supply the ATimes, PSetup, and Psolve function pointers and s1 and s2 scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (V, Hes, givens, and yg)
- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the GMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

8.12.2 SUNLinearSolver_SPGMR functions

The SUNLINSOL_SPGMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPGMR

Return value

Notes

Call LS = SUNLinSol_SPGMR(y, pretype, maxl);

Description The function SUNLinSol_SPGMR creates and allocates memory for a SPGMR

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

 ${\tt pretype}$ (int) flag indicating the desired type of preconditioning, allowed values

are:

- PREC_NONE (0)
- PREC_LEFT (1)
- PREC_RIGHT (2)
- PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

maxl (int) the number of Krylov basis vectors to use. Values ≤ 0 will result in the default value (5).

This returns a SUNLinearSolver object. If either y is incompatible then this

routine will return NULL.

This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations).

If y is incompatible, then this routine will return NULL.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPGMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result

in inferior performance.

Deprecated Name For backward compatibility, the wrapper function SUNSPGMR with idential input

and output arguments is also provided.

F2003 Name FSUNLinSol_SPGMR

The SUNLINSOL_SPGMR module defines implementations of all "iterative" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_SPGMR
- SUNLinSolInitialize_SPGMR
- SUNLinSolSetATimes_SPGMR
- SUNLinSolSetPreconditioner_SPGMR
- $\bullet \ {\tt SUNLinSolSetScalingVectors_SPGMR}$
- SUNLinSolSetup_SPGMR
- SUNLinSolSolve_SPGMR
- SUNLinSolNumIters_SPGMR
- SUNLinSolResNorm_SPGMR
- SUNLinSolResid_SPGMR
- SUNLinSolLastFlag_SPGMR
- SUNLinSolSpace_SPGMR

• SUNLinSolFree_SPGMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPGMR module also defines the following additional user-callable functions.

SUNLinSol_SPGMRSetPrecType

Call retval = SUNLinSol_SPGMRSetPrecType(LS, pretype);

Description The function SUNLinSol_SPGMRSetPrecType updates the type of preconditioning

to use in the SUNLINSOL_SPGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPGMR object to update

pretype (int) flag indicating the desired type of preconditioning, allowed values

match those discussed in SUNLinSol_SPGMR.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPGMRSetPrecType with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPGMRSetPrecType

SUNLinSol_SPGMRSetGSType

Call retval = SUNLinSol_SPGMRSetGSType(LS, gstype);

Description The function SUNLinSol_SPGMRSetPrecType sets the type of Gram-Schmidt or-

thogonalization to use in the SUNLINSOL_SPGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPGMR object to update

gstype (int) flag indicating the desired orthogonalization algorithm; allowed val-

ues are:

• MODIFIED_GS (1)

• CLASSICAL_GS (2)

Any other integer input will result in a failure, returning error code

SUNLS_ILL_INPUT.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPGMRSetGSType with iden-

tial input and output arguments is also provided.

F2003 Name FSUNLinSol_SPGMRSetGSType

SUNLinSol_SPGMRSetMaxRestarts

Call retval = SUNLinSol_SPGMRSetMaxRestarts(LS, maxrs);

Description The function SUNLinSol_SPGMRSetMaxRestarts sets the number of GMRES restarts

to allow in the SUNLINSOL_SPGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPGMR object to update

maxrs (int) integer indicating number of restarts to allow. A negative input will

result in the default of 0.

Return value This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or

SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPGMRSetMaxRestarts with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPGMRSetMaxRestarts

8.12.3 SUNLinearSolver SPGMR Fortran interfaces

The SUNLINSOL_SPGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_spgmr_mod FORTRAN module defines interfaces to all SUNLINSOL_SPGMR 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 SUNLinSol_SPGMR is interfaced as FSUNLinSol_SPGMR.

The Fortran 2003 sunlinsol_spgmr_mod, and linking to the library libsundials_fsunlinsolspgmr_mod.lib in addition to the C library. For details on where the library and module file fsunlinsol_spgmr_mod.mod are installed see Appendix A. We note that the module is accessible from the Fortran 2003 sundials integrators without separately linking to the libsundials_fsunlinsolspgmr_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPGMR module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNSPGMRINIT

Call FSUNSPGMRINIT(code, pretype, maxl, ier)

Description The function FSUNSPGMRINIT can be called for Fortran programs to create a SUNLIN-

SOL_SPGMR object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating Krylov subspace size

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPGMR.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPGMR module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSSPGMRINIT

Call FSUNMASSSPGMRINIT(pretype, maxl, ier)

Description The function FSUNMASSSPGMRINIT can be called for Fortran programs to create a SUN-

LINSOL_SPGMR object for mass matrix linear systems.

Arguments pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating Krylov subspace size

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPGMR.

The SUNLinSol_SPGMRSetPrecType, SUNLinSol_SPGMRSetGSType and

SUNLinSol_SPGMRSetMaxRestarts routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPGMRSETGSTYPE

Call FSUNSPGMRSETGSTYPE(code, gstype, ier)

Description The function FSUNSPGMRSETGSTYPE can be called for Fortran programs to change the

Gram-Schmidt orthogonaliation algorithm.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

gstype (int*) flag indicating the desired orthogonalization algorithm.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetGSType for complete further documentation of this routine.

FSUNMASSSPGMRSETGSTYPE

Call FSUNMASSSPGMRSETGSTYPE(gstype, ier)

Description The function FSUNMASSSPGMRSETGSTYPE can be called for Fortran programs to change

the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPGMRSETGSTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetGSType for complete further documentation of this routine.

FSUNSPGMRSETPRECTYPE

Call FSUNSPGMRSETPRECTYPE(code, pretype, ier)

Description The function FSUNSPGMRSETPRECTYPE can be called for Fortran programs to change the

type of preconditioning to use.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating the type of preconditioning to use.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetPrecType for complete further documentation of this routine.

FSUNMASSSPGMRSETPRECTYPE

Call FSUNMASSSPGMRSETPRECTYPE(pretype, ier)

Description The function FSUNMASSSPGMRSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPGMRSETPRECTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetPrecType for complete further documentation of this routine.

FSUNSPGMRSETMAXRS

Call FSUNSPGMRSETMAXRS(code, maxrs, ier)

Description The function FSUNSPGMRSETMAXRS can be called for Fortran programs to change the

maximum number of restarts allowed for SPGMR.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

maxrs (int*) maximum allowed number of restarts.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetMaxRestarts for complete further documentation of this rou-

tine.

FSUNMASSSPGMRSETMAXRS

Call FSUNMASSSPGMRSETMAXRS(maxrs, ier)

Description The function FSUNMASSSPGMRSETMAXRS can be called for Fortran programs to change

the maximum number of restarts allowed for SPGMR for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPGMRSETMAXRS above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPGMRSetMaxRestarts for complete further documentation of this rou-

tine.

8.12.4 SUNLinearSolver_SPGMR content

The $\mathtt{SUNLINSOL_SPGMR}$ module defines the content field of a $\mathtt{SUNLinearSolver}$ as the following structure:

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

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

- number of GMRES basis vectors to use (default is 5),

- flag for type of preconditioning to employ (default is none),

gstype - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

 ${\tt max_restarts}$ - number of GMRES restarts to allow (default is 0),

 ${\tt numiters} \qquad {\tt -number\ of\ iterations\ from\ the\ most-recent\ solve},$

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,

 v_i is a vector of type NVECTOR.,

Hes - the $(\max 1 + 1) \times \max 1$ Hessenberg matrix. It is stored row-wise so that the (i,j)th

element is given by Hes[i][j].,

 ${\tt givens} \qquad {\tt -a \ length \ 2*maxl \ array \ which \ represents \ the \ Givens \ rotation \ matrices \ that \ arise \ in \ the}$

GMRES algorithm. These matrices are F_0, F_1, \ldots, F_j , where

are represented in the givens vector as givens [0] = c_0 , givens [1] = s_0 , givens [2]

= c_1 , givens[3] = s_1 , ... givens[2j] = c_j , givens[2j+1] = s_j .,

xcor - a vector which holds the scaled, preconditioned correction to the initial guess,

yg - a length (maxl+1) array of realtype values used to hold "short" vectors (e.g. y and

g),

vtemp - temporary vector storage.

8.13 The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [30]) iterative linear solver. The SUNLINSOL_SPFGMR module is designed to be compatible with any NVECTOR 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). When using Classical Gram-Schmidt, the optional function N_VDotProdMulti may be supplied for increased efficiency. Unlike the other Krylov iterative linear solvers supplied with SUNDIALS, SPFGMR is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

To access the SUNLINSOL_SPFGMR module, include the header file sunlinsol/sunlinsol_spfgmr.h. We note that the SUNLINSOL_SPFGMR module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolspfgmr module library.

8.13.1 SUNLinearSolver_SPFGMR description

This solver is constructed to perform the following operations:

- During construction, the xcor and vtemp arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPFGMR to supply the ATimes, PSetup, and Psolve function pointers and s1 and s2 scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (V, Hes, givens, and yg)
- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

SUNLinear Solver SPFGMR functions 8.13.2

The SUNLINSOL_SPFGMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPFGMR

Notes

Call LS = SUNLinSol_SPFGMR(y, pretype, maxl);

Description The function SUNLinSol_SPFGMR creates and allocates memory for a SPFGMR

SUNLinearSolver object.

Arguments (N_Vector) a template for cloning vectors needed within the solver

pretype (int) flag indicating the desired type of preconditioning, allowed values are:

- PREC_NONE (0)
- PREC_LEFT (1)
- PREC_RIGHT (2)
- PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

maxl (int) the number of Krylov basis vectors to use. Values < 0 will result in the default value (5).

Return value This returns a SUNLinearSolver object. If either y is incompatible then this routine will return NULL.

> This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPFGMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

F2003 Name FSUNLinSol_SPFGMR

SUNSPFGMR The SUNLINSOL_SPFGMR module defines implementations of all "iterative" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_SPFGMR
- SUNLinSolInitialize_SPFGMR
- SUNLinSolSetATimes_SPFGMR
- SUNLinSolSetPreconditioner_SPFGMR
- SUNLinSolSetScalingVectors_SPFGMR
- SUNLinSolSetup_SPFGMR
- SUNLinSolSolve_SPFGMR
- SUNLinSolNumIters_SPFGMR
- SUNLinSolResNorm_SPFGMR
- SUNLinSolResid_SPFGMR
- SUNLinSolLastFlag_SPFGMR
- SUNLinSolSpace_SPFGMR
- SUNLinSolFree_SPFGMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPFGMR module also defines the following additional user-callable functions.

SUNLinSol_SPFGMRSetPrecType

Call retval = SUNLinSol_SPFGMRSetPrecType(LS, pretype);

Description The function SUNLinSol_SPFGMRSetPrecType updates the type of preconditioning

to use in the SUNLINSOL_SPFGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPFGMR object to update

pretype (int) flag indicating the desired type of preconditioning, allowed values

match those discussed in SUNLinSol_SPFGMR.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPFGMRSetPrecType with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPFGMRSetPrecType

SUNLinSol_SPFGMRSetGSType

Call retval = SUNLinSol_SPFGMRSetGSType(LS, gstype);

Description The function SUNLinSol_SPFGMRSetPrecType sets the type of Gram-Schmidt or-

thogonalization to use in the SUNLINSOL_SPFGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPFGMR object to update

gstype (int) flag indicating the desired orthogonalization algorithm; allowed values are:

• MODIFIED_GS (1)

• CLASSICAL_GS (2)

Any other integer input will result in a failure, returning error code SUNLS_ILL_INPUT.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPFGMRSetGSType with iden-

tial input and output arguments is also provided.

F2003 Name FSUNLinSol_SPFGMRSetGSType

|SUNLinSol_SPFGMRSetMaxRestarts

Call retval = SUNLinSol_SPFGMRSetMaxRestarts(LS, maxrs);

Description The function SUNLinSol_SPFGMRSetMaxRestarts sets the number of GMRES

restarts to allow in the SUNLINSOL_SPFGMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPFGMR object to update

maxrs (int) integer indicating number of restarts to allow. A negative input will

result in the default of 0.

Return value This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or

SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPFGMRSetMaxRestarts with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPFGMRSetMaxRestarts

8.13.3 SUNLinearSolver_SPFGMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_spfgmr_mod FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR 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 SUNLinSol_SPFGMR is interfaced as FSUNLinSol_SPFGMR.

The FORTRAN 2003 SUNLINSOL_SPFGMR interface module can be accessed with the use statement, i.e. use fsunlinsol_spfgmr_mod, and linking to the library libsundials_fsunlinsolspfgmr_mod.lib in addition to the C library. For details on where the library and module file

fsunlinsol_spfgmr_mod.mod are installed see Appendix A. We note that the module is accessible from the Fortran 2003 sundials integrators without separately linking to the libsundials_fsunlinsolspfgmr_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPFGMR module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNSPFGMRINIT

Call FSUNSPFGMRINIT(code, pretype, maxl, ier)

Description The function FSUNSPFGMRINIT can be called for Fortran programs to create a SUNLIN-

SOL_SPFGMR object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating Krylov subspace size

Return value \mathtt{ier} is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called after the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPFGMR.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPFGMR module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSSPFGMRINIT

Call FSUNMASSSPFGMRINIT(pretype, maxl, ier)

Description The function FSUNMASSSPFGMRINIT can be called for Fortran programs to create a SUN-

LINSOL_SPFGMR object for mass matrix linear systems.

Arguments pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating Krylov subspace size

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPFGMR.

The SUNLinSol_SPFGMRSetPrecType, SUNLinSol_SPFGMRSetGSType and

SUNLinSol_SPFGMRSetMaxRestarts routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPFGMRSETGSTYPE

Call FSUNSPFGMRSETGSTYPE(code, gstype, ier)

Description The function FSUNSPFGMRSETGSTYPE can be called for Fortran programs to change the

Gram-Schmidt orthogonaliation algorithm.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

gstype (int*) flag indicating the desired orthogonalization algorithm.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetGSType for complete further documentation of this routine.

FSUNMASSSPFGMRSETGSTYPE

Call FSUNMASSSPFGMRSETGSTYPE(gstype, ier)

Description The function FSUNMASSSPFGMRSETGSTYPE can be called for Fortran programs to change

the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPFGMRSETGSTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetGSType for complete further documentation of this routine.

FSUNSPFGMRSETPRECTYPE

Call FSUNSPFGMRSETPRECTYPE(code, pretype, ier)

Description The function FSUNSPFGMRSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning to use.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating the type of preconditioning to use.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetPrecType for complete further documentation of this routine.

FSUNMASSSPFGMRSETPRECTYPE

Call FSUNMASSSPFGMRSETPRECTYPE(pretype, ier)

Description The function FSUNMASSSPFGMRSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPFGMRSETPRECTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetPrecType for complete further documentation of this routine.

FSUNSPFGMRSETMAXRS

Call FSUNSPFGMRSETMAXRS(code, maxrs, ier)

Description The function FSUNSPFGMRSETMAXRS can be called for Fortran programs to change the

maximum number of restarts allowed for SPFGMR.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

maxrs (int*) maximum allowed number of restarts.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetMaxRestarts for complete further documentation of this rou-

tine.

FSUNMASSSPFGMRSETMAXRS

Call FSUNMASSSPFGMRSETMAXRS(maxrs, ier)

Description The function FSUNMASSSPFGMRSETMAXRS can be called for Fortran programs to change

the maximum number of restarts allowed for SPFGMR for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPFGMRSETMAXRS above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPFGMRSetMaxRestarts for complete further documentation of this rou-

tine.

8.13.4 SUNLinearSolver_SPFGMR content

The SUNLINSOL_SPFGMR module defines the *content* field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_SPFGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector *V;
  N_Vector *Z;
  realtype **Hes;
  realtype *givens;
  N_Vector xcor;
  realtype *yg;
  N_Vector vtemp;
};
These entries of the content field contain the following information:
               - number of FGMRES basis vectors to use (default is 5),
maxl
pretype
               - flag for type of preconditioning to employ (default is none),
              - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),
gstype
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,
              - function pointer to preconditioner setup routine,
Psetup
Psolve
              - function pointer to preconditioner solve routine,
PData
              - pointer to structure for Psetup and Psolve,
               - vector pointers for supplied scaling matrices (default is NULL),
s1, s2
V
               - the array of Krylov basis vectors v_1, \ldots, v_{\mathtt{maxl}+1}, stored in V[0], \ldots, V[\mathtt{maxl}]. Each
               v_i is a vector of type NVECTOR.,
Z
               - the array of preconditioned Krylov basis vectors z_1, \ldots, z_{\max 1+1}, stored in Z[0], \ldots
               Z[max1]. Each z_i is a vector of type NVECTOR.,
               - the (maxl + 1) × maxl Hessenberg matrix. It is stored row-wise so that the (i,j)th
Hes
               element is given by Hes[i][j].,
```

givens

- a length 2*maxl array which represents the Givens rotation matrices that arise in the FGMRES algorithm. These matrices are F_0, F_1, \ldots, F_j , where

are represented in the givens vector as givens [0] = c_0 , givens [1] = s_0 , givens [2]

= c_1 , givens[3] = s_1 , ... givens[2j] = c_j , givens[2j+1] = s_j .

xcor - a vector which holds the scaled, preconditioned correction to the initial guess,

yg - a length (maxl+1) array of realtype values used to hold "short" vectors (e.g. y and g),

vtemp - temporary vector storage.

8.14 The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [32]) iterative linear solver. The SUNLINSOL_SPBCGS module is designed to be compatible with any NVECTOR 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.

To access the SUNLINSOL_SPBCGS module, include the header file sunlinsol/sunlinsol_spbcgs.h. We note that the SUNLINSOL_SPBCGS module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolspbcgs module library.

8.14.1 SUNLinearSolver_SPBCGS description

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPBCGS to supply the ATimes, PSetup, and Psolve function pointers and s1 and s2 scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the SPBCGS iteration is performed. This will include scaling and preconditioning if those options have been supplied.

8.14.2 SUNLinearSolver_SPBCGS functions

The SUNLINSOL_SPBCGS module provides the following user-callable constructor for creating a SUNLinearSolver object.

Notes

SUNLinSol_SPBCGS

Call LS = SUNLinSol_SPBCGS(y, pretype, maxl);

Description The function SUNLinSol_SPBCGS creates and allocates memory for a SPBCGS

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

pretype (int) flag indicating the desired type of preconditioning, allowed values

are:

• PREC_NONE (0)

• PREC_LEFT (1)

• PREC_RIGHT (2)

• PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

maxl (int) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value This returns a SUNLinearSolver object. If either y is incompatible then this

routine will return NULL.

This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations).

If y is incompatible, then this routine will return NULL.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPBCGS object to use any of the preconditioning options with these solvers, this use mode is not supported and may result

 $in\ inferior\ performance.$

Deprecated Name For backward compatibility, the wrapper function SUNSPBCGS with idential input

and output arguments is also provided.

F2003 Name FSUNLinSol_SPBCGS

The SUNLINSOL_SPBCGS module defines implementations of all "iterative" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_SPBCGS
- SUNLinSolInitialize_SPBCGS
- SUNLinSolSetATimes_SPBCGS
- SUNLinSolSetPreconditioner_SPBCGS
- SUNLinSolSetScalingVectors_SPBCGS
- SUNLinSolSetup_SPBCGS
- SUNLinSolSolve_SPBCGS
- SUNLinSolNumIters_SPBCGS
- SUNLinSolResNorm_SPBCGS
- SUNLinSolResid_SPBCGS
- $\bullet \ {\tt SUNLinSolLastFlag_SPBCGS} \\$
- SUNLinSolSpace_SPBCGS

• SUNLinSolFree_SPBCGS

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPBCGS module also defines the following additional user-callable functions.

SUNLinSol_SPBCGSSetPrecType

Call retval = SUNLinSol_SPBCGSSetPrecType(LS, pretype);

Description The function SUNLinSol_SPBCGSSetPrecType updates the type of preconditioning

to use in the SUNLINSOL_SPBCGS object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPBCGS object to update

pretype (int) flag indicating the desired type of preconditioning, allowed values

match those discussed in SUNLinSol_SPBCGS.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPBCGSSetPrecType with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPBCGSSetPrecType

SUNLinSol_SPBCGSSetMaxl

Call retval = SUNLinSol_SPBCGSSetMaxl(LS, maxl);

Description The function SUNLinSol_SPBCGSSetMaxl updates the number of linear solver iter-

ations to allow.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPBCGS object to update

max1 (int) flag indicating the number of iterations to allow. Values ≤ 0 will result

in the default value (5).

Return value This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or

SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPBCGSSetMax1 with idential

input and output arguments is also provided.

F2003 Name FSUNLinSol_SPBCGSSetMaxl

8.14.3 SUNLinearSolver_SPBCGS Fortran interfaces

The SUNLINSOL_SPBCGS module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_spbcgs_mod FORTRAN module defines interfaces to all SUNLINSOL_SPBCGS 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 SUNLinSol_SPBCGS is interfaced as FSUNLinSol_SPBCGS.

The FORTRAN 2003 SUNLINSOL_SPBCGS interface module can be accessed with the use statement, i.e. use fsunlinsol_spbcgs_mod, and linking to the library libsundials_fsunlinsolspbcgs_mod.lib in addition to the C library. For details on where the library and module file

fsunlinsol_spbcgs_mod.mod are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fsunlinsolspbcgs_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPBCGS module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNSPBCGSINIT

Call FSUNSPBCGSINIT(code, pretype, maxl, ier)

Description The function FSUNSPBCGSINIT can be called for Fortran programs to create a SUNLIN-

SOL_SPBCGS object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating desired preconditioning type
maxl (int*) flag indicating number of iterations to allow

Return value \mathtt{ier} is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called after the NVECTOR object has been initialized.

Allowable values for pretype and max1 are the same as for the C function

 ${\tt SUNLinSol_SPBCGS}.$

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPBCGS module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSSPBCGSINIT

Call FSUNMASSSPBCGSINIT(pretype, maxl, ier)

Description The function FSUNMASSSPBCGSINIT can be called for Fortran programs to create a sun-

LINSOL_SPBCGS object for mass matrix linear systems.

Arguments pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating number of iterations to allow

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPBCGS.

The SUNLinSol_SPBCGSSetPrecType and SUNLinSol_SPBCGSSetMaxl routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPBCGSSETPRECTYPE

Call FSUNSPBCGSSETPRECTYPE(code, pretype, ier)

Description The function FSUNSPBCGSSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning to use.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating the type of preconditioning to use.

Return value \mathtt{ier} is a \mathtt{int} return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPBCGSSetPrecType for complete further documentation of this routine.

FSUNMASSSPBCGSSETPRECTYPE

Call FSUNMASSSPBCGSSETPRECTYPE(pretype, ier)

Description The function FSUNMASSSPBCGSSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPBCGSSETPRECTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPBCGSSetPrecType for complete further documentation of this routine.

FSUNSPBCGSSETMAXL

Call FSUNSPBCGSSETMAXL(code, maxl, ier)

Description The function FSUNSPBCGSSETMAXL can be called for Fortran programs to change the

maximum number of iterations to allow.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

maxl (int*) the number of iterations to allow.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPBCGSSetMaxl for complete further documentation of this routine.

FSUNMASSSPBCGSSETMAXL

Call FSUNMASSSPBCGSSETMAXL(maxl, ier)

Description The function FSUNMASSSPBCGSSETMAXL can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPBCGSSETMAXL above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPBCGSSetMaxl for complete further documentation of this routine.

8.14.4 SUNLinearSolver_SPBCGS content

The $sunlingol_sphisms$ module defines the content field of a sunlinearSolver as the following structure:

```
struct _SUNLinearSolverContent_SPBCGS {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
```

```
N_Vector r;
  N_Vector r_star;
  N_Vector p;
  N_Vector q;
  N_Vector u;
  N_Vector Ap;
  N_Vector vtemp;
};
These entries of the content field contain the following information:
           - number of SPBCGS iterations to allow (default is 5),
           - flag for type of preconditioning to employ (default is none),
pretype
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,
           - function pointer to perform Av product,
ATimes
ATData
           - pointer to structure for ATimes,
           - function pointer to preconditioner setup routine,
Psetup
           - function pointer to preconditioner solve routine,
Psolve
PData
           - pointer to structure for Psetup and Psolve,
           - vector pointers for supplied scaling matrices (default is NULL),
s1, s2
           - a NVECTOR which holds the current scaled, preconditioned linear system residual,
           - a NVECTOR which holds the initial scaled, preconditioned linear system residual,
r_star
p, q, u, Ap, vtemp - NVECTORS used for workspace by the SPBCGS algorithm.
```

8.15 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [16]) iterative linear solver. The SUNLINSOL_SPTFQMR module is designed to be compatible with any NVECTOR 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.

To access the SUNLINSOL_SPTFQMR module, include the header file sunlinsol/sunlinsol_sptfqmr.h. We note that the SUNLINSOL_SPTFQMR module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolsptfqmr module library.

8.15.1 SUNLinearSolver_SPTFQMR description

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPTFQMR to supply the ATimes, PSetup, and Psolve function pointers and s1 and s2 scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the TFQMR iteration is performed. This will include scaling and preconditioning if those options have been supplied.

8.15.2 SUNLinearSolver_SPTFQMR functions

The SUNLINSOL_SPTFQMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPTFQMR

Notes

Call LS = SUNLinSol_SPTFQMR(y, pretype, maxl);

SUNLinearSolver object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver pretype (int) flag indicating the desired type of preconditioning, allowed values

- PREC_NONE (0)
- PREC_LEFT (1)
- PREC_RIGHT (2)
- PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

(int) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value This returns a SUNLinearSolver object. If either y is incompatible then this

routine will return NULL.

This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPTFQMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

Deprecated Name For backward compatibility, the wrapper function SUNSPTFQMR with idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPTFQMR

maxl

The SUNLINSOL_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_SPTFQMR
- SUNLinSolInitialize_SPTFQMR
- SUNLinSolSetATimes_SPTFQMR
- SUNLinSolSetPreconditioner_SPTFQMR
- SUNLinSolSetScalingVectors_SPTFQMR

- SUNLinSolSetup_SPTFQMR
- SUNLinSolSolve_SPTFQMR
- SUNLinSolNumIters_SPTFQMR
- SUNLinSolResNorm_SPTFQMR
- SUNLinSolResid_SPTFQMR
- SUNLinSolLastFlag_SPTFQMR
- SUNLinSolSpace_SPTFQMR
- SUNLinSolFree_SPTFQMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPTFQMR module also defines the following additional user-callable functions.

SUNLinSol_SPTFQMRSetPrecType

Call retval = SUNLinSol_SPTFQMRSetPrecType(LS, pretype);

Description The function SUNLinSol_SPTFQMRSetPrecType updates the type of preconditioning

to use in the SUNLINSOL_SPTFQMR object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPTFQMR object to update

pretype (int) flag indicating the desired type of preconditioning, allowed values

match those discussed in SUNLinSol_SPTFQMR.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNSPTFQMRSetPrecType with

idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPTFQMRSetPrecType

SUNLinSol_SPTFQMRSetMaxl

Call retval = SUNLinSol_SPTFQMRSetMax1(LS, max1);

Description The function SUNLinSol_SPTFQMRSetMaxl updates the number of linear solver iterations

to allow.

Arguments LS (SUNLinearSolver) the SUNLINSOL_SPTFQMR object to update

 \mathtt{maxl} (int) flag indicating the number of iterations to allow; values ≤ 0 will result in

the default value (5)

Return value This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or

SUNLS_SUCCESS.

F2003 Name FSUNLinSol_SPTFQMRSetMax1

 ${\bf SUNSPTFQMRSetMaxl}$

8.15.3 SUNLinearSolver_SPTFQMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_sptfqmr_mod FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR 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 SUNLinSol_SPTFQMR is interfaced as FSUNLinSol_SPTFQMR.

The Fortran 2003 sunlinsol_spfgmr interface module can be accessed with the use statement, i.e. use fsunlinsol_sptfqmr_mod, and linking to the library libsundials_fsunlinsolsptfqmr_mod. lib in addition to the C library. For details on where the library and module file

fsunlinsol_sptfqmr_mod.mod are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fsunlinsolsptfqmr_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPTFQMR module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNSPTFQMRINIT

Call FSUNSPTFQMRINIT(code, pretype, maxl, ier)

Description The function FSUNSPTFQMRINIT can be called for Fortran programs to create a SUNLIN-SOL_SPTFQMR object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating number of iterations to allow

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and max1 are the same as for the C function SUNLinSol_SPTFQMR.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPTFQMR module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSSPTFQMRINIT

Call FSUNMASSSPTFQMRINIT(pretype, maxl, ier)

Description The function FSUNMASSSPTFQMRINIT can be called for Fortran programs to create a

SUNLINSOL_SPTFQMR object for mass matrix linear systems.

Arguments pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating number of iterations to allow

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and maxl are the same as for the C function

SUNLinSol_SPTFQMR.

The SUNLinSol_SPTFQMRSetPrecType and SUNLinSol_SPTFQMRSetMaxl routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPTFQMRSETPRECTYPE

Call FSUNSPTFQMRSETPRECTYPE(code, pretype, ier)

Description The function FSUNSPTFQMRSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning to use.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating the type of preconditioning to use.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetPrecType for complete further documentation of this rou-

tine.

FSUNMASSSPTFQMRSETPRECTYPE

Call FSUNMASSSPTFQMRSETPRECTYPE(pretype, ier)

Description The function FSUNMASSSPTFQMRSETPRECTYPE can be called for Fortran programs to

change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPTFQMRSETPRECTYPE above, except that code is

not needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetPrecType for complete further documentation of this rou-

tine.

FSUNSPTFQMRSETMAXL

Call FSUNSPTFQMRSETMAXL(code, maxl, ier)

Description The function FSUNSPTFQMRSETMAXL can be called for Fortran programs to change the

maximum number of iterations to allow.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

maxl (int*) the number of iterations to allow.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

FSUNMASSSPTFQMRSETMAXL

Call FSUNMASSSPTFQMRSETMAXL(maxl, ier)

Description The function FSUNMASSSPTFQMRSETMAXL can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPTFQMRSETMAXL above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value \mathtt{ier} is a \mathtt{int} return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

8.15.4 SUNLinearSolver_SPTFQMR content

The SUNLINSOL_SPTFQMR module defines the *content* field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_SPTFQMR {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector r_star;
  N_Vector q;
  N_Vector d;
  N_Vector v;
  N_Vector p;
  N_Vector *r;
  N_Vector u;
  N_Vector vtemp1;
  N_Vector vtemp2;
  N_Vector vtemp3;
};
These entries of the content field contain the following information:
          - number of TFQMR iterations to allow (default is 5),
maxl
          - flag for type of preconditioning to employ (default is none),
pretype
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,
          - function pointer to preconditioner setup routine,
Psetup
Psolve
          - function pointer to preconditioner solve routine,
          - pointer to structure for Psetup and Psolve,
PData
s1, s2
          - vector pointers for supplied scaling matrices (default is NULL),
          - a NVECTOR which holds the initial scaled, preconditioned linear system residual,
r_star
q, d, v, p, u - NVECTORS used for workspace by the SPTFQMR algorithm,
          - array of two NVECTORS used for workspace within the SPTFQMR algorithm,
vtemp1, vtemp2, vtemp3 - temporary vector storage.
```

8.16 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementation of the PCG (Preconditioned Conjugate Gradient [18]) iterative linear solver. The SUNLINSOL_PCG module is designed to be compatible with any NVECTOR 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.

To access the SUNLINSOL_PCG module, include the header file sunlinsol/sunlinsol_pcg.h. We note that the SUNLINSOL_PCG module is accessible from SUNDIALS packages without separately linking to the libsundials_sunlinsolpcg module library.

8.16.1 SUNLinearSolver_PCG description

Unlike all of the other iterative linear solvers supplied with Sundials, PCG should only be used on symmetric linear systems (e.g. mass matrix linear systems encountered in ARKODE). As a result, the explanation of the role of scaling and preconditioning matrices given in general must be modified in this scenario. The PCG algorithm solves a linear system Ax = b where A is a symmetric $(A^T = A)$, real-valued matrix. Preconditioning is allowed, and is applied in a symmetric fashion on both the right and left. Scaling is also allowed and is applied symmetrically. We denote the preconditioner and scaling matrices as follows:

- P is the preconditioner (assumed symmetric),
- S is a diagonal matrix of scale factors.

The matrices A and P are not required explicitly; only routines that provide A and P^{-1} as operators are required. The diagonal of the matrix S is held in a single NVECTOR, supplied by the user.

In this notation, PCG applies the underlying CG algorithm to the equivalent transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{8.3}$$

where

$$\tilde{A} = SP^{-1}AP^{-1}S,$$

$$\tilde{b} = SP^{-1}b,$$

$$\tilde{x} = S^{-1}Px.$$
(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:

$$\begin{split} &\|\tilde{b}-\tilde{A}\tilde{x}\|_2<\delta\\ \Leftrightarrow & \\ &\|SP^{-1}b-SP^{-1}Ax\|_2<\delta\\ \Leftrightarrow & \\ &\|P^{-1}b-P^{-1}Ax\|_S<\delta \end{split}$$

where $||v||_S = \sqrt{v^T S^T S v}$, with an input tolerance δ .

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_PCG to supply the ATimes, PSetup, and Psolve function pointers and s scaling vector.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

8.16.2 SUNLinearSolver_PCG functions

The SUNLINSOL_PCG module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_PCG

Notes

Call LS = SUNLinSol_PCG(y, pretype, maxl);

Description The function SUNLinSol_PCG creates and allocates memory for a PCG SUNLinearSolver

object.

Arguments y (N_Vector) a template for cloning vectors needed within the solver

pretype (int) flag indicating whether to use preconditioning. Since the PCG algorithm is designed to only support symmetric preconditioning, then any of the pretype inputs PREC_LEFT (1), PREC_RIGHT (2), or PREC_BOTH (3)

will result in use of the symmetric preconditioner; any other integer input will result in the default (no preconditioning).

 $\verb|maxl| \qquad (\verb|int|) \ the \ number \ of \ linear \ iterations \ to \ allow; \ values \le 0 \ will \ result \ in$

the default value (5).

Return value This returns a SUNLinearSolver object. If either y is incompatible then this

routine will return NULL.

This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

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.

Deprecated Name For backward compatibility, the wrapper function SUNPCG with idential input and output arguments is also provided.

F2003 Name FSUNLinSol_PCG

The SUNLINSOL_PCG module defines implementations of all "iterative" linear solver operations listed in Sections 8.1.1 - 8.1.3:

- SUNLinSolGetType_PCG
- SUNLinSolInitialize_PCG
- SUNLinSolSetATimes_PCG
- SUNLinSolSetPreconditioner_PCG

- SUNLinSolSetScalingVectors_PCG since PCG only supports symmetric scaling, the second NVECTOR argument to this function is ignored
- SUNLinSolSetup_PCG
- SUNLinSolSolve_PCG
- SUNLinSolNumIters_PCG
- SUNLinSolResNorm_PCG
- SUNLinSolResid_PCG
- SUNLinSolLastFlag_PCG
- SUNLinSolSpace_PCG
- SUNLinSolFree_PCG

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_PCG module also defines the following additional user-callable functions.

SUNLinSol_PCGSetPrecType

Call	retval =	SUNLinSol	_PCGSetPrec	Type(LS.	pretype):

Description The function SUNLinSol_PCGSetPrecType updates the flag indicating use of pre-

conditioning in the SUNLINSOL_PCG object.

Arguments LS (SUNLinearSolver) the SUNLINSOL_PCG object to update

pretype (int) flag indicating use of preconditioning, allowed values match those

discussed in SUNLinSol_PCG.

Return value This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal

pretype), SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNPCGSetPrecType with iden-

tial input and output arguments is also provided.

F2003 Name FSUNLinSol_PCGSetPrecType

SUNLinSol_PCGSetMaxl

Call retval = SUNLinSol_PCGSetMaxl(LS, maxl);

Description The function SUNLinSol_PCGSetMaxl updates the number of linear solver iterations

to allow.

Arguments LS (SUNLinearSolver) the SUNLINSOL_PCG object to update

 $\verb|maxl (int)| flag indicating the number of iterations to allow; values \leq 0 will result$

in the default value (5)

Return value This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or

SUNLS_SUCCESS.

Deprecated Name For backward compatibility, the wrapper function SUNPCGSetMaxl with idential

input and output arguments is also provided.

F2003 Name FSUNLinSol_PCGSetMax1

8.16.3 SUNLinearSolver_PCG Fortran interfaces

The SUNLINSOL_PCG module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The fsunlinsol_pcg_mod FORTRAN module defines interfaces to all SUNLINSOL_PCG 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 SUNLinSol_PCG is interfaced as FSUNLinSol_PCG.

The FORTRAN 2003 SUNLINSOL_PCG interface module can be accessed with the use statement, i.e. use fsunlinsol_pcg_mod, and linking to the library libsundials_fsunlinsolpcg_mod.lib in addition to the C library. For details on where the library and module file fsunlinsol_pcg_mod.mod are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators without separately linking to the libsundials_fsunlinsolpcg_mod library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_PCG module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNPCGINIT

Call FSUNPCGINIT(code, pretype, maxl, ier)

Description The function FSUNPCGINIT can be called for Fortran programs to create a SUNLIN-

SOL_PCG object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating desired preconditioning type
maxl (int*) flag indicating number of iterations to allow

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See

printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for pretype and max1 are the same as for the C function SUNLinSol_PCG.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_PCG module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSPCGINIT

Call FSUNMASSPCGINIT(pretype, maxl, ier)

Description The function FSUNMASSPCGINIT can be called for Fortran programs to create a SUNLIN-

SOL_PCG object for mass matrix linear systems.

Arguments pretype (int*) flag indicating desired preconditioning type

maxl (int*) flag indicating number of iterations to allow

Return value $\verb"ier"$ is a $\verb"int"$ return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes This routine must be called after the NVECTOR object has been initialized.

Allowable values for pretype and max1 are the same as for the C function SUNLinSol_PCG.

The SUNLinSol_PCGSetPrecType and SUNLinSol_PCGSetMaxl routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNPCGSETPRECTYPE

Call FSUNPCGSETPRECTYPE(code, pretype, ier)

Description The function FSUNPCGSETPRECTYPE can be called for Fortran programs to change the

type of preconditioning to use.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3

for KINSOL, and 4 for ARKODE).

pretype (int*) flag indicating the type of preconditioning to use.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetPrecType for complete further documentation of this routine.

FSUNMASSPCGSETPRECTYPE

Call FSUNMASSPCGSETPRECTYPE(pretype, ier)

Description The function FSUNMASSPCGSETPRECTYPE can be called for Fortran programs to change

the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNPCGSETPRECTYPE above, except that code is not

needed since mass matrix linear systems only arise in ARKODE.

Return value \mathtt{ier} is a \mathtt{int} return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetPrecType for complete further documentation of this routine.

FSUNPCGSETMAXL

Call FSUNPCGSETMAXL(code, maxl, ier)

Description The function FSUNPCGSETMAXL can be called for Fortran programs to change the maxi-

mum number of iterations to allow.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for

KINSOL, and 4 for ARKODE).

maxl (int*) the number of iterations to allow.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetMaxl for complete further documentation of this routine.

FSUNMASSPCGSETMAXL

Call FSUNMASSPCGSETMAXL(maxl, ier)

Description The function FSUNMASSPCGSETMAXL can be called for Fortran programs to change the

type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNPCGSETMAXL above, except that code is not needed

since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise.

See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetMaxl for complete further documentation of this routine.

8.16.4 SUNLinearSolver_PCG content

The SUNLINSOL_PCG module defines the content field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_PCG {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s;
  N_Vector r;
  N_Vector p;
  N_Vector z;
  N_Vector Ap;
};
These entries of the content field contain the following information:
           - number of PCG iterations to allow (default is 5),
maxl
           - flag for use of preconditioning (default is none),
numiters - number of iterations from the most-recent solve,
           - 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,
           - function pointer to preconditioner setup routine,
Psetup
Psolve
           - function pointer to preconditioner solve routine,
PData
           - pointer to structure for Psetup and Psolve,
           - vector pointer for supplied scaling matrix (default is NULL),
           - a NVECTOR which holds the preconditioned linear system residual,
p, z, Ap - NVECTORs used for workspace by the PCG algorithm.
```

8.17 SUNLinearSolver Examples

There are SUNLinearSolver examples that may be installed for each implementation; these make use of the functions in test_sunlinsol.c. These example functions show simple usage of the SUNLinearSolver family of functions. The inputs to the examples depend on the linear solver type, and are output to stdout if the example is run without the appropriate number of command-line arguments.

The following is a list of the example functions in test_sunlinsol.c:

- Test_SUNLinSolGetType: Verifies the returned solver type against the value that should be returned.
- Test_SUNLinSolInitialize: Verifies that SUNLinSolInitialize can be called and returns successfully.

- Test_SUNLinSolSetup: Verifies that SUNLinSolSetup can be called and returns successfully.
- Test_SUNLinSolSolve: Given a SUNMATRIX object A, NVECTOR objects x and b (where Ax = b) and a desired solution tolerance tol, this routine clones x into a new vector y, calls SUNLinSolSolve to fill y as the solution to Ay = b (to the input tolerance), verifies that each entry in x and y match to within 10*tol, and overwrites x with y prior to returning (in case the calling routine would like to investigate further).
- Test_SUNLinSolSetATimes (iterative solvers only): Verifies that SUNLinSolSetATimes can be called and returns successfully.
- Test_SUNLinSolSetPreconditioner (iterative solvers only): Verifies that SUNLinSolSetPreconditioner can be called and returns successfully.
- Test_SUNLinSolSetScalingVectors (iterative solvers only): Verifies that SUNLinSolSetScalingVectors can be called and returns successfully.
- Test_SUNLinSolLastFlag: Verifies that SUNLinSolLastFlag can be called, and outputs the result to stdout.
- Test_SUNLinSolNumIters (iterative solvers only): Verifies that SUNLinSolNumIters can be called, and outputs the result to stdout.
- Test_SUNLinSolResNorm (iterative solvers only): Verifies that SUNLinSolResNorm can be called, and that the result is non-negative.
- Test_SUNLinSolResid (iterative solvers only): Verifies that SUNLinSolResid can be called.
- Test_SUNLinSolSpace verifies that SUNLinSolSpace can be called, and outputs the results to stdout.

We'll note that these tests should be performed in a particular order. For either direct or iterative linear solvers, Test_SUNLinSolInitialize must be called before Test_SUNLinSolSolve, 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.

Appendix A

SUNDIALS Package Installation Procedure

The installation of any SUNDIALS package is accomplished by installing the SUNDIALS suite as a whole, according to the instructions that follow. The same procedure applies whether or not the downloaded file contains one or all solvers in SUNDIALS.

The SUNDIALS suite (or individual solvers) are distributed as compressed archives (.tar.gz). The name of the distribution archive is of the form *solver-x.y.z.tar.gz*, where *solver* is one of: sundials, cvode, cvodes, arkode, ida, idas, or kinsol, and x.y.z represents the version number (of the SUNDIALS suite or of the individual solver). To begin the installation, first uncompress and expand the sources, by issuing

% tar xzf solver-x.y.z.tar.gz

This will extract source files under a directory *solver*-x.y.z.

Starting with version 2.6.0 of SUNDIALS, CMake is the only supported method of installation. The explanations of the installation procedure begins with a few common observations:

• The remainder of this chapter will follow these conventions:

solverdir is the directory solver-x.y.z created above; i.e., the directory containing the SUNDI-ALS 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/CMAKE_INSTALL_LIBDIR, with instdir and CMAKE_INSTALL_LIBDIR specified at configuration time.

- For sundials CMake-based installation, in-source builds are prohibited; in other words, the build directory builddir can **not** be the same as solverdir and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.
- The installation directory *instdir* can **not** be the same as the source directory *solverdir*.
- By default, only the libraries and header files are exported to the installation directory *instdir*. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the *installed* SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as "templates" for your own problems. CMake installs CMakeLists.txt files



and also (as an option available only under Unix/Linux) Makefile files. Note this installation approach also allows the option of building the SUNDIALS examples without having to install them. (This can be used as a sanity check for the freshly built libraries.)

• Even if generation of shared libraries is enabled, only static libraries are created for the FCMIX modules. (Because of the use of fixed names for the Fortran user-provided subroutines, FCMIX shared libraries would result in "undefined symbol" errors at link time.)

A.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Makefiles, as well as KDevelop, Visual Studio, and (Apple) XCode project files from the same configuration file. In addition, CMake also provides a GUI front end and which allows an interactive build and installation process.

The SUNDIALS build process requires CMake version 3.1.3 or higher and a working C compiler. On Unix-like operating systems, it also requires Make (and curses, including its development libraries, for the GUI front end to CMake, ccmake), while on Windows it requires Visual Studio. CMake is continually adding new features, and the latest version can be downloaded from http://www.cmake.org. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use ccmake, while Windows users will be able to use CMakeSetup.

As previously noted, when using CMake to configure, build and install SUNDIALS, it is always required to use a separate build directory. While in-source builds are possible, they are explicitly prohibited by the SUNDIALS CMake scripts (one of the reasons being that, unlike autotools, CMake does not provide a make distclean procedure and it is therefore difficult to clean-up the source tree after an in-source build). By ensuring a separate build directory, it is an easy task for the user to clean-up all traces of the build by simply removing the build directory. CMake does generate a make clean which will remove files generated by the compiler and linker.

A.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The *instdir* defaults to /usr/local and can be changed by setting the CMAKE_INSTALL_PREFIX variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the cmake command, or from a curses-based GUI by using the ccmake command. Examples for using both methods will be presented. For the examples shown it is assumed that there is a top level SUNDIALS directory with appropriate source, build and install directories:

```
% mkdir (...)sundials/instdir
% mkdir (...)sundials/builddir
% cd (...)sundials/builddir
```

Building with the GUI

Using CMake with the GUI follows this general process:

- Select and modify values, run configure (c key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
 - If it is a boolean (ON/OFF) it will toggle the value
 - If it is string or file, it will allow editing of the string

- For file and directories, the <tab> key can be used to complete
- Repeat until all values are set as desired and the generate option is available (g key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (t key)
- To search for a variable press / key, and to repeat the search, press the n key

To build the default configuration using the GUI, from the *builddir* enter the ccmake command and point to the *solverdir*:

% ccmake ../solverdir

The default configuration screen is shown in Figure A.1.

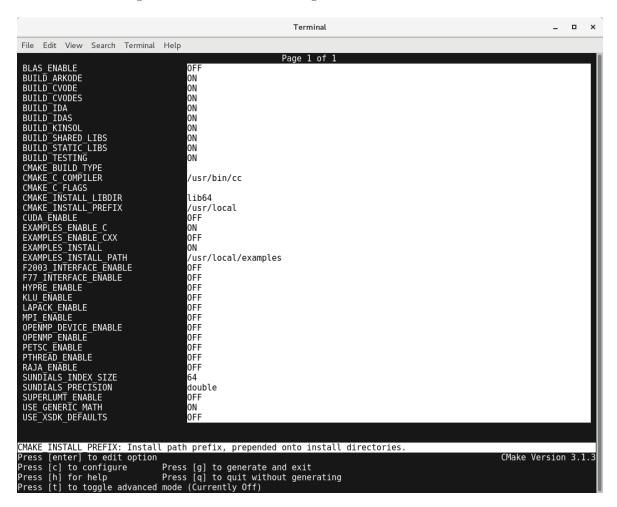


Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the CMAKE_INSTALL_PREFIX and the EXAMPLES_INSTALL_PATH as shown in figure A.2.

Pressing the (g key) will generate makefiles including all dependencies and all rules to build SUN-DIALS on this system. Back at the command prompt, you can now run:



Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

% make

To install SUNDIALS in the installation directory specified in the configuration, simply run:

% make install

Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the cmake command. The following will build the default configuration:

```
% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../solverdir
% make
% make install
```

A.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

BLAS_ENABLE - Enable BLAS support

Default: OFF

Note: Setting this option to ON will trigger additional CMake options. See additional informa-

tion on building with BLAS enabled in A.1.4.

BLAS_LIBRARIES - BLAS library

Default: /usr/lib/libblas.so

Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system

paths.

BUILD_ARKODE - Build the ARKODE library

Default: ON

BUILD_CVODE - Build the CVODE library

Default: ON

BUILD_CVODES - Build the CVODES library

Default: ON

BUILD_IDA - Build the IDA library

Default: ON

BUILD_IDAS - Build the IDAS library

Default: ON

BUILD_KINSOL - Build the KINSOL library

Default: ON

BUILD_SHARED_LIBS - Build shared libraries

Default: ON

BUILD_STATIC_LIBS - Build static libraries

Default: ON

CMAKE_BUILD_TYPE - Choose the type of build, options are: None (CMAKE_C_FLAGS used), Debug, Release, RelWithDebInfo, and MinSizeRel

Default:

Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by CMAKE_<language>_FLAGS.

CMAKE_C_COMPILER - C compiler

Default: /usr/bin/cc

 ${\tt CMAKE_C_FLAGS}$ - 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

 ${\tt CMAKE_CXX_COMPILER}$ - C^{++} compiler

Default: /usr/bin/c++

Note: A C++ compiler (and all related options) are only triggered if C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ applications by default without setting any additional configuration options.

CMAKE_CXX_FLAGS - Flags for C++ compiler

Default:

CMAKE_CXX_FLAGS_DEBUG - Flags used by the C++ compiler during debug builds

Default: -g

CMAKE_CXX_FLAGS_MINSIZEREL - Flags used by the C++ compiler during release minsize builds

Default: -Os -DNDEBUG

CMAKE_CXX_FLAGS_RELEASE - Flags used by the C++ compiler during release builds

Default: -O3 -DNDEBUG

CMAKE_Fortran_COMPILER - Fortran compiler

Default: /usr/bin/gfortran

Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (FCMIX_ENABLE is ON) or BLAS/LAPACK support is enabled (BLAS_ENABLE or LAPACK_ENABLE is ON).

CMAKE_Fortran_FLAGS - Flags for Fortran compiler

Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the Fortran compiler during debug builds

Default: -g

CMAKE_Fortran_FLAGS_MINSIZEREL - Flags used by the Fortran compiler during release minsize builds

Default: -Os

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the Fortran compiler during release builds

Default: -O3

CMAKE_INSTALL_PREFIX - Install path prefix, prepended onto install directories

Default: /usr/local

Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories include and CMAKE_INSTALL_LIBDIR of CMAKE_INSTALL_PREFIX, respectively.

CMAKE_INSTALL_LIBDIR - Library installation directory

Default:

Note: This is the directory within CMAKE_INSTALL_PREFIX that the SUNDIALS libraries will be installed under. The default is automatically set based on the operating system using the GNUInstallDirs CMake module.

Fortran_INSTALL_MODDIR - Fortran module installation directory

Default: fortran

CUDA_ENABLE - Build the SUNDIALS CUDA vector module.

Default: OFF

EXAMPLES_ENABLE_C - Build the SUNDIALS C examples

Default: ON

EXAMPLES_ENABLE_CUDA - Build the SUNDIALS CUDA examples

Default: OFF

Note: You need to enable CUDA support to build these examples.

 ${\tt EXAMPLES_ENABLE_CXX}$ - Build the sundials C^{++} examples

Default: OFF unless Trilinos_ENABLE is ON.

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples

Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90 examples

Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F2003 - Build the SUNDIALS Fortran2003 examples

Default: ON (if F2003_INTERFACE_ENABLE 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.

F77_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 77 interfaces

Default: OFF

F2003_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 2003 interfaces

Default: OFF

HYPRE_ENABLE - Enable hypre support

Default: OFF

Note: See additional information on building with hypre enabled in A.1.4.

HYPRE_INCLUDE_DIR - Path to hypre header files

HYPRE_LIBRARY_DIR - Path to hypre installed library files

KLU_ENABLE - Enable KLU support

Default: OFF

Note: See additional information on building with KLU enabled in A.1.4.

KLU_INCLUDE_DIR - Path to SuiteSparse header files

KLU_LIBRARY_DIR - Path to SuiteSparse installed library files

LAPACK_ENABLE - Enable LAPACK support

Default: OFF

Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in A.1.4.

LAPACK_LIBRARIES - LAPACK (and BLAS) libraries

Default: /usr/lib/liblapack.so;/usr/lib/libblas.so

Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

MPI_ENABLE - Enable MPI support. 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 (MPI_ENABLE is ON) and C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than MPI_ENABLE.

MPI_Fortran_COMPILER - mpif77 or mpif90 program

Default:

Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON) and Fortran-C support is enabled (F77_INTERFACE_ENABLE or F2003_INTERFACE_ENABLE is ON).

MPIEXEC_EXECUTABLE - Specify the executable for running MPI programs

Default: mpirun

Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON).

OPENMP_ENABLE - Enable OpenMP support (build the OpenMP NVECTOR).

Default: OFF

OPENMP_DEVICE_ENABLE - Enable OpenMP device offloading (build the OpenMPDEV nvector) if supported by the provided compiler.

Default: OFF

SKIP_OPENMP_DEVICE_CHECK - advanced option - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.

Default: OFF

PETSC_ENABLE - Enable PETSc support

Default: OFF

Note: See additional information on building with PETSc enabled in A.1.4.

PETSC_INCLUDE_DIR - Path to PETSc header files

PETSC_LIBRARY_DIR - Path to PETSc installed library files

PTHREAD_ENABLE - Enable Pthreads support (build the Pthreads NVECTOR).

Default: OFF

RAJA_ENABLE - Enable RAJA support (build the RAJA NVECTOR).

Default: OFF

Note: You need to enable CUDA in order to build the RAJA vector module.

SUNDIALS_F77_FUNC_CASE - advanced option - Specify the case to use in the Fortran name-mangling scheme, options are: lower or upper

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (lower) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_UNDERSCORES must also be set.

SUNDIALS_F77_FUNC_UNDERSCORES - advanced option - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: none, one, or two

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (one) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_CASE must also be set.

SUNDIALS_INDEX_TYPE - advanced option - Integer type used for SUNDIALS indices. The size must match the size provided for the

SUNDIALS_INDEX_SIZE option.

Default:

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_PRECISION - Precision used in SUNDIALS, options are: double, single, or extended Default: double

 ${\tt SUPERLUDIST_ENABLE - Enable \ SuperLU_DIST \ support}$

Default: OFF

Note: See additional information on building with SuperLU_DIST enabled in A.1.4.

SUPERLUDIST_INCLUDE_DIR - Path to SuperLU_DIST header files (typically SRC directory)

SUPERLUDIST_LIBRARY_DIR - Path to SuperLU_DIST installed library files

SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST

 ${\tt SUPERLUDIST_OpenMP - Enable \ SUNDIALS \ support \ for \ SuperLU_DIST \ built \ with \ OpenMP}$

Default: OFF

Note: SuperLU_DIST must be built with OpenMP support for this option to function properly. Additionally the environment variable OMP_NUM_THREADS must be set to the desired number of threads.

SUPERLUMT_ENABLE - Enable SUPERLUMT support

Default: OFF

Note: See additional information on building with Superlumt enabled in A.1.4.

SUPERLUMT_INCLUDE_DIR - Path to SuperLU_MT header files (typically SRC directory)

 ${\tt SUPERLUMT_LIBRARY_DIR}$ - Path to SuperLU_MT installed library files

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP

Default: Pthread

Trilinos_ENABLE - Enable Trilinos support (build the Tpetra NVECTOR).

Default: OFF

Trilinos_DIR - Path to the Trilinos install directory.

Default:

TRILINOS_INTERFACE_C_COMPILER - advanced option - Set the C compiler for building the Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_COMPILER or MPI_C_COMPILER if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_C_COMPILER_FLAGS - advanced option - Set the C compiler flags for Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

 $Default:\ The\ C\ compiler\ flags\ exported\ from\ the\ found\ Trilinos\ installation\ if\ {\tt USE_XSDK_DEFAULTS=OFF}.$

CMAKE_C_FLAGS if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same flags that were used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER - advanced option - Set the C++ compiler for builing Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C++ compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=0FF.

CMAKE_CXX_COMPILER or MPI_CXX_COMPILER if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER_FLAGS - advanced option - Set the C++ compiler flags for Trili-

nos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

 $Default: \ The \ C^{++} \ compiler \ flags \ exported \ from \ the \ found \ Trilinos \ installation \ if \ {\tt USE_XSDK_DEFAULTS=OFF}.$

CMAKE_CXX_FLAGS if USE_XSDK_DEFAULTS=ON.

Note: Is is recommended to use the same flags that were used to build the Trilinos library.

USE_GENERIC_MATH - Use generic (stdc) math libraries

Default: ON

xSDK Configuration Options

SUNDIALS supports CMake configuration options defined by the Extreme-scale Scientific Software Development Kit (xSDK) community policies (see https://xsdk.info for more information). xSDK CMake options are unused by default but may be activated by setting USE_XSDK_DEFAULTS to ON.

When xSDK options are active, they will overwrite the corresponding SUNDIALS option and may have different default values (see details below). As such the equivalent SUNDIALS options should not be used when configuring with xSDK options. In the GUI front end to CMake (ccmake), setting USE_XSDK_DEFAULTS to ON will hide the corresponding SUNDIALS options as advanced CMake variables. During configuration, messages are output detailing which xSDK flags are active and the equivalent SUNDIALS options that are replaced. Below is a complete list xSDK options and the corresponding SUNDIALS options if applicable.

TPL_BLAS_LIBRARIES - BLAS library

Default: /usr/lib/libblas.so

SUNDIALS equivalent: BLAS_LIBRARIES

Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system

paths.

TPL_ENABLE_BLAS - Enable BLAS support

Default: OFF

SUNDIALS equivalent: BLAS_ENABLE

TPL_ENABLE_HYPRE - Enable hypre support

Default: OFF

SUNDIALS equivalent: HYPRE_ENABLE

TPL_ENABLE_KLU - Enable KLU support

Default: OFF

SUNDIALS equivalent: KLU_ENABLE

TPL_ENABLE_PETSC - Enable PETSc support

Default: OFF

SUNDIALS equivalent: PETSC_ENABLE



TPL_ENABLE_LAPACK - Enable LAPACK support

Default: OFF

SUNDIALS equivalent: LAPACK_ENABLE

TPL_ENABLE_SUPERLUDIST - Enable SuperLU_DIST support

Default: OFF

SUNDIALS equivalent: SUPERLUDIST_ENABLE

TPL_ENABLE_SUPERLUMT - Enable SuperLU_MT support

Default: OFF

SUNDIALS equivalent: SUPERLUMT_ENABLE

 ${\tt TPL_HYPRE_INCLUDE_DIRS~-~Path~to~hypre~header~files}$

SUNDIALS equivalent: HYPRE_INCLUDE_DIR

TPL_HYPRE_LIBRARIES - hypre library

SUNDIALS equivalent: N/A

 ${\tt TPL_KLU_INCLUDE_DIRS}$ - Path to KLU header files

SUNDIALS equivalent: KLU_INCLUDE_DIR

TPL_KLU_LIBRARIES - KLU library

SUNDIALS equivalent: N/A

TPL_LAPACK_LIBRARIES - LAPACK (and BLAS) libraries

Default: /usr/lib/liblapack.so;/usr/lib/libblas.so

SUNDIALS equivalent: LAPACK_LIBRARIES

Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system

paths.

TPL_PETSC_INCLUDE_DIRS - Path to PETSc header files

SUNDIALS equivalent: PETSC_INCLUDE_DIR

TPL_PETSC_LIBRARIES - PETSc library

SUNDIALS equivalent: N/A

TPL_SUPERLUDIST_INCLUDE_DIRS - Path to SuperLU_DIST header files

 ${\tt SUNDIALS\ equivalent:\ SUPERLUDIST_INCLUDE_DIR}$

TPL_SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST in-

cluding the SuperLU_DIST library itself
SUNDIALS equivalent: SUPERLUDIST_LIBRARIES

TPL_SUPERLUDIST_OPENMP - Enable SUNDIALS support for SuperLU_DIST built with OpenMP

SUNDIALS equivalent: SUPERLUDIST_OPENMP

TPL_SUPERLUMT_LIBRARIES - SuperLU_MT library

SUNDIALS equivalent: N/A

 ${\tt TPL_SUPERLUMT_THREAD_TYPE~-~SuperLU_MT~library~thread~type}$

SUNDIALS equivalent: SUPERLUMT_THREAD_TYPE

USE_XSDK_DEFAULTS - Enable xSDK default configuration settings

Default: OFF

SUNDIALS equivalent: N/A

Note: Enabling xSDK defaults also sets CMAKE_BUILD_TYPE to Debug

XSDK_ENABLE_FORTRAN - Enable SUNDIALS Fortran interfaces

Default: OFF

SUNDIALS equivalent: F77_INTERFACE_ENABLE/F2003_INTERFACE_ENABLE

```
    XSDK_INDEX_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64
        Default: 32
        SUNDIALS equivalent: SUNDIALS_INDEX_SIZE
    XSDK_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad
        Default: double
        SUNDIALS equivalent: SUNDIALS_PRECISION
```

A.1.3 Configuration examples

The following examples will help demonstrate usage of the CMake configure options.

To configure SUNDIALS using the default C and Fortran compilers, and default mpic and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> /home/myname/sundials/solverdir
%
% make install
%
```

To disable installation of the examples, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/solverdir
%
% make install
%
```

A.1.4 Working with external Libraries

The SUNDIALS suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries. When building SUNDIALS as a shared library external libraries any used with SUNDIALS must also be build as a shared library or as a static library compiled with the -fPIC flag.



Building with BLAS

SUNDIALS does not utilize BLAS directly but it may be needed by other external libraries that SUNDIALS can be built with (e.g. LAPACK, PETSC, SuperLU_MT, etc.). To enable BLAS, set the BLAS_ENABLE option to ON. If the directory containing the BLAS library is in the LD_LIBRARY_PATH environment variable, CMake will set the BLAS_LIBRARIES variable accordingly, otherwise CMake will attempt to find the BLAS library in standard system locations. To explicitly tell CMake what libraries to use, the BLAS_LIBRARIES variable can be set to the desired library. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
```

```
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/myblaspath/lib/libblas.so \
> -DSUPERLUMT_ENABLE=ON \
> -DSUPERLUMT_INCLUDE_DIR=/mysuperlumtpath/SRC
> -DSUPERLUMT_LIBRARY_DIR=/mysuperlumtpath/lib
> /home/myname/sundials/solverdir
%
make install
%
```



When allowing CMake to automatically locate the LAPACK library, CMake may also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES must be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were lower and one respectively.

Building with LAPACK

To enable LAPACK, set the LAPACK_ENABLE option to ON. If the directory containing the LAPACK library is in the LD_LIBRARY_PATH environment variable, CMake will set the LAPACK_LIBRARIES variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the LAPACK_LIBRARIES variable can be set to the desired libraries. When setting the LAPACK location explicitly the location of the corresponding BLAS library will also need to be set. Example:



```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/mylapackpath/lib/libblas.so \
> -DLAPACK_ENABLE=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/solverdir
%
% make install
%
```



When allowing CMake to automatically locate the LAPACK library, CMake may also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES must be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were lower and one respectively.

Building with KLU

The KLU libraries are part of SuiteSparse, a suite of sparse matrix software, available from the Texas A&M University website: http://faculty.cse.tamu.edu/davis/suitesparse.html. SUNDIALS has been tested with SuiteSparse version 5.3.0. To enable KLU, set KLU_ENABLE to ON, set KLU_INCLUDE_DIR to the include path of the KLU installation and set KLU_LIBRARY_DIR to the lib path of the KLU installation. The CMake configure will result in populating the following variables: AMD_LIBRARY, AMD_LIBRARY_DIR, BTF_LIBRARY_DIR, COLAMD_LIBRARY, COLAMD_LIBRARY_DIR, and KLU_LIBRARY.

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt. SUNDIALS has been tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set SUPERLUMT_ENABLE to ON, set SUPERLUMT_INCLUDE_DIR to the SRC path of the SuperLU_MT installation, and set the variable SUPERLUMT_LIBRARY_DIR to the lib path of the SuperLU_MT installation. At the same time, the variable SUPERLUMT_THREAD_TYPE must be set to either Pthread or OpenMP.



Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either OPENMP_ENABLE or PTHREAD_ENABLE set to ON then SuperLU_MT should be set to use the same threading type.

Building with SuperLU_DIST

The SuperLU_DIST libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_dist. SUNDIALS has been tested with SuperLU_DIST greater than 6.1. To enable SuperLU_DIST, set SUPERLUDIST_ENABLE to ON, set SUPERLUDIST_INCLUDE_DIR to the include directory of the SuperLU_DIST installation (typically SRC), and set the variable

SUPERLUDIST_LIBRARY_DIR to the path to library directory of the SuperLU_DIST installation (typically lib). At the same time, the variable SUPERLUDIST_LIBRARIES must be set to a semi-colon separated list of other libraries SuperLU_DIST depends on. For example, if SuperLU_DIST was built with LAPACK, then include the LAPACK library in this list. If SuperLU_DIST was built with OpenMP support, then you may set SUPERLUDIST_OPENMP to ON to utilize the OpenMP functionality of SuperLU_DIST.



Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having PTHREAD_ENABLE set to ON then SuperLU_DIST should not be set to use OpenMP.

Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: http://www.mcs.anl.gov/SUNDIALS has been tested with PETSc version 3.10.3. To enable PETSc, set PETSC_ENABLE to ON, set PETSC_INCLUDE_DIR to the include path of the PETSc installation, and set the variable PETSC_LIBRARY_DIR to the lib path of the PETSc installation.

Building with hypre

The hypre libraries are available for download from the Lawrence Livermore National Laboratory website: http://computation.llnl.gov/projects/hypre. SUNDIALS has been tested with hypre version 2.14.0. To enable hypre, set HYPRE_ENABLE to ON, set HYPRE_INCLUDE_DIR to the include path of the hypre installation, and set the variable HYPRE_LIBRARY_DIR to the lib path of the hypre installation.

Building with CUDA

SUNDIALS CUDA modules and examples have been tested with version 9.0 of the CUDA toolkit. To build them, you need to install the Toolkit and compatible NVIDIA drivers. Both are available for download from the NVIDIA website: https://developer.nvidia.com/cuda-downloads. To enable CUDA, set CUDA_ENABLE to ON. If CUDA is installed in a nonstandard location, you may be prompted to set the variable CUDA_TOOLKIT_ROOT_DIR with your CUDA Toolkit installation path. To enable CUDA examples, set EXAMPLES_ENABLE_CUDA to ON.

Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from https://github.com/LLNL/RAJA. SUNDIALS RAJA modules and examples have

been tested with RAJA version 0.6. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set CUDA_ENABLE and RAJA_ENABLE to ON. If RAJA is installed in a nonstandard location you will be prompted to set the variable RAJA_DIR with the path to the RAJA CMake configuration file. To enable building the RAJA examples set EXAMPLES_ENABLE_CUDA to ON.

Building with Trilinos

Trilinos is a suite of numerical libraries developed by Sandia National Laboratories. It can be obtained at https://github.com/trilinos/Trilinos. SUNDIALS Trilinos modules and examples have been tested with Trilinos version 12.14. To enable Trilinos, set Trilinos_ENABLE to ON. If Trilinos is installed in a nonstandard location you will be prompted to set the variable Trilinos_DIR with the path to the Trilinos CMake configuration file. It is desireable to build the Trilinos vector interface with same compiler and options that were used to build Trilinos. CMake will try to find the correct compiler settings automatically from the Trilinos configuration file. If that is not successful, the compilers and options can be manually set with the following CMake variables:

- Trilinos_INTERFACE_C_COMPILER
- Trilinos_INTERFACE_C_COMPILER_FLAGS
- Trilinos_INTERFACE_CXX_COMPILER
- Trilinos_INTERFACE_CXX_COMPILER_FLAGS

A.1.5 Testing the build and installation

If SUNDIALS was configured with EXAMPLES_ENABLE_<language> options to ON, then a set of regression tests can be run after building with the make command by running:

% make test

Additionally, if EXAMPLES_INSTALL was also set to ON, then a set of smoke tests can be run after installing with the make install command by running:

% make test_install

A.2 Building and Running Examples

Each of the SUNDIALS solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set at least of the EXAMPLES_ENABLE_<language> options to ON, and set EXAMPLES_INSTALL to ON. Specify the installation path for the examples with the variable EXAMPLES_INSTALL_PATH. CMake will generate CMakeLists.txt configuration files (and Makefile files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

Either the CMakeLists.txt file or the traditional Makefile may be used to build the examples as well as serve as a template for creating user developed solutions. To use the supplied Makefile simply run make to compile and generate the executables. To use CMake from within the installed example directory, run cmake (or ccmake to use the GUI) followed by make to compile the example code. Note that if CMake is used, it will overwrite the traditional Makefile with a new CMake-generated Makefile. The resulting output from running the examples can be compared with example output bundled in the SUNDIALS distribution.

NOTE: There will potentially be differences in the output due to machine architecture, compiler versions, use of third party libraries etc.



A.3 Configuring, building, and installing on Windows

CMake can also be used to build SUNDIALS on Windows. To build SUNDIALS for use with Visual Studio the following steps should be performed:

- 1. Unzip the downloaded tar file(s) into a directory. This will be the solverdir
- 2. Create a separate builddir
- 3. Open a Visual Studio Command Prompt and cd to builddir
- 4. Run cmake-gui ../solverdir
 - (a) Hit Configure
 - (b) Check/Uncheck solvers to be built
 - (c) Change CMAKE_INSTALL_PREFIX to instdir
 - (d) Set other options as desired
 - (e) Hit Generate
- 5. Back in the VS Command Window:
 - (a) Run msbuild ALL_BUILD.vcxproj
 - (b) Run msbuild INSTALL.vcxproj

The resulting libraries will be in the *instdir*. The SUNDIALS project can also now be opened in Visual Studio. Double click on the ALL_BUILD.vcxproj file to open the project. Build the whole *solution* to create the SUNDIALS libraries. To use the SUNDIALS libraries in your own projects, you must set the include directories for your project, add the SUNDIALS libraries to your project solution, and set the SUNDIALS libraries as dependencies for your project.

A.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

% make install

will install the libraries under *libdir* and the public header files under *includedir*. The values for these directories are *instdir*/CMAKE_INSTALL_LIBDIR and *instdir*/include, respectively. The location can be changed by setting the CMake variable CMAKE_INSTALL_PREFIX. Although all installed libraries reside under *libdir*/CMAKE_INSTALL_LIBDIR, the public header files are further organized into subdirectories under *includedir*/include.

The installed libraries and exported header files are listed for reference in Table A.1. The file extension .lib is typically .so for shared libraries and .a for static libraries. Note that, in the Tables, names are relative to libdir for libraries and to includedir for header files.

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the <code>includedir/include/sundials</code> directory since they are explicitly included by the appropriate solver header files (e.g., <code>cvode_dense.h</code> includes <code>sundials_dense.h</code>). However, it is both legal and safe to do so, and would be useful, for example, if the functions declared in <code>sundials_dense.h</code> are to be used in building a preconditioner.

Table A.1: SUNDIALS libraries and header files

	Libraries	ALS libraries and header files n/a
SHARED	Header files	
	Header files	sundials/sundials_config.h
		sundials/sundials_fconfig.h
		sundials/sundials_types.h
		sundials/sundials_math.h
		sundials/sundials_nvector.h
		sundials/sundials_fnvector.h
		sundials/sundials_matrix.h
		sundials/sundials_linearsolver.h
		sundials/sundials_iterative.h
		sundials/sundials_direct.h
		sundials/sundials_dense.h
		sundials/sundials_band.h
		sundials/sundials_nonlinearsolver.h
		sundials/sundials_version.h
		sundials/sundials_mpi_types.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.lib
		libsundials_fnvecserial_mod.lib
		libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module	fnvector_serial_mod.mod
	files	
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.lib
		libsundials_fnvecparallel.a
		$libsundials_fnvecparallel_mod.lib$
	Header files	nvector/nvector_parallel.h
	Module	fnvector_parallel_mod.mod
	files	
NVECTOR_MANYVECTOR	Libraries	libsundials_nvecmanyvector.lib
	Header files	nvector/nvector_manyvector.h
NVECTOR_MPIMANYVECTOR	Libraries	libsundials_nvecmpimanyvector.lib
	Header files	nvector/nvector_mpimanyvector.h
NVECTOR_MPIPLUSX	Libraries	libsundials_nvecmpiplusx.lib
	Header files	nvector/nvector_mpiplusx.h
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.lib
		libsundials_fnvecopenmp_mod.lib
		libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h
	Module	fnvector_openmp_mod.mod
	files	
	•	continued on next page

NVECTOR_OPENMPDEV	Libraries	libsundials_nvecopenmpdev.lib	
	Header files	nvector/nvector_openmpdev.h	
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.lib	
		libsundials_fnvecpthreads_mod.lib	
		libsundials_fnvecpthreads.a	
	Header files	nvector/nvector_pthreads.h	
	Module	fnvector_pthreads_mod.mod	
	files	•	
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp.lib	
	Header files	nvector/nvector_parhyp.h	
NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.lib	
	Header files	nvector/nvector_petsc.h	
NVECTOR_CUDA	Libraries	libsundials_nveccuda.lib	
	Header files		
		nvector/cuda/ThreadPartitioning.hpp	
		nvector/cuda/Vector.hpp	
		nvector/cuda/VectorKernels.cuh	
NVECTOR_RAJA	Libraries	libsundials_nveccudaraja.lib	
	Header files	nvector/nvector_raja.h	
	1100001 11100	nvector/raja/Vector.hpp	
NVECTOR_TRILINOS	Libraries	libsundials_nvectrilinos.lib	
	Header files	nvector/nvector_trilinos.h	
	Troduct into	nvector/trilinos/SundialsTpetraVectorInterface.hpp	
		nvector/trilinos/SundialsTpetraVectorKernels.hpp	
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.lib	
		libsundials_fsunmatrixband_mod.lib	
		libsundials_fsunmatrixband.a	
	Header files		
	Module	fsunmatrix_band_mod.mod	
	files		
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.lib	
	215101105	libsundials_fsunmatrixdense_mod.lib	
		libsundials_fsunmatrixdense.a	
	Header files	sunmatrix/sunmatrix_dense.h	
	Module	fsunmatrix_dense_mod.mod	
	files		
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse.lib	
		libsundials_fsunmatrixsparse_mod.lib	
		libsundials_fsunmatrixsparse.a	
	Header files	sunmatrix/sunmatrix_sparse.h	
	Module	fsunmatrix_sparse_mod.mod	
	files	T	

SUNMATRIX_SLUNRLOC	Libraries	libsundials_sunmatrixslunrloc.lib
~ 0111111111111111111111111111111111111	Header files	sunmatrix/sunmatrix_slunrloc.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.lib
SUNLINSOL_BAND	Distarios	libsundials_fsunlinsolband_mod.lib
		libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module	fsunlinsol_band_mod.mod
	files	isummsor-survemou
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.lib
		$libsundials_fsunlinsoldense_mod. lib$
		libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	Module	fsunlinsol_dense_mod.mod
	files	
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.lib
		libsundials_fsunlinsolklu_mod.lib
		libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module	fsunlinsol_klu_mod.mod
	files	
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.lib
		libsundials_fsunlinsollapackband.a
	Header files	sunlinsol/sunlinsol_lapackband.h
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.lib
		libsundials_fsunlinsollapackdense.a
	Header files	sunlinsol/sunlinsol_lapackdense.h
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.lib
		libsundials_fsunlinsolpcg_mod.lib
		libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module	fsunlinsol_pcg_mod.mod
	files	
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.lib
		libsundials_fsunlinsolspbcgs_mod.lib
		libsundials_fsunlinsolspbcgs.a
	Header files	
	Module	fsunlinsol_spbcgs_mod.mod
	files	
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.lib
		libsundials_fsunlinsolspfgmr_mod.lib
		libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h

continued from last page				
1 0	Module	fsunlinsol_spfgmr_mod.mod		
	files			
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.lib		
		libsundials_fsunlinsolspgmr_mod.lib		
		libsundials_fsunlinsolspgmr.a		
	Header files	sunlinsol/sunlinsol_spgmr.h		
	Module	fsunlinsol_spgmr_mod.mod		
	files			
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.lib		
•		libsundials_fsunlinsolsptfqmr_mod.lib		
		libsundials_fsunlinsolsptfqmr.a		
	Header files	sunlinsol/sunlinsol_sptfqmr.h		
	Module	fsunlinsol_sptfqmr_mod.mod		
	files	-		
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.lib		
		libsundials_fsunlinsolsuperlumt.a		
	Header files	sunlinsol/sunlinsol_superlumt.h		
SUNLINSOL_SUPERLUDIST	Libraries	libsundials_sunlinsolsuperludist.lib		
		libsundials_fsunlinsolsuperludist.a		
	Header files	sunlinsol/sunlinsol_superludist.h		
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnewton.lib		
		libsundials_fsunnonlinsolnewton_mod.lib		
		libsundials_fsunnonlinsolnewton.a		
	Header files	sunnonlinsol/sunnonlinsol_newton.h		
	Module	fsunnonlinsol_newton_mod.mod		
	files			
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint.lib		
		libsundials_fsunnonlinsolfixedpoint.a		
		libsundials_fsunnonlinsolfixedpoint_mod.lib		
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h		
	Module	fsunnonlinsol_fixedpoint_mod.mod		
	files			
CVODE	Libraries	libsundials_cvode.lib		
		libsundials_fcvode.a		
		libsundials_fcvode_mod. lib		
	Header files	cvode/cvode.h cvode/cvode_impl.h		
		cvode/cvode_direct.h cvode/cvode_ls.h		
		cvode/cvode_spils.h cvode/cvode_bandpre.h		
		cvode/cvode_bbdpre.h		
	Module	fcvode_mod.mod		
	files			
CVODES	Libraries	libsundials_cvodes.lib		
		continued on next page		

continued from last p	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h
	11000401 11100	cvodes/cvodes_direct.h	cvodes/cvodes_ls.h
		cvodes/cvodes_spils.h	cvodes/cvodes_bandpre.h
		cvodes/cvodes_bbdpre.h	evodes/evodes_sanapre.n
ARKODE	Libraries	libsundials_arkode.lib	
		libsundials_farkode.a	
		libsundials_farkode_mod.lib	
	Header files	arkode/arkode.h	arkode/arkode_impl.h
		arkode/arkode_ls.h	arkode/arkode_bandpre.h
		arkode/arkode_bbdpre.h	
	Module	farkode_mod.mod	farkode_arkstep_mod.mod
	files		
		farkode_erkstep_mod.mod	farkode_mristep_mod.mod
IDA	Libraries	libsundials_ida.lib	
		libsundials_fida.a	
		libsundials_fida_mod.lib	
	Header files	ida/ida.h	ida/ida_impl.h
		ida/ida_direct.h	ida/ida_ls.h
		ida/ida_spils.h	$ida/ida_bbdpre.h$
	Module	fida_mod.mod	
	files		
IDAS	Libraries	libsundials_idas.lib	
	Header files	idas/idas.h	idas/idas_impl.h
		idas/idas_direct.h	$idas/idas_ls.h$
		idas/idas_spils.h	idas/idas_bbdpre.h
KINSOL	Libraries	libsundials_kinsol.lib	
		libsundials_fkinsol.a	
		libsundials_fkinsol_mod.lib	
	Header files	kinsol/kinsol.h	kinsol/kinsol_impl.h
		kinsol/kinsol_direct.h	kinsol/kinsol_ls.h
		kinsol/kinsol_spils.h	kinsol/kinsol_bbdpre.h
	Module	fkinsol_mod.mod	• -
	files		

Appendix B

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.

B.1 KINSOL input constants

		KINSOL main solver module		
KIN_ETACHOICE1	1	Use Eisenstat and Walker Choice 1 for η .		
KIN_ETACHOICE2	2	Use Eisenstat and Walker Choice 2 for η .		
KIN_ETACONSTANT	,			
KIN_NONE 0 Use inexact Newton globalization.				
KIN_LINESEARCH 1 Use linesearch globalization.				
	I	terative linear solver modules		
PREC_NONE	0	No preconditioning		
PREC_RIGHT	2	Preconditioning on the right.		
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.		
CLASSICAL_GS	2 Use classical Gram-Schmidt procedure.			

B.2 KINSOL output constants

KINSOL main solver module				
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 kin_mem 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 KINMalloc.		
KIN_MEM_FAIL	-4	A memory allocation failed.		

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KIN_LINESEARCH_NONCONV	-5	The linesearch algorithm was unable to find an iterate suffi-
		ciently 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 β -condition
		for nbcfails iterations.
KIN_LINSOLV_NO_RECOVERY	-9	The user-supplied routine preconditioner slve function failed re-
		coverably, 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 man-
		ner.
KIN_SYSFUNC_FAIL	-13	The system function failed in an unrecoverable manner.
KIN_FIRST_SYSFUNC_ERR	-14	The system function failed recoverably at the first call.
KIN_REPTD_SYSFUNC_ERR	-15	The system function had repeated recoverable errors.

KINLS linear solver interface

KINLS_SUCCESS	0	Successful function return.
KINLS_MEM_NULL	-1	The kin_mem 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 NVECTOR
		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 SUNMATRIX module.
KINLS_SUNLS_FAIL	-8	An error occurred with the current SUNLINSOL module.

Appendix C

SUNDIALS Release History

Table C.1: Release History

Da	ate	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Jun	2019	5.0.0-dev.1	4.0.0-dev.1	5.0.0-dev.1	5.0.0-dev.1	5.0.0-dev.1	4.0.0-dev.1	5.0.0-dev.1
Mar	2019	5.0.0-dev.0	4.0.0-dev.1 4.0.0-dev.0	5.0.0-dev.1 5.0.0-dev.0	5.0.0-dev.1 5.0.0-dev.0	5.0.0-dev.1 5.0.0-dev.0	4.0.0-dev.1 4.0.0-dev.0	5.0.0-dev.1 5.0.0-dev.0
	2019							
Feb		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
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	$\frac{2.3.0}{2.2.2}$	_	2.2.2

continued from last page								
Da	ate	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Jan	2005	2.0.1	_	2.2.1	2.1.1	2.2.1	_	2.2.1
Dec	2004	2.0.0	_	2.2.0	2.1.0	2.2.0	_	2.2.0
Jul	2002	1.0.0	_	2.0.0	1.0.0	2.0.0	_	2.0.0
Mar	2002	_	_	$1.0.0^{3}$	_	_	_	_
Feb	1999	_	_	_	_	$1.0.0^4$	_	_
Aug	1998	_	_	_	_	_	_	$1.0.0^{5}$
Jul	1997	_	_	$1.0.0^2$	_	_	_	_
Sep	1994	_	_	$1.0.0^{1}$	_	_	_	_
¹ CVO	¹ CVODE written, ² PVODE written, ³ CVODE and PVODE combined, ⁴ IDA written, ⁵ KINSOL written							

Bibliography

- [1] KLU Sparse Matrix Factorization Library. http://faculty.cse.tamu.edu/davis/suitesparse.html.
- [2] SuperLU_DIST Parallel Sparse Matrix Factorization Library. http://crd-legacy.lbl.gov/xiaoye/-SuperLU/.
- [3] SuperLU_MT Threaded Sparse Matrix Factorization Library. http://crd-legacy.lbl.gov/xiaoye/-SuperLU/.
- [4] D. G. Anderson. Iterative procedures for nonlinear integral equations. *J. Assoc. Comput. Machinery*, 12:547–560, 1965.
- [5] P. N. Brown. A local convergence theory for combined inexact-Newton/finite difference projection methods. SIAM J. Numer. Anal., 24(2):407–434, 1987.
- [6] P. N. Brown and A. C. Hindmarsh. Reduced Storage Matrix Methods in Stiff ODE Systems. *J. Appl. Math. & Comp.*, 31:49–91, 1989.
- [7] P. N. Brown and Y. Saad. Hybrid Krylov Methods for Nonlinear Systems of Equations. SIAM J. Sci. Stat. Comput., 11:450–481, 1990.
- [8] G. D. Byrne. Pragmatic Experiments with Krylov Methods in the Stiff ODE Setting. In J.R. Cash and I. Gladwell, editors, Computational Ordinary Differential Equations, pages 323–356, Oxford, 1992. Oxford University Press.
- [9] A. M. Collier and R. Serban. Example Programs for KINSOL v5.0.0-dev.1. Technical Report UCRL-SM-208114, LLNL, 2019.
- [10] T. A. Davis and P. N. Ekanathan. Algorithm 907: KLU, a direct sparse solver for circuit simulation problems. *ACM Trans. Math. Softw.*, 37(3), 2010.
- [11] R. S. Dembo, S. C. Eisenstat, and T. Steihaug. Inexact Newton Methods. SIAM J. Numer. Anal., 19:400–408, 1982.
- [12] J. W. Demmel, J. R. Gilbert, and X. S. Li. An asynchronous parallel supernodal algorithm for sparse gaussian elimination. SIAM J. Matrix Analysis and Applications, 20(4):915–952, 1999.
- [13] J. E. Dennis and R. B. Schnabel. Numerical Methods for Unconstrained Optimization and Non-linear Equations. SIAM, Philadelphia, 1996.
- [14] S. C. Eisenstat and H. F. Walker. Choosing the Forcing Terms in an Inexact Newton Method. SIAM J. Sci. Comput., 17:16–32, 1996.
- [15] H. Fang and Y. Saad. Two classes of secant methods for nonlinear acceleration. Numer. Linear Algebra Appl., 16:197–221, 2009.
- [16] R. W. Freund. A Transpose-Free Quasi-Minimal Residual Algorithm for Non-Hermitian Linear Systems. SIAM J. Sci. Comp., 14:470–482, 1993.

284 BIBLIOGRAPHY

[17] Laura Grigori, James W. Demmel, and Xiaoye S. Li. Parallel symbolic factorization for sparse LU with static pivoting. SIAM J. Scientific Computing, 29(3):1289–1314, 2007.

- [18] M. R. Hestenes and E. Stiefel. Methods of Conjugate Gradients for Solving Linear Systems. J. Research of the National Bureau of Standards, 49(6):409–436, 1952.
- [19] A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker, and C. S. Woodward. SUNDIALS, suite of nonlinear and differential/algebraic equation solvers. ACM Trans. Math. Softw., (31):363–396, 2005.
- [20] A. C. Hindmarsh, R. Serban, and A. Collier. Example Programs for IDA v5.0.0-dev.1. Technical Report UCRL-SM-208113, LLNL, 2019.
- [21] A. C. Hindmarsh, R. Serban, and D. R. Reynolds. Example Programs for CVODE v5.0.0-dev.1. Technical report, LLNL, 2019. UCRL-SM-208110.
- [22] Seth R. Johnson, Andrey Prokopenko, and Katherine J. Evans. Automated fortran-c++ bindings for large-scale scientific applications. arXiv:1904.02546 [cs], 2019.
- [23] C. T. Kelley. Iterative Methods for Solving Linear and Nonlinear Equations. SIAM, Philadelphia, 1995.
- [24] X. S. Li. An overview of SuperLU: Algorithms, implementation, and user interface. *ACM Trans. Math. Softw.*, 31(3):302–325, September 2005.
- [25] Xiaoye S. Li and James W. Demmel. SuperLU_DIST: A scalable distributed-memory sparse direct solver for unsymmetric linear systems. ACM Trans. Mathematical Software, 29(2):110–140, June 2003.
- [26] X.S. Li, J.W. Demmel, J.R. Gilbert, L. Grigori, M. Shao, and I. Yamazaki. SuperLU Users' Guide. Technical Report LBNL-44289, Lawrence Berkeley National Laboratory, September 1999. http://crd.lbl.gov/~xiaoye/SuperLU/. Last update: August 2011.
- [27] P. A. Lott, H. F. Walker, C. S. Woodward, and U. M. Yang. An accelerated Picard method for nonlinear systems related to variably saturated flow. *Adv. Wat. Resour.*, 38:92–101, 2012.
- [28] J. M. Ortega and W. C. Rheinbolt. *Iterative solution of nonlinear equations in several variables*. SIAM, Philadelphia, 2000. Originally published in 1970 by Academic Press.
- [29] Daniel R. Reynolds. Example Programs for ARKODE v4.0.0-dev.1. Technical report, Southern Methodist University, 2019.
- [30] Y. Saad. A flexible inner-outer preconditioned GMRES algorithm. SIAM J. Sci. Comput., 14(2):461–469, 1993.
- [31] Y. Saad and M. H. Schultz. GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems. SIAM J. Sci. Stat. Comp., 7:856–869, 1986.
- [32] H. A. Van Der Vorst. Bi-CGSTAB: A Fast and Smoothly Converging Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems. SIAM J. Sci. Stat. Comp., 13:631–644, 1992.
- [33] H. F. Walker and P. Ni. Anderson acceleration for fixed-point iterations. SIAM Jour. Num. Anal., 49(4):1715–1735, 2011.

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