User Documentation for KINSOL v2.4.0

Aaron M. Collier, Alan C. Hindmarsh, Radu Serban, and Carol S. Woodward
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

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Chapter 1

Introduction

KINSOL is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers. This suite consists of CVODE, KINSOL, and IDA, and variants of these. KINSOL is a general-purpose nonlinear system solver based on Newton-Krylov solver technology.

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 solution of partial differential equations [2]. 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, preventing 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 into 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 tolerances and has a more modular design to provide flexibility for future enhancements.

At present, KINSOL contains three Krylov methods: the GMRES (Generalized Minimal RESidual) [9], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [10], and TFQMR (Transpose-Free Quasi-Minimal Residual) [7] linear iterative methods. As Krylov methods, these require almost no matrix storage 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 three Krylov methods in KINSOL, we recommend GMRES as the best overall choice. However, users are encouraged to compare all three, especially if encountering convergence failures with GMRES. Bi-CGStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size.

In the process of translating 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 has been created. This module facilitated extension to multiprosessor environments with minimal impact on the rest of the solver. The new 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 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.

There are several motivations for choosing the C language for KINSOL. First, a general movement away from FORTRAN and toward C in scientific computing is 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 v2.4.0

KINSPBCG, KINSPTFQMR, KINDENSE, and KINBAND modules have been added to interface with the Scaled Preconditioned Bi-CGStab (SPBCG), Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR), DENSE, and BAND linear solver modules, respectively (for details see Chapter 5). 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 §2.

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 systems has been further improved to make it more robust.

Changes in v2.2.1

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

Changes in v2.2.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the iopt and ropt arrays. Instead, 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 5.

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 set-type functions.

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 3, then Chapter 5 through §5.5.3 only, and looking at examples in [3]. In a different direction, a more expert user with a nonlinear system may want to (a) use a package preconditioner (§5.7), (b) supply his/her own Jacobian or preconditioner routines (§5.6), (c) supply a new NVECTOR module (Chapter 7), or even (d) supply a different linear solver module (§4.2 and Chapter 9).

The structure of this document is as follows:

- In Chapter 2 we begin with instructions for the installation of KINSOL, within the structure of SUNDIALS.

- In Chapter 3, 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 (§4.1) and the software organization of the KINSOL solver (§4.2).

- Chapter 5 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 6, we describe FKINSOL, an interface module for the use of KINSOL with FORTRAN applications.

- Chapter 7 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, and details on the two NVECTOR implementations provided with SUNDIALS: a serial implementation (§7.1) and a parallel implementation based on MPI (§7.2).

- Chapter 8 describes the interfaces to the linear solver modules, so that a user can provide his/her own such module.

- Chapter 9 describes in detail the generic linear solvers shared by all SUNDIALS solvers.

- Finally, Chapter 10 lists the constants used for input to and output from KINSOL.

Finally, the reader should be aware of the following notational conventions in this user guide: program listings and identifiers (such as `KINMalloc`) 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. In the index, page numbers that appear in bold indicate the main reference for that entry.

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

Chapter 2

KINSOL Installation Procedure

The installation of KINSOL 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 solvers other than KINSOL. [1]

Generally speaking, the installation procedure outlined in §2.1 below will work on commodity LINUX/UNIX systems without modification. Users are still encouraged, however, to carefully read the entire chapter before attempting to install the SUNDIALS suite, in case non-default choices are desired for compilers, compilation options, or the like. In lieu of reading the option list below, the user may invoke the configuration script with the help flag to view a complete listing of available options, which may be done by issuing

```
% ./configure --help
```

from within the sundials directory.

In the descriptions below, *build_tree* refers to the directory under which the user wants to build and/or install the SUNDIALS package. By default, the SUNDIALS libraries and header files are installed under the subdirectories *build_tree*/lib and *build_tree*/include, respectively. Also, *source_tree* refers to the directory where the SUNDIALS source code is located. The chosen *build_tree* may be different from the *source_tree*, thus allowing for multiple installations of the SUNDIALS suite with different configuration options.

Concerning the installation procedure outlined below, after invoking the tar command with the appropriate options, the contents of the SUNDIALS archive (or the *source_tree*) will be extracted to a directory named sundials. Since the name of the extracted directory is not version-specific it is recommended that the user refrain from extracting the archive to a directory containing a previous version/release of the SUNDIALS suite. If the user is only upgrading and the previous installation of SUNDIALS is not needed, then the user may remove the previous installation by issuing

```
% rm -rf sundials
```

from a shell command prompt.

Even though the installation procedure given below presupposes that the user will use the default vector modules supplied with the distribution, using the SUNDIALS suite with a user-supplied vector module normally will not require any changes to the build procedure.

---

[1]Files for both the serial and parallel versions of KINSOL are included in the distribution. For users in a serial computing environment, the files specific to parallel environments (which may be deleted) are as follows: all files in nvec_par; kinbbdpre.c, kinbbdpre_impl.h (in kinsol/source/); kinsol/include/kinbbdpre.h; fkinbbd.c, fkinbbd.h (in kinsol/fcmix/); all files in kinsol/examples_par/; all files in kinsol/fcmix/examples_par/. (By "serial version" of KINSOL we mean the KINSOL solver with the serial NVECTOR module attached, and similarly for "parallel version".)

2.1 Installation steps

To install the SUNDIALS suite, given a downloaded file named *sundials_file*.`tar.gz`, issue the following commands from a shell command prompt, while within the directory where *source_tree* is to be located.

1. `gunzip` *sundials_file*.`tar.gz`

2. `tar -xf` *sundials_file*.`tar`   [creates `sundials` directory]

3. `cd` *build_tree*

4. *path_to_source_tree*/`configure` *options*   [options can be absent]

5. `make`

6. `make install`

7. `make examples`

8. If system storage space conservation is a priority, then issue
   `make clean`
   and/or
   `make examples_clean`
   from a shell command prompt to remove unneeded object files.

2.2 Configuration options

The installation procedure given above will generally work without modification; however, if the system includes multiple MPI implementations, then certain configure script-related options may be used to indicate which MPI implementation should be used. Also, if the user wants to use non-default language compilers, then, again, the necessary shell environment variables must be appropriately redefined. The remainder of this section provides explanations of available configure script options.

General options

`--prefix=PREFIX`

Location for architecture-independent files.

Default: `PREFIX=`*build_tree*

`--includedir=DIR`

Alternate location for installation of header files.

Default: `DIR=PREFIX/include`

`--libdir=DIR`

Alternate location for installation of libraries.

Default: `DIR=PREFIX/lib`

`--disable-examples`

All available example programs are automatically built unless this option is given. The example executables are stored under the following subdirectories of the associated solver:

build_tree/*solver*/`examples_ser` : serial C examples

build_tree/*solver*/`examples_par` : parallel C examples (MPI-enabled)

build_tree/*solver*/`fcmix/examples_ser`: serial FORTRAN examples

build_tree/*solver*/`fcmix`/`examples_par`: parallel FORTRAN examples (MPI-enabled)

Note: Some of these subdirectories may not exist depending upon the solver and/or the configuration options given.

`--disable-`*solver*

Although each existing solver module is built by default, support for a given solver can be explicitly disabled using this option. The valid values for *solver* are: `cvode`, `cvodes`, `ida`, and `kinsol`.

`--with-cppflags=ARG`

Specify additional C preprocessor flags (e.g., `ARG=-I<include_dir>` if necessary header files are located in nonstandard locations).

`--with-cflags=ARG`

Specify additional C compilation flags.

`--with-ldflags=ARG`

Specify additional linker flags (e.g., `ARG=-L<lib_dir>` if required libraries are located in nonstandard locations).

`--with-libs=ARG`

Specify additional libraries to be used (e.g., `ARG=-l<foo>` to link with the library named `libfoo.a` or `libfoo.so`).

`--with-precision=ARG`

By default, SUNDIALS will define a real number (internally referred to as `realtype`) to be a double-precision floating-point numeric data type (`double` C-type); however, this option may be used to build SUNDIALS with `realtype` alternatively defined as a single-precision floating-point numeric data type (`float` C-type) if `ARG=single`, or as a `long double` C-type if `ARG=extended`.

Default: `ARG=double`

Users should *not* build SUNDIALS with support for single-precision floating-point arithmetic on 32- or 64-bit systems. This will almost certainly result in unreliable numerical solutions. The configuration option `--with-precision=single` is intended for systems on which single-precision arithmetic involves at least 14 decimal digits.

⚠️

Options for Fortran support

`--disable-f77`

Using this option will disable all FORTRAN support. The FCVODE, FKINSOL, FIDA, and FNVECTOR modules will not be built, regardless of availability.

`--with-fflags=ARG`

Specify additional FORTRAN compilation flags.

The configuration script will attempt to automatically determine the function name mangling scheme required by the specified FORTRAN compiler, but the following two options may be used to override the default behavior.

`--with-f77underscore=ARG`

This option pertains to the FCVODE, FKINSOL, FIDA, and FNVECTOR FORTRAN-C interface modules and is used to specify the number of underscores to append to function names so FORTRAN routines can properly link with the associated SUNDIALS libraries. Valid values for `ARG` are: `none`, `one` and `two`.

Default: `ARG=one`

`--with-f77case=ARG`

> Use this option to specify whether the external names of the FCVODE, FKINSOL, FIDA, and FN-VECTOR FORTRAN-C interface functions should be lowercase or uppercase so FORTRAN routines can properly link with the associated SUNDIALS libraries. Valid values for `ARG` are: `lower` and `upper`.
>
> Default: `ARG=lower`

Options for MPI support

The following configuration options are only applicable to the parallel SUNDIALS packages:

`--disable-mpi`

> Using this option will completely disable MPI support.

`--with-mpicc=ARG`

`--with-mpif77=ARG`

> By default, the configuration utility script will use the MPI compiler scripts named `mpicc` and `mpif77` to compile the parallelized SUNDIALS subroutines; however, for reasons of compatibility, different executable names may be specified via the above options. Also, `ARG=no` can be used to disable the use of MPI compiler scripts, thus causing the serial C and FORTRAN compilers to be used to compile the parallelized SUNDIALS functions and examples.

`--with-mpi-root=MPIDIR`

> This option may be used to specify which MPI implementation should be used. The SUNDIALS configuration script will automatically check under the subdirectories `MPIDIR/include` and `MPIDIR/lib` for the necessary header files and libraries. The subdirectory `MPIDIR/bin` will also be searched for the C and FORTRAN MPI compiler scripts, unless the user uses `--with-mpicc=no` or `--with-mpif77=no`.

`--with-mpi-incdir=INCDIR`

`--with-mpi-libdir=LIBDIR`

`--with-mpi-libs=LIBS`

> These options may be used if the user would prefer not to use a preexisting MPI compiler script, but instead would rather use a serial complier and provide the flags necessary to compile the MPI-aware subroutines in SUNDIALS.
>
> Often an MPI implementation will have unique library names and so it may be necessary to specify the appropriate libraries to use (e.g., `LIBS=-lmpich`).
>
> Default: `INCDIR=MPIDIR/include` and `LIBDIR=MPIDIR/lib`

`--with-mpi-flags=ARG`

> Specify additional MPI-specific flags.

Options for library support

By default, only static libraries are built, but the following option may be used to build shared libraries on supported platforms.

`--enable-shared`

> Using this particular option will result in both static and shared versions of the available SUNDIALS libraries being built if the system supports shared libraries. To build only shared libraries also specify `--disable-static`.

Note: The FCVODE, FKINSOL, and FIDA libraries can only be built as static libraries because they contain references to externally defined symbols, namely user-supplied FORTRAN subroutines. Although the FORTRAN interfaces to the serial and parallel implementations of the supplied NVECTOR module do not contain any unresolvable external symbols, the libraries are still built as static libraries for the purpose of consistency.

Environment variables

The following environment variables can be locally (re)defined for use during the configuration of SUNDIALS. See the next section for illustrations of these.

CC

F77

Since the configuration script uses the first C and FORTRAN compilers found in the current executable search path, then each relevant shell variable (`CC` and `F77`) must be locally (re)defined in order to use a different compiler. For example, to use `xcc` (executable name of chosen compiler) as the C language compiler, use `CC=xcc` in the configure step.

CFLAGS

FFLAGS

Use these environment variables to override the default C and FORTRAN compilation flags.

2.3 Configuration examples

The following examples are meant to help demonstrate proper usage of the configure options:

```
% configure CC=gcc F77=g77 --with-cflags=-g3 --with-fflags=-g3 \
            --with-mpicc=/usr/apps/mpich/1.2.4/bin/mpicc \
            --with-mpif77=/usr/apps/mpich/1.2.4/bin/mpif77
```

The above example builds SUNDIALS using `gcc` as the serial C compiler, `g77` as the serial FORTRAN compiler, `mpicc` as the parallel C compiler, `mpif77` as the parallel FORTRAN compiler, and appends the `-g3` compilaton flag to the list of default flags.

```
% configure CC=gcc --disable-examples --with-mpicc=no \
            --with-mpi-root=/usr/apps/mpich/1.2.4 \
            --with-mpi-libs=-lmpich
```

This example again builds SUNDIALS using `gcc` as the serial C compiler, but the `--with-mpicc=no` option explicitly disables the use of the corresponding MPI compiler script. In addition, since the `--with-mpi-root` option is given, the compilation flags `-I/usr/apps/mpich/1.2.4/include` and `-L/usr/apps/mpich/1.2.4/lib` are passed to `gcc` when compiling the MPI-enabled functions. The `--disable-examples` option disables the examples (which means a FORTRAN compiler is not required). The `--with-mpi-libs` option is required so that the configure script can check if `gcc` can link with the appropriate MPI library.

2.4 Installed libraries and exported header files

Using the standard SUNDIALS build system, the command

```
% make install
```

will install the libraries under *libdir* and the public header files under *incdir*. The default values for these directories are *build_tree*/lib and *build_tree*/include, respectively, but can be changed using the configure script options --prefix, --includedir and --libdir (see §2.2). For example, a global installation of SUNDIALS on a *NIX system could be accomplished using

```
% configure --prefix=/usr/local
```

Although all installed libraries reside under *libdir*, the public header files are further organized into subdirectories under *incdir*.

The installed libraries and exported header files are listed for reference in Table 2.1. The file extension *.lib* is typically `.so` for shared libraries and `.a` for static libraries (see *Options for library support* for additional details).

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the *incdir*/sundials directory since they are explicitly included by the appropriate solver header files (*e.g.*, cvode_dense.h includes sundials_dense.h). However, it is both legal and safe to do so (*e.g.*, the functions declared in sundials_smalldense.h could be used in building a preconditioner).

2.5 Building SUNDIALS without the configure script

If the `configure` script cannot be used (*e.g.*, when building SUNDIALS under Microsoft Windows without using Cygwin), or if the user prefers to own the build process (*e.g.*, when SUNDIALS is incorporated into a larger project with its own build system), then the header and source files for a given module can be copied from the *source_tree* to some other location and compiled separately.

The following files are required to compile a SUNDIALS solver module:

- public header files located under *source_tree*/*solver*/include

- implementation header files and source files located under *source_tree*/*solver*/source

- (optional) FORTRAN/C interface files located under *source_tree*/*solver*/fcmix

- shared public header files located under *source_tree*/shared/include

- shared source files located under *source_tree*/shared/source

- (optional) NVECTOR_SERIAL header and source files located under *source_tree*/nvec_ser

- (optional) NVECTOR_PARALLEL header and source files located under *source_tree*/nvec_par

- configuration header file sundials_config.h (see below)

A sample header file that, appropriately modified, can be used as sundials_config.h (otherwise created automatically by the `configure` script) is provided below. The various preprocessor macros defined within sundials_config.h have the following uses:

- Precision of the SUNDIALS realtype type

  Only one of the macros SUNDIALS_SINGLE_PRECISION, SUNDIALS_DOUBLE_PRECISION and SUNDIALS_EXTENDED_PRECISION should be defined to indicate if the SUNDIALS realtype type is an alias for `float`, `double`, or `long double`, respectively.

- Use of generic math functions

  If SUNDIALS_USE_GENERIC_MATH is defined, then the functions in sundials_math.(h,c) will use the `pow`, `sqrt`, `fabs`, and `exp` functions from the standard math library (see `math.h`), regardless of the definition of `realtype`. Otherwise, if `realtype` is defined to be an alias for the `float` C-type, then SUNDIALS will use `powf`, `sqrtf`, `fabsf`, and `expf`. If `realtype` is instead defined to be a synonym for the `long double` C-type, then `powl`, `sqrtl`, `fabsl`, and `expl` will be used.

Table 2.1: SUNDIALS libraries and header files (names are relative to *libdir* for libraries and to *incdir* for header files)

SHARED	Libraries	n/a	
	Header files	sundials/sundials_types.h	sundials/sundials_math.h
		sundials/sundials_config.h	sundias/sundials_nvector.h
		sundials/sunials_smalldense.h	sundials/sundials_dense.h
		sundials/sundials_iterative.h	sundials/sundials_band.h
		sundials/sundials_spbcgs.h	sundials/sundials_sptfqmr.h
		sundials/sundials_spgmr.h	
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib*	libsundials_fnvecserial.a
	Header files	nvector_serial.h	
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib*	libsundials_fnvecparallel.a
	Header files	nvector_parallel.h	
CVODE	Libraries	libsundials_cvode.*lib*	libsundials_fcvode.a
	Header files	cvode.h	
		cvode/cvode_dense.h	cvode/cvode_band.h
		cvode/cvode_diag.h	cvode/cvode_spils.h
		cvode/cvode_bandpre.h	cvode/cvode_bbdpre.h
		cvode/cvode_spgmr.h	cvode/cvode_spbcgs.h
		cvode/cvode_sptfqmr.h	cvode/cvode_impl.h
CVODES	Libraries	libsundials_cvodes.*lib*	
	Header files	cvodes.h	cvodea.h
		cvodes/cvodes_dense.h	cvodes/cvodes_band.h
		cvodes/cvodes_diag.h	cvodes/cvodes_spils.h
		cvodes/cvodes_bandpre.h	cvodes/cvodes_bbdpre.h
		cvodes/cvodes_spgmr.h	cvodes/cvodes_spbcgs.h
		cvodes/cvodes_sptfqmr.h	cvodes/cvodes_impl.h
		cvodes/cvodea_impl.h	
IDA	Libraries	libsundials_ida.*lib*	libsundials_fida.a
	Header files	ida.h	
		ida/ida_dense.h	ida/ida_band.h
		ida/ida_spils.h	ida/ida_spgmr.h
		ida/ida_spbcgs.h	ida/ida_sptfqmr.h
		ida/ida_bbdpre.h	ida/ida_impl.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a
	Header files	kinsol.h	
		kinsol/kinsol_dense.h	kinsol/kinsol_band.h
		kinsol/kinsol_spils.h	kinsol/kinsol_spgmr.h
		kinsol/kinsol_spbcgs.h	kinsol/kinsol_sptfqmr.h
		kinsol/kinsol_bbdpre.h	kinsol/kinsol_impl.h

Note: Although the `powf/powl`, `sqrtf/sqrtl`, `fabsf/fabsl`, and `expf/expl` routines are not specified in the ANSI C standard, they are ISO C99 requirements. Consequently, these routines will only be used if available.

- Fortran name-mangling scheme

  The macros given below are used to transform the C-language function names defined in the Fortran-C inteface modules in a manner consistent with the preferred Fortran compiler, thus allowing native C functions to be called from within a Fortran subroutine. The name-mangling scheme can be specified either by appropriately defining the parameterized macros (using the stringization operator, `##`, if necessary)

    – `F77_FUNC(name,NAME)`
    – `F77_FUNC_(name,NAME)`

  or by defining *one* macro from each of the following lists:

    – `SUNDIALS_CASE_LOWER` or `SUNDIALS_CASE_UPPER`
    – `SUNDIALS_UNDERSCORE_NONE`, `SUNDIALS_UNDERSCORE_ONE`, or `SUNDIALS_UNDERSCORE_TWO`

  For example, to specify that mangled C-language function names should be lowercase with one underscore appended include either

  ```
  #define F77_FUNC(name,NAME) name ## _
  #define F77_FUNC_(name,NAME) name ## _
  ```

  or

  ```
  #define SUNDIALS_CASE_LOWER 1
  #define SUNDIALS_UNDERSCORE_ONE 1
  ```

  in the `sundials_config.h` header file.

- Use of an MPI communicator other than `MPI_COMM_WORLD` in Fortran

  If the macro `SUNDIALS_MPI_COMM_F2C` is defined, then the MPI implementation used to build SUNDIALS defines the type `MPI_Fint` and the function `MPI_Comm_f2c`, and it is possible to use MPI communicators other than `MPI_COMM_WORLD` with the Fortran-C interface modules.

```
 1   /*
 2    * -----------------------------------------------------------------
 3    * Copyright (c) 2005, The Regents of the University of California.
 4    * Produced at the Lawrence Livermore National Laboratory.
 5    * All rights reserved.
 6    * For details, see sundials/shared/LICENSE.
 7    * -----------------------------------------------------------------
 8    * SUNDIALS configuration header file
 9    * -----------------------------------------------------------------
10    */
11
12
13   /* Define SUNDIALS version number
14    * ------------------------------ */
15
16   #define SUNDIALS_PACKAGE_VERSION "2.2.0"
17
18   /* Define precision of SUNDIALS data type 'realtype'
19    * ------------------------------------------------- */
20
21   /* Define SUNDIALS data type 'realtype' as 'double' */
22   #define SUNDIALS_DOUBLE_PRECISION 1
23
24   /* Define SUNDIALS data type 'realtype' as 'float' */
25   /* #define SUNDIALS_SINGLE_PRECISION 1 */
26
27   /* Define SUNDIALS data type 'realtype' as 'long double' */
28   /* #define SUNDIALS_EXTENDED_PRECISION 1 */
29
30   /* Use generic math functions
31    * -------------------------- */
32
33   #define SUNDIALS_USE_GENERIC_MATH 1
34
35   /* FCMIX: Define Fortran name-mangling macro
36    * ----------------------------------------- */
37
38   #define F77_FUNC(name,NAME) name ## _
39   #define F77_FUNC_(name,NAME) name ## _
40
41   /* FCMIX: Define case of function names
42    * ------------------------------------ */
43
44   /* FCMIX: Make function names lowercase */
45   /* #define SUNDIALS_CASE_LOWER 1 */
46
47   /* FCMIX: Make function names uppercase */
48   /* #define SUNDIALS_CASE_UPPER 1 */
49
50   /* FCMIX: Define number of underscores to append to function names
51    * -------------------------------------------------------------- */
52
53   /* FCMIX: Do NOT append any underscores to functions names */
54   /* #define SUNDIALS_UNDERSCORE_NONE 1 */
55
56   /* FCMIX: Append ONE underscore to function names */
57   /* #define SUNDIALS_UNDERSCORE_ONE 1 */
58
59   /* FCMIX: Append TWO underscores to function names */
60   /* #define SUNDIALS_UNDERSCORE_TWO 1 */
61
62   /* FNVECTOR: Allow user to specify different MPI communicator
63    * --------------------------------------------------------- */
64
65   #define SUNDIALS_MPI_COMM_F2C 1
```

Chapter 3

Mathematical Considerations

KINSOL solves nonlinear algebraic systems in real N-space,

$$F(u) = 0, \quad F : \mathbf{R}^N \to \mathbf{R}^N, \tag{3.1}$$

given an initial guess u_0.

Basic Newton iteration

Depending on the linear solver used, KINSOL can employ either an Inexact Newton method [1, 2, 4, 5, 8], or a Modified Newton method. At the highest level, KINSOL implements the following iteration scheme:

1. Set $u_0 =$ an initial guess

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

Here, u_n is the nth 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 2(a), KINSOL provides a choice of five methods:

- dense direct solver,

- band direct solver,

- scaled preconditioned GMRES (Generalized Minimal Residual method),

- scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method), or

- scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method).

When using one of the direct linear solvers, the linear system in 2(a) is solved exactly thus resulting in a Modified Newton method (the Jacobian matrix is normally outdated; see below[1]). Note that the direct linear solvers (dense and band) can only be used with serial vector representations.

---

[1] KINSOL allows the user to enforce a Jacobian evaluation at each iteration thus allowing for an Exact Newton iteration.

On the other hand, using any of the iterative linear solvers (GMRES, Bi-CGStab, or TFQMR), the linear system in 2(a) is solved only approximately thus resulting in an Inexact Newton method. In the latter case, right preconditioning is available if the preconditioning setup and solve routines are 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.

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 direct linear solvers, or the preconditioner matrix P in the case of iterative linear solvers) as infrequently as possible to balance the high costs of matrix operations against other costs. Specifically, these updates occur when:

- the problem is initialized,

- $\|\lambda\delta_{n-1}\|_{D_u,\infty} > 1.5$ (Inexact Newton only),

- mbset$= 10$ nonlinear iterations have passed since the last update,

- the linear solver failed recoverably with outdated Jacobian information,

- the global strategy failed with outdated Jacobian information, or

- $\|\lambda\delta_n\|_{D_u,\infty} <$ STEPTOL with outdated Jacobian 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.

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:

$$\|z\|_{D_u} = \|D_u z\|_2, \;\; \|z\|_{D_F} = \|D_F z\|_2, \;\; \|z\|_{D_u,\infty} = \|D_u z\|_\infty, \;\text{and}\; \|z\|_{D_F,\infty} = \|D_F z\|_\infty \qquad (3.2)$$

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 (3.6) and (3.8) 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 [5] 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)

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

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):

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

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} = $ STEPMAX$/\|\delta_n\|_{D_u}$). In the above expressions, v^j indicates the jth component of a vector v.

For more details, the reader is referred to [5].

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 $U^{1/3}$. For the latter, the Newton method will terminate when the maximum scaled step is below a given tolerance

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

where 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 ith 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 (over all i) 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 Modified Newton method (i.e.; when a direct linear solver is used), in addition to the strategy described below 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

$$\|D_u F(u_n)\|_2 > \omega\|D_u F(u_m)\|_2,$$

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

$$\omega = \min\left(\omega_{min}\, e^{\max(0,\beta-1)}, \omega_{max}\right), \tag{3.3}$$

with β defined as

$$\beta = \frac{\|D_u F(u_n)\|_2}{\text{FTOL}}, \tag{3.4}$$

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 [6]. 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 [6].

Difference quotient Jacobian approximations

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

$$J^{ij} = [F^i(u + \sigma_j e^j) - F^i(u)]/\sigma_j . \tag{3.5}$$

The increments σ_j are given by

$$\sigma_j = \sqrt{U}\ \max\left\{|u^j|, 1/D_u^j\right\} , \tag{3.6}$$

where U is the unit roundoff. 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.

In the case of a Krylov method, 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

$$J(u)v \approx [F(u + \sigma v) - F(u)]/\sigma \tag{3.7}$$

where u is the current approximation to a root of (3.1), and σ is a scalar. The choice of σ is taken from [2] and is given by

$$\sigma = \frac{\max\{|u^T v|, u_{typ}^T |v|\}}{\|v\|_2}\text{sign}(u^T v)\sqrt{U} , \tag{3.8}$$

where u_{typ} is a vector of typical values for the absolute values of the solution (and can be taken to be inverses of the scale factors given for u as described below), and U is unit roundoff. Convergence of the Newton method is maintained as long as the value of σ remains appropriately small as shown in [1].

Chapter 4

Code Organization

4.1 SUNDIALS organization

The family of solvers referred to as SUNDIALS consists of the solvers CVODE (for ODE systems), KINSOL (for nonlinear algebraic systems), and IDA (for differential-algebraic systems). In addition, variants of these which also do sensitivity analysis calculations are available or in development. CVODES, an extension of CVODE that provides both forward and adjoint sensitivity capabilities is available, while IDAS is currently in development.

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Fig. 4.1). The following is a list of the solver packages presently available:

- CVODE, a solver for stiff and nonstiff ODEs $dy/dt = f(t, y)$;

- CVODES, a solver for stiff and nonstiff ODEs $dy/dt = f(t, y, p)$ with sensitivity analysis capabilities;

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

- IDA, a solver for differential-algebraic systems $F(t, y, y') = 0$.

4.2 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 4.2. 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 modules is specified, and is then invoked as needed.

At present, the package includes the following five KINSOL linear system modules:

- KINDENSE: LU factorization and backsolving with dense matrices;

- KINBAND: LU factorization and backsolving with banded matrices;

- KINSPGMR: scaled preconditioned GMRES method;

- KINSPBCG: scaled preconditioned Bi-CGStab method;

- KINSPTFQMR: scaled preconditioned TFQMR method.
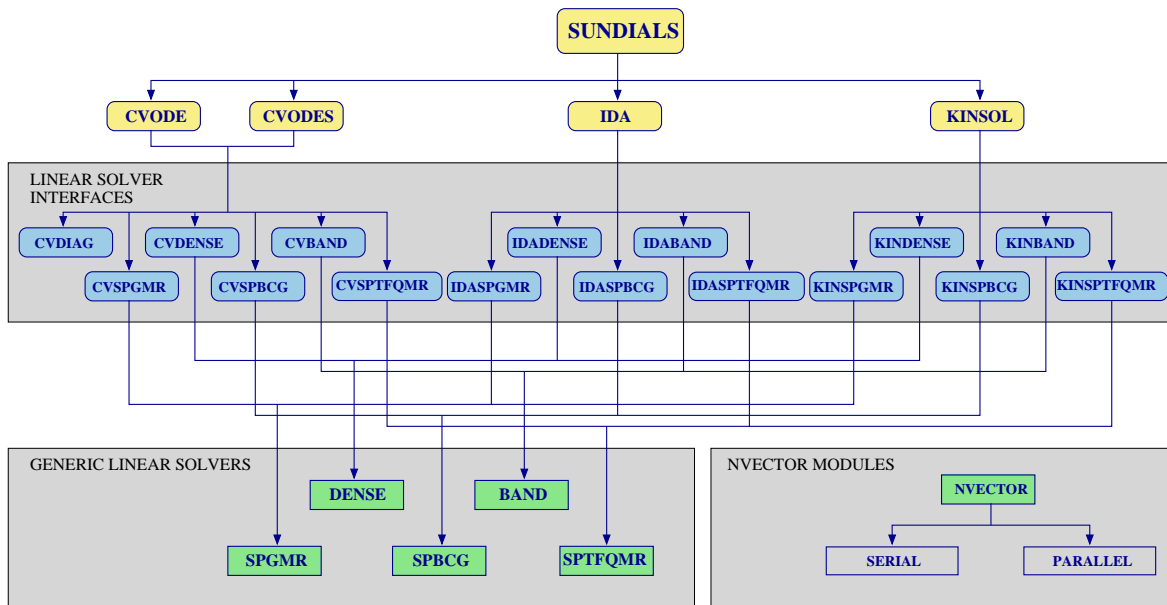
(a) High-level diagram
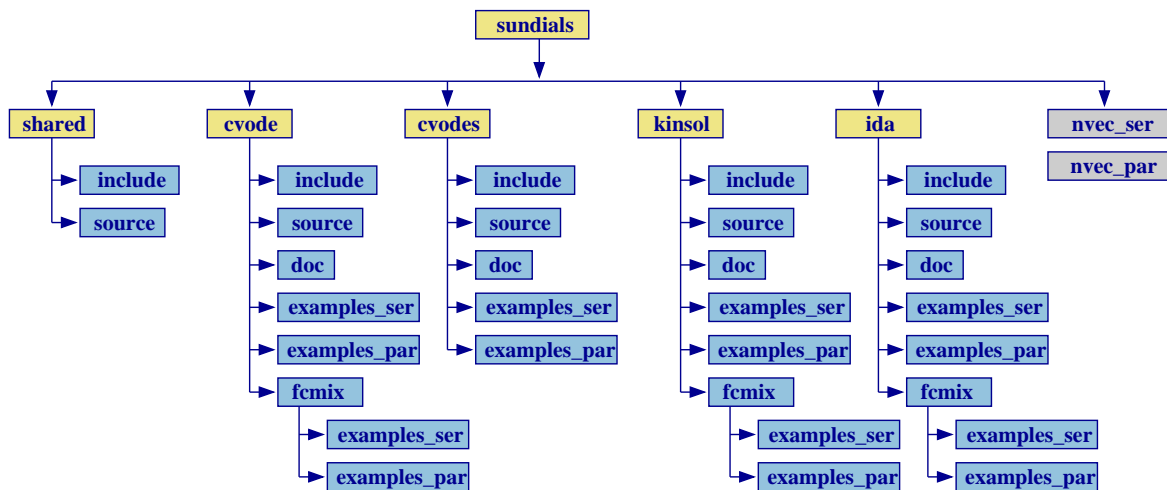
(b) Directory structure of the source tree

Figure 4.1: Organization of the SUNDIALS suite

Figure 4.2: 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.

This set of linear solver modules is intended to be expanded in the future as new algorithms are developed.

In the case of the direct methods KINDENSE and KINBAND, the package includes an algorithm for the approximation of the Jacobian by difference quotients, but the user also has the option of supplyi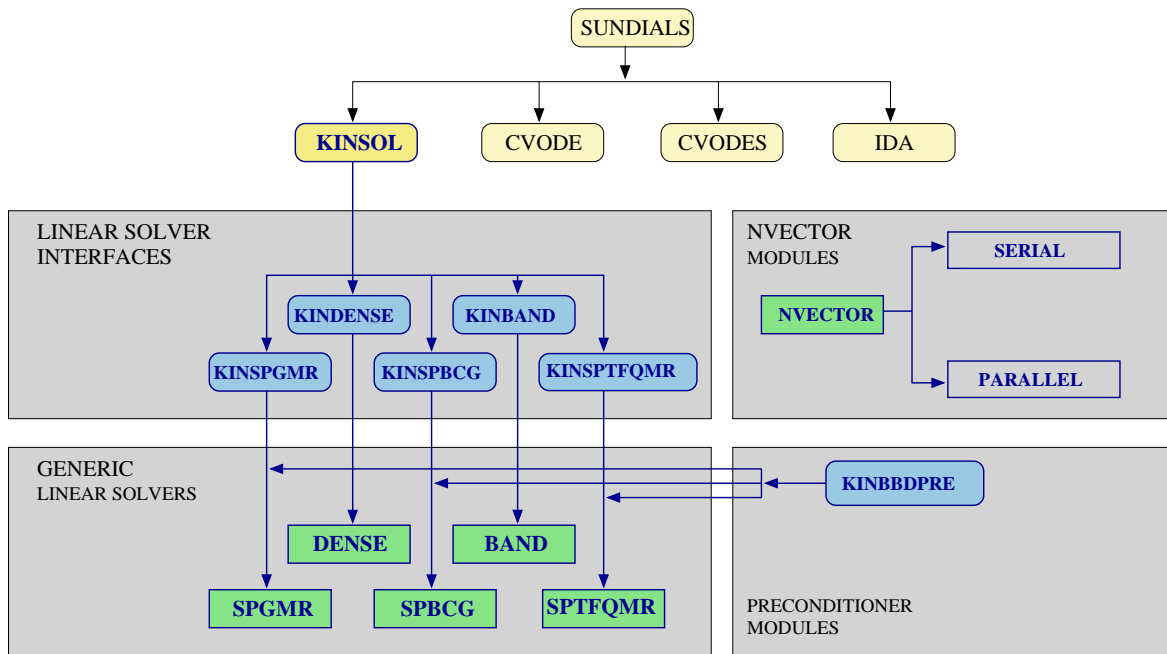ng the Jacobian (or an approximation to it) directly. In the case of the Krylov methods KINSPGMR, KINSPBCG and KINSPTFQMR, the package includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector of appropriate length. Again, the user has the option of providing a routine for this operation. For the Krylov methods, the preconditioning must be supplied by the user, in twho phases: setup (preprocessing of Jacobian data) and solve.

Each KINSOL linear solver module consists of four routines, devoted to (1) memory allocation and initialization, (2) setup of the matrix data involved, (3) solution of the system, and (4) freeing of memory. The setup and solution phases are separate because the evaluation of Jacobians and preconditioners is done only periodically during the integration, 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.

These modules are also decomposed in another way. Each of the modules KINDENSE, KINBAND, KINSPGMR, KINSPBCG, and KINSPTFQMR is a set of interface routines built on top of a generic solver module, name DENSE, BAND, SPGMR, SPBCG, and SPTFQMR, respectively. The interface deals with the use of these methods in the KINSOL context, whereas the generic solver is independent of the context. While the generic solvers here were generated with SUNDIALS in mind, our intention is that they be usable in other applications as general-purpose solvers. This separation also allows for any generic solver to be replaced by an improved version, with no necessity to revise the KINSOL package elsewhere.

KINSOL also provides a preconditioner module called KINBBDPRE for use with any of the Krylov iterative liear solvers. It works in conjunction with NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix, as further described in §5.7.

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 different problems are solved by intermixed calls to the package from one user program.

Chapter 5

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 final section describes the FORTRAN/C interface module, which supports users with applications written in FORTRAN77. The listings of the sample programs in the companion document [3] 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.

The user should be aware that not all linear solver modules are compatible with all NVECTOR implementations. For example, NVECTOR_PARALLEL is not compatible with the direct dense or direct band linear solvers since these linear solver modules need to form the complete system Jacobian. The following KINSOL modules can only be used with NVECTOR_SERIAL: KINDENSE and KINBAND. The preconditioner module KINBBDPRE can only be used with NVECTOR_PARALLEL.

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 Chapter 10.

5.1   Access to library and header files

At this point, it is assumed that the installation of KINSOL, following the procedure described in Chapter 2, 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 or two 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`

- *incdir*/`include/kinsol`

- *incdir*/`include/sundials`

The directories *libdir* and *incdir* are the install libray and include directories. For a default installation, these are *build_tree*/`lib` and *build_tree*/`include`, respectively, where *build_tree* was defined in Chapter 2.

5.2   Data types

The `sundials_types.h` file contains the definition of the type `realtype`, which is used by the SUNDIALS solvers for all floating-point data. The type `realtype` can be `float`, `double`, or `long double`, with the default being `double`. The user can change the precision of the SUNDIALS solvers arithmetic at the configuration stage (see §2.2).

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 the typedef for `realtype` matches this choice). 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 §2.2).

5.3   Header files

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

- `kinsol.h`, the header file for KINSOL, which defines several types and various constants, and includes function prototypes.

`kinsol.h` also includes `sundials_types.h`, which defines the types `realtype` and `booleantype` and constants `FALSE` and `TRUE`.

The calling program must also include an NVECTOR implementation header file (see Chapter 7 for details). For the two NVECTOR implementations that are included in the KINSOL package, the corresponding header files are:

- `nvector_serial.h`, which defines the serial implementation, NVECTOR_SERIAL;

- `nvector_parallel.h`, which defines the parallel MPI implementation, NVECTOR_PARALLEL.

Note that both of these files include in turn the header file `sundials_nvector.h`, which defines the abstract `N_Vector` type.

Finally, a linear solver module header file is required. The header files corresponding to the various linear solver options in KINSOL are:

- `kinsol_dense.h`, which is used with the dense direct linear solver in the context of KINSOL. This in turn includes a header file (`sundials_dense.h`) which defines the `DenseMat` type and corresponding accessor macros;

- `kinsol_band.h`, which is used with the band direct linear solver in the context of KINSOL. This in turn includes a header file (`sundials_band.h`) which defines the `BandMat` type and corresponding accessor macros;

- `kinsol_spgmr.h`, which is used with the Krylov solver SPGMR in the context of KINSOL;

- `kinsol_spbcgs.h`, which is used with the Krylov solver SPBCG in the context of KINSOL;

- `kinsol_sptfqmr.h`, which is used with the Krylov solver SPTFQMR in the context of KINSOL;

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

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the `kinkryx` example [3], preconditioning is done with a block-diagonal matrix. For this, the header `sundials_smalldense.h` is included.

5.4   A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the solution of a nonlinear problem. Some steps are independent of the NVECTOR implementation used; where this is not the case, usage specifications are given for the two implementations provided with KINSOL: Steps marked with [**P**] correspond to NVECTOR_PARALLEL, while steps marked with [**S**] correspond to NVECTOR_SERIAL.

1. [**P**] **Initialize MPI**

   Call `MPI_Init(&argc, &argv);` to initialize MPI if used by the user's program, aside from the internal use in NVECTOR_PARALLEL. Here `argc` and `argv` are the command line argument counter and array received by `main`.

2. **Set problem dimensions**

   [**S**] Set `N`, the problem size N.

   [**P**] Set `Nlocal`, the local vector length (the sub-vector length for this process); `N`, the global vector length (the problem size N, and the sum of all the values of `Nlocal`); and the active set of processes.

3. **Set vector with initial guess**

   To set the vector `u` of initial values, use functions defined by a particular NVECTOR implementation. If a `realtype` array `udata` already exists, containing the initial guess of u_0, make the call:

   [**S**] `u = N_VMake_Serial(N, udata);`

   [**P**] `u = N_VMake_Parallel(comm, Nlocal, N, udata);`

   Otherwise, make the call:

   [**S**] `u = N_VNew_Serial(N);`

   [**P**] `u = N_VNew_Parallel(comm, Nlocal, N);`

   and load initial values into the structure defined by:

   [**S**] `NV_DATA_S(u)`

   [**P**] `NV_DATA_P(u)`

   Here `comm` is the MPI communicator, set in one of two ways: If a proper subset of active processes is to be used, `comm` must be set by suitable MPI calls. Otherwise, to specify that all processes are to be used, `comm` must be `MPI_COMM_WORLD`.

4. **Create KINSOL object**

   Call `kin_mem = KINCreate();` to create the KINSOL memory block. `KINCreate` returns a pointer to the KINSOL memory structure. See §5.5.1 for details.

5. **Set optional inputs**

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

6. **Allocate internal memory**

   Call `KINMalloc(...);` to specify the problem defining function F, allocate internal memory for KINSOL, and initialize KINSOL. `KINMalloc` returns a flag to indicate success or an illegal argument value. See §5.5.1 for details.

7. **Attach linear solver module**

   Initialize the linear solver module with one of the following calls (for details see §5.5.2).

   [**S**] `ier = KINDense(...);`

   [**S**] `ier = KINBand(...);`

   `ier = KINSpgmr(...);`

   `ier = KINSpbcg(...);`

   `ier = KINSptfqmr(...);`

8. **Set linear solver optional inputs**

   Call `KIN*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See §5.5.4 for details.

9. **Solve problem**

   Call `ier = KINSol(...);` to solve the nonlinear problem for a given initial guess. See §5.5.3 for details.

10. **Get optional outputs**

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

11. **Deallocate memory for solution vector**

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

    [**S**] `N_VDestroy_Serial(u);`

    [**P**] `N_VDestroy_Parallel(u);`

12. **Free solver memory**

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

13. [**P**] **Finalize MPI**

    Call `MPI_Finalize();` to terminate MPI.

5.5 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 §5.5.4, 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 §5.4 for the correct order of these calls.

5.5.1   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`.

| KINMalloc |

Call	`flag = KINMalloc(kin_mem, func, tmpl);`	
Description	The function `KINMalloc` specifies the problem-defining function, allocates internal memory, and initializes KINSOL.	
Arguments	`kin_mem`	(`void *`) pointer to the KINSOL memory block returned by `KINCreate`.
	`func`	(`KINSysFn`) is the C function which computes F in the nonlinear problem. This function has the form `func(u, fval, f_data)` (for full details see §5.6.1).
	`tmpl`	(`N_Vector`) is an `N_Vector` which is used as a template to create (by cloning) necessary vectors in `kin_mem`.
Return value	The return flag `flag` (of type `int`) will be one of the following:	
	`KIN_SUCCESS`	The call to `KINMalloc` 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 `KINMalloc` has an illegal value.
Notes	If an error occurred, `KINMalloc` 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 `KINMalloc`.
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.

5.5.2   Linear solver specification functions

As previously explained, Newton iteration requires the solution of linear systems of the form (2). There are five KINSOL linear solvers currently available for this task: KINDENSE, KINBAND, KINSPGMR, KINSPBCG, and KINSPTFQMR. The first two are direct solvers and their names indicate the type of approximation used for the Jacobian $J = \partial F / \partial u$; KINDENSE and KINBAND work with dense and banded approximations to J, respectively. The last three KINSOL linear solvers — KINSPGMR, KINSPBCG, and

KINSPTFQMR — are Krylov iterative solvers, which use scaled preconditioned GMRES, scaled precon-
ditioned Bi-CGStab, and scaled preconditioned TFQMR, respectively. Together, they are referred to
as KINSPILS (from scaled preconditioned iterative linear solvers).

To specify a KINSOL linear solver, after the call to KINCreate but before any calls to KINSol,
the user's program must call one of the functions KINDense, KINBand, KINSpgmr, KINSpbcg, or
KINSptfqmr, as documented below. The first argument passed to these functions is the KINSOL mem-
ory pointer returned by KINCreate. A call to one of these functions links the main KINSOL nonlinear
solver to a linear solver and allows the user to specify parameters which are specific to a particular
solver, such as the half-bandwidths in the KINBAND case. The use of each of the linear solvers involves
certain constants and possibly some macros, that are likely to be needed in the user code. These are
available in the corresponding header file associated with the linear solver, as specified below.

In each case, the linear solver module used by KINSOL is actually built on top of a generic linear
system solver, which may be of interest in itself. These generic solvers, denoted DENSE, BAND, SPGMR,
SPBCG, and SPTFQMR, are described separately in Chapter 9.

KINDense

Call	`flag = KINDense(kin_mem, N);`
Description	The function KINDense selects the KINDENSE linear solver.
	The user's main function must include the `kinsol_dense.h` header file.
Arguments	`kin_mem` (`void *`) pointer to the KINSOL memory block.
	`N` (`long int`) problem dimension.
Return value	The return value `flag` (of type `int`) is one of

            KINDENSE_SUCCESS   The KINDENSE initialization was successful.
            KINDENSE_MEM_NULL   The `kin_mem` pointer is NULL.
            KINDENSE_ILL_INPUT   The KINDENSE solver is not compatible with the current NVECTOR
                                     module.
            KINDENSE_MEM_FAIL   A memory allocation request failed.

Notes	The KINDENSE linear solver may not be compatible with a particular implementation of the NVECTOR module. Of the two NVECTOR modules provided by SUNDIALS, only NVECTOR_SERIAL is compatible, while NVECTOR_PARALLEL is not.

KINBand

Call	`flag = KINBand(kin_mem, N, mupper, mlower);`
Description	The function KINBand selects the KINBAND linear solver.
	The user's main function must include the `kinsol_band.h` header file.
Arguments	`kin_mem` (`void *`) pointer to the KINSOL memory block.
	`N` (`long int`) problem dimension.
	`mupper` (`long int`) upper half-bandwidth of the problem Jacobian (or of the approximation of it).
	`mlower` (`long int`) lower half-bandwidth of the problem Jacobian (or of the approximation of it).
Return value	The return value `flag` (of type `int`) is one of

            KINBAND_SUCCESS   The KINBAND initialization was successful.
            KINBAND_MEM_NULL   The `kin_mem` pointer is NULL.
            KINBAND_ILL_INPUT   The KINBAND solver is not compatible with the current NVECTOR
                                  module, or one of the Jacobian half-bandwidths is outside its valid
                                  range ($0\ldots$ N-1).
            KINBAND_MEM_FAIL   A memory allocation request failed.

Notes   The KINBAND linear solver may not be compatible with a particular implementation of the NVECTOR module. Of the two NVECTOR modules provided by SUNDIALS, only NVECTOR_SERIAL is compatible, while NVECTOR_PARALLEL is not. The half-bandwidths are to be set so that the nonzero locations (i, j) in the banded (approximate) Jacobian satisfy $-\texttt{mlower} \leq j - i \leq \texttt{mupper}$.

KINSpgmr

Call   `flag = KINSpgmr(kin_mem, maxl);`

Description   The function `KINSpgmr` selects the KINSPGMR linear solver.

The user's main function must include the `kinsol_spgmr.h` header file.

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

`maxl`   (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL= 5`.

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

KINSPILS_SUCCESS   The KINSPGMR initialization was successful.

KINSPILS_MEM_NULL   The `kin_mem` pointer is NULL.

KINSPILS_ILL_INPUT   The NVECTOR module used does not implement a required operation.

KINSPILS_MEM_FAIL   A memory allocation request failed.

Notes   The KINSPGMR solver uses a scaled preconditioned GMRES iterative method to solve the linear system (2).

Within KINSOL, only right preconditioning is available. For specification of the preconditioner, see §5.5.4 and §5.6.

If preconditioning is done, user-supplied functions define the right preconditioner matrices P, which approximate the Newton matrix from (2).

KINSpbcg

Call   `flag = KINSpbcg(kin_mem, maxl);`

Description   The function `KINSpbcg` selects the KINSPBCG linear solver.

The user's main function must include the `kinsol_spbcgs.h` header file.

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

`maxl`   (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL= 5`.

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

KINSPILS_SUCCESS   The KINSPBCG initialization was successful.

KINSPILS_MEM_NULL   The `kin_mem` pointer is NULL.

KINSPILS_ILL_INPUT   The NVECTOR module used does not implement a required operation.

KINSPILS_MEM_FAIL   A memory allocation request failed.

Notes   The KINSPBCG solver uses a scaled preconditioned Bi-CGStab iterative method to solve the linear system (2).

Within KINSOL, only right preconditioning is available. For specification of the preconditioner, see §5.5.4 and §5.6.

If preconditioning is done, user-supplied functions define the right preconditioner matrices P, which approximate the Newton matrix from (2).

KINSptfqmr

Call	`flag = KINSptfqmr(kin_mem, maxl);`
Description	The function `KINSptfqmr` selects the KINSPTFQMR linear solver.
	The user's main function must include the `kinsol_sptfqmr.h` header file.
Arguments	`kin_mem` (`void *`) pointer to the KINSOL memory block.
	`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL`= 5.
Return value	The return value `flag` (of type `int`) is one of:

`KINSPILS_SUCCESS`	The KINSPTFQMR initialization was successful.
`KINSPILS_MEM_NULL`	The `kin_mem` pointer is `NULL`.
`KINSPILS_ILL_INPUT`	The NVECTOR module used does not implement a required operation.
`KINSPILS_MEM_FAIL`	A memory allocation request failed.

Notes	The KINSPTFQMR solver uses a scaled preconditioned TFQMR iterative method to solve the linear system (2).
	Within KINSOL, only right preconditioning is available. For specification of the preconditioner, see §5.5.4 and §5.6.
	If preconditioning is done, user-supplied functions define the right preconditioner matrices P, which approximate the Newton matrix from (2).

5.5.3 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 `KINSol`, but which upon return contains an approximate solution of the nonlinear system $F(u) = 0$ the computed solution vector.
	`strategy` (`int`) globalization strategy applied to the Newton method. It must be one of `KIN_NONE` or `KIN_LINESEARCH`.
	`u_scale` (`N_Vector`) vector containing diagonal elements of scaling matrix D_u for vector `u` chosen so that the components of $D_u \cdot$`u` (as a matrix multiplication) all have about 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 $F(u)$.
Return value	On return, `KINSol` returns the approximate solution in the vector `u`. 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 $u = u_0$ satisfied the system $F(u) = 0$ within the tolerances specified.

KIN_STEP_LT_STPTOL

KINSOL stopped based on scaled step length. This means that the current iterate may be an approximate solution of the given nonlinear system, but it is also quite possible that the algorithm is "stalled" (making insufficient progress) near an invalid solution, or that the scalar `scsteptol` is too large (see `KINSetScaledStepTol` in §5.5.4 to change `scsteptol` from its default value).

KIN_MEM_NULL

The KINSOL memory block pointer was `NULL`.

KIN_ILL_INPUT

An input parameter was invalid.

KIN_NO_MALLOC

The KINSOL memory was not allocated by a call to `KINMalloc`.

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 finite 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 $\|D_u p\|_{L2} > 0.99$ `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 $\|D_F F(u)\|_{L2}$ asymptotes from above to a finite 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 linear solver initialization routine (`linit`) encountered an error.

KIN_LSETUP_FAIL

The user-supplied routine `pset` (used to set up the preconditioner data) encountered an unrecoverable error.

KIN_LSOLVE_FAIL

Either the user-supplied routine `psolve` (used to to solve the preconditioned linear system) encountered an unrecoverable error, or the linear solver routine (`lsolve`) encountered an error condition.

KIN_SYSFUNC_FAIL

The system function failed in an unrecoverable manner.

KIN_FIRST_SYSFUNC_ERR

The system function failed recoverably at the first call.

KIN_REPTD_SYSFUNC_ERR

The system function had repeated recoverable errors. No recovery is possible.

Notes   The components of vectors `u_scale` and `f_scale` should be strictly positive.

               `KIN_SUCCESS` = 0, `KIN_INITIAL_GUESS_OK` = 1, and `KIN_STEP_LT_STPTOL` = 2. All
               remaining return values are negative and therefore a test `flag` < 0 will trap all `KINSol`
               failures.

5.5.4   Optional input functions

KINSOL provides an extensive list of functions that can be used to change from their default values
various optional input parameters that control the behavior of the KINSOL solver. Table 5.1 lists
all optional input functions in KINSOL which are then described in detail in the remainder of this
section, beginning with those for the main KINSOL solver and continuing with those for the linear
solver modules. For the most casual use of KINSOL, the reader can skip to §5.6.

   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.

5.5.4.1   Main solver optional input functions

The calls listed here can be executed in any order.
However, if `KINSetErrHandlerFn` or `KINSetErrFile` are to be called, that call should be first, 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 C error handler function (see §5.6.2).

               `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 `ehfun` and data pointer `eh_data` have been successfully set.

               `KIN_MEM_NULL` The `kin_mem` pointer is `NULL`.

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

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

`KINSetErrFile`

Call   `flag = KINSetErrFile(kin_mem, errfp);`

Description   The function `KINSetErrFile` specifies the pointer to the file where all KINSOL messages
               should be directed in case 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`.

Table 5.1: Optional inputs for KINSOL, KINDENSE, and KINSPILS

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	`KINSetFdata`	`NULL`
Verbosity level of output	`KINSetPrintLevel`	0
Max. number of nonlinear iterations	`KINSetNumMaxIters`	200
No initial preconditioner setup	`KINSetNoInitSetup`	`FALSE`
No residual monitoring*	`KINSetNoResMon`	`FALSE`
Max. iterations without prec. 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`	`FALSE`
Max. scaled length of Newton step	`KINSetMaxNewtonStep`	$1000\|D_u u_0\|_2$
Max. number of β-condition failures	`KINSetMaxBetaFails`	10
Rel. error for F.D. Jv	`KINSetRelErrFunc`	$\sqrt{\text{uround}}$
Function-norm stopping tolerance	`KINSetFuncNormTol`	$\sqrt[3]{\text{uround}}$
Scaled-step stopping tolerance	`KINSetScaledSteptol`	$\text{uround}^{2/3}$
Inequality constraints on solution	`KINSetConstraints`	`NULL`
Nonlinear system function	`KINSetSysFunc`	none
KINDENSE linear solver		
Dense Jacobian function and data	`KINDenseSetJacFn`	internal DQ, `NULL`
KINBAND linear solver		
Band Jacobian function and data	`KINBandSetJacFn`	internal DQ, `NULL`
KINSPILS linear solvers		
Max. number of restarts**	`KINSpilsSetMaxRestarts`	0
Preconditioner functions and data	`KINSpilsSetPreconditioner`	`NULL, NULL, NULL`
Jacobian-times-vector function and data	`KINSpilsSetJacTimesVecFn`	internal DQ, `NULL`

* Only for KINDENSE and KINBAND
** Only for KINSPGMR

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`).

               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.

| 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 C info handler function (see §5.6.3).

               `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 `ihfun` and data pointer `ih_data` have been successfully set.

               `KIN_MEM_NULL` The `kin_mem` pointer is `NULL`.

Notes   The default internal info handler function directs informative (non-error) messages to
               the file specified by the file pointer `infofp` (see `KINSetInfoFile` below).

| 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`.

| 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 the linear
                 solver.

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.

`KINSetFdata`

Call `flag = KINSetFdata(kin_mem, f_data);`

Description The function `KINSetFdata` specifies the pointer to user-defined memory that is to be passed to the user-supplied function implementing the nonlinear system residual.

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

          `f_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 The default value for `f_data` is NULL.

`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 setup function should be made or not.

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

          `noInitSetup` (`booleantype`) flag controlling whether or not an initial call to the preconditioner setup function is made.

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 `FALSE`, meaning that an initial call to the preconditioner setup function will be made.

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 or not residual monitoring is
                used.

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 `FALSE`, meaning that
                the nonlinear residual will be monitored. Otherwise, `noNNIResMon` is set to `TRUE`.

                Residual monitoring is only available for use with the direct linear solver modules (mean-
                ing KINDENSE and KINBAND).

KINSetMaxSetupCalls

Call   `flag = KINSetMaxSetupCalls(kin_mem, msbset);`

Description   The function `KINSetMaxSetupCalls` specifies the maximum number of nonlinear itera-
                tions that can be performed between calls to the preconditioner 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 setup function.

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` $= 10$.

KINSetMaxSubSetupCalls

Call   `flag = KINSetMaxSubSetupCalls(kin_mem, msbsetsub);`

Description   The function `KINSetMaxSubSetupCalls` 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.

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` $= 5$.

                Residual monitoring is only available for use with the direct linear solver modules (mean-
                ing KINDENSE and KINBAND).

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. `etachoice` must be one of `KIN_ETACHOICE1`, `KIN_ETACHOICE2`, or `KIN_ETACONSTANT` (see Chapter 3 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`.

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.

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 `eta` had an illegal value

Notes   The default value for `eta` is 0.1. The valid values are $0.0 < \texttt{eta} \le 1.0$.

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.

              `ealpha`   (`realtype`) value of the α parameter.

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 valid values for `ealpha` are $1.0 < \texttt{ealpha} \le 2.0$. If $\texttt{ealpha} = 0.0$, then its value is set to 2.0.

           The valid values for `egamma` are $0.0 < \texttt{egamma} \le 1.0$. If $\texttt{egamma} = 0.0$, then its value is set to 0.9.

`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.

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 omega is 0.9. The valid values are $0.0 < $ omega $ < 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 for ω.

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

              omegamin (realtype) value of the ω_{min} parameter.

              omegamax (realtype) value of the ω_{max} parameter.

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 valid values for omegamin and omegamax are $0.0 < $ omegamin $ < $ omegamax $ < 1.0$. If
              omegamin $= 0.0$, then its value is set to 0.00001. If omegamax $= 0.0$, then its value is
              set to 0.9.

`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.

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 FALSE.

`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.

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 step was non-positive.

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 failures in the linesearch algorithm.

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

mxnbcf (realtype) maximum number of β-condition failures.

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 non-positive.

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 of the Jacobian-vector product.

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

relfunc (realtype) relative error in $F(u)$.

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 non-positive.

Notes The default value for relfunc is $\sqrt{\text{unit roundoff}}$.

| 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.

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 fnormtol is $\sqrt[3]{\text{unit roundoff}}$.

KINSetScaledStepTol

Call	`flag = KINSetScaledStepTol(kin_mem, scsteptol);`
Description	The function `KINSetScaledStepTol` specifies the scalar used as a stopping tolerance on 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..
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
	$\quad\quad$ 0.0 then no constraint is imposed on u_i.
	$\quad\quad$ 1.0 then u_i will be constrained to be $u_i > 0.0$.
	$\quad\quad$ -1.0 then u_i will be constrained to be $u_i < 0.0$.
	$\quad\quad$ 2.0 then u_i will be constrained to be $u_i \geq 0.0$.
	$\quad\quad$ -2.0 then u_i will be constrained to be $u_i \leq 0.0$.
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.
	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 $F(u)$.
Arguments	`kin_mem` (`void *`) pointer to the KINSOL memory block.
	`func` (`KINSysFn`) user-supplied function that evaluates $F(u)$.
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 `KINMalloc`. 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.

5.5.4.2 Dense linear solver

The KINDENSE solver needs a function to compute a dense approximation to the Jacobian matrix $J(u)$. This function must be of type KINDenseJacFn. The user can supply his/her own dense Jacobian function, or use the default difference quotient function KINDenseDQJac that comes with the KINDENSE solver. To specify a user-supplied Jacobian function djac and associated user data jac_data, KINDENSE provides the function KINDenseSetJacFn. The KINDENSE solver passes the pointer jac_data to its dense Jacobian function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer jac_data may be identical to f_data, if the latter was specified through KINSetFdata.

KINDenseSetJacFn

Call	flag = KINDenseSetJacFn(kin_mem, djac, jac_data);
Description	The function KINDenseSetJacFn specifies the dense Jacobian approximation function to be used and the pointer to user data.
Arguments	kin_mem (void *) pointer to the KINSOL memory block.
	djac (KINDenseJacFn) user-defined dense Jacobian approximation function.
	jac_data (void *) pointer to the user-defined data structure.
Return value	The return value flag (of type int) is one of
	KINDENSE_SUCCESS The optional value has been successfully set.
	KINDENSE_MEM_NULL The kin_mem pointer is NULL.
	KINDENSE_LMEM_NULL The KINDENSE linear solver has not been initialized.
Notes	By default, KINDENSE uses the difference quotient function KINDenseDQJac. If NULL is passed to djac, this default function is used.
	The function type KINDenseJacFn is described in §5.6.4.

5.5.4.3 Band linear solver

The KINDENSE solver needs a function to compute a banded approximation to the Jacobian matrix $J(u)$. This function must be of type KINBandJacFn. The user can supply his/her own banded Jacobian approximation function, or use the default difference quotient function KINBandDQJac that comes with the KINBAND solver. To specify a user-supplied Jacobian function bjac and associated user data jac_data, KINBAND provides the function KINBandSetJacFn. The KINBAND solver passes the pointer jac_data to its banded Jacobian approximation function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer jac_data may be identical to f_data, if the latter was specified through KINSetFdata.

KINBandSetJacFn

Call	flag = KINBandSetJacFn(cvode_mem, bjac, jac_data);
Description	The function KINBandSetJacFn specifies the banded Jacobian approximation function to be used and the pointer to user data.
Arguments	kin_mem (void *) pointer to the KINSOL memory block.
	bjac (KINBandJacFn) user-defined banded Jacobian approximation function.
	jac_data (void *) pointer to the user-defined data structure.
Return value	The return value flag (of type int) is one of
	KINBAND_SUCCESS The optional value has been successfully set.
	KINBAND_MEM_NULL The kin_mem pointer is NULL.

KINBAND_LMEM_NULL The KINBAND linear solver has not been initialized.

Notes   By default, KINBAND uses the difference quotient function KINBandDQJac. If NULL is passed to bjac, this default function is used.

The function type KINBandJacFn is described in §5.6.5.

5.5.4.4   SPILS linear solvers

If any preconditioning is to be done with one of the KINSPILS linear solvers, then the user must supply a preconditioner solve function psolve and specify its name in a call to KINSpilsSetPreconditioner.

The evaluation and preprocessing of any Jacobian-related data needed by the user's preconditioner solve function is done in the optional user-supplied function psetup. Both of these functions are fully specified in §5.6. If used, the psetup function should also be specified in the call to KINSpilsSetPreconditioner. Optionally, a KINSPILS solver passes the pointer p_data received through KINSpilsSetPreconditioner to the preconditioner psetup and psolve functions. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied preconditioner functions without using global data in the program. The pointer p_data may be identical to f_data, if the latter was specified through KINSetFdata.

Ther KINSPILS solvers require 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 difference quotient function KINSpilsDQJtimes that comes with the KINSPILS solvers. A user-defined Jacobian-vector function must be of type KINSpilsJacTimesVecFn and can be specified through a call to KINSpilsSetJacTimesVecFn (see §5.6.6 for specification details). As with the preconditioner user data structure p_data, the user can also specify, in the call to KINSpilsSetJacTimesVecFn, a pointer to a user-defined data structure, jac_data, which the KINSPILS solver passes to the Jacobian-times-vector function jtimes each time it is called. The pointer jac_data may be identical to p_data and/or f_data.

KINSpilsSetPreconditioner

Call   flag = KINSpilsSetPreconditioner(kin_mem, psetup, psolve, p_data);

Description   The function KINSpilsSetPreconditioner specifies the preconditioner setup and solve functions and the pointer to user data.

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

             psetup   (KINSpilsPrecSetupFn) user-defined preconditioner setup function.

             psolve   (KINSpilsPrecSolveFn) user-defined preconditioner solve function.

             p_data   (void *) pointer to the user-defined data structure.

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

             KINSPILS_SUCCESS   The optional value has been successfully set.

             KINSPILS_MEM_NULL   The kin_mem pointer is NULL.

             KINSPILS_LMEM_NULL The KINSPILS linear solver has not been initialized.

Notes   The function type KINSpilsPrecSolveFn is described in §5.6.7. The function type KINSpilsPrecSetupFn is described in §5.6.8.

KINSpilsSetJacTimesVecFn

Call   flag = KINSpilsSetJacTimesVecFn(kin_mem, jtimes, jac_data);

Description   The function KINSpilsSetJacTimesFn specifies the Jacobian-vector function to be used and the pointer to user data.

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

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

             jac_data (void *) pointer to the user-defined data structure.

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

      `KINSPILS_SUCCESS`   The optional value has been successfully set.

      `KINSPILS_MEM_NULL`   The `kin_mem` pointer is `NULL`.

      `KINSPILS_LMEM_NULL` The KINSPILS linear solver has not been initialized.

Notes   By default, the KINSPILS linear solvers use an internal difference quotient function `KINSpilsDQJtimes`. If `NULL` is passed to `jtimes`, this default function is used.

         The function type `KINSpilsJacTimesVecFn` is described in §5.6.6.

`KINSpilsSetMaxRestarts`

Call   `flag = KINSpilsSetMaxRestarts(kin_mem, maxrs);`

Description   The function `KINSpilsSetMaxRestarts` specifies the maximum number of times the iterative linear solver can be restarted.

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

          `maxrs`   (`int`) maximum number of restarts.

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

      `KINSPILS_SUCCESS`   The optional value has been successfully set.

      `KINSPILS_ILL_INPUT` The maximum number of restarts specified is negative.

      `KINSPILS_MEM_NULL`   The `kin_mem` pointer is `NULL`.

      `KINSPILS_LMEM_NULL` The linear solver has not been initialized.

Notes   The default value is 0 (meaning no restarts).

         This option is available only for the KINSPGMR linear solver.

5.5.5   Optional output functions

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

Table 5.2: Optional outputs from KINSOL, KINDENSE, KINBAND, and KINSPILS

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 F	`KINGetFuncNorm`
Scaled norm of the step	`KINGetStepLength`
KINDENSE linear solver	
Size of KINDENSE real and integer workspaces	`KINDenseGetWorkSpace`
No. of Jacobian evaluations	`KINDenseGetNumJacEvals`
No. of r.h.s. calls for finite diff. Jacobian evals.	`KINDenseGetNumFuncEvals`
Last return from a KINDENSE function	`KINDenseGetLastFlag`
	continued on next page

continued from last page	
Optional output	**Function name**
KINBAND linear solver	
Size of KINBAND real and integer workspaces	KINBandGetWorkSpace
No. of Jacobian evaluations	KINBandGetNumJacEvals
No. of r.h.s. calls for finite diff. Jacobian evals.	KINBandGetNumFuncEvals
Last return from a KINBAND function	KINBandGetLastFlag
KINSPILS linear solvers	
Size of real and integer workspaces	KINSpilsGetWorkSpace
No. of linear iterations	KINSpilsGetNumLinIters
No. of linear convergence failures	KINSpilsGetNumConvFails
No. of preconditioner evaluations	KINSpilsGetNumPrecEvals
No. of preconditioner solves	KINSpilsGetNumPrecSolves
No. of Jacobian-vector product evaluations	KINSpilsGetNumJtimesEvals
No. of fct. calls for finite diff. Jacobian-vector evals.	KINSpilsGetNumFuncEvals
Last return from a linear solver function	KINSpilsGetLastFlag

5.5.5.1   Main solver optional output functions

KINSOL provides several user-callable functions that can be used to obtain different quantities that may be of interest to the user, such as solver workspace requirements and solver performance statistics. These optional output functions are described next.

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.

5.5.5.2   Dense linear solver

The following optional outputs are available from the KINDENSE module: workspace requirements, number of calls to the Jacobian routine, number of calls to the system function routine for finite-difference Jacobian approximation, and last return value from a KINDENSE function.

`KINDenseGetWorkSpace`

Call   `flag = KINDenseGetWorkSpace(kin_mem, &lenrwLS, &leniwLS);`

Description   The function `KINDenseGetWorkSpace` returns the KINDENSE 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 KINDENSE workspace.

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

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

KINDENSE_SUCCESS   The optional output value has been successfully set.

KINDENSE_MEM_NULL   The `kin_mem` pointer is NULL.

KINDENSE_LMEM_NULL The KINDENSE linear solver has not been initialized.

Notes   In terms of the problem size N, the actual size of the real workspace is $2N^2$ `realtype` words, and the actual size of the integer workspace is N integer words.

`KINDenseGetNumJacEvals`

Call   `flag = KINDenseGetNumJacEvals(kin_mem, &njevals);`

Description   The function `KINDenseGetNumJacEvals` returns the number of calls to the dense 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

KINDENSE_SUCCESS   The optional output value has been successfully set.

KINDENSE_MEM_NULL   The `kin_mem` pointer is NULL.

KINDENSE_LMEM_NULL The KINDENSE linear solver has not been initialized.

`KINDenseGetNumFuncEvals`

Call   `flag = KINDenseGetNumFuncEvals(kin_mem, &nfevalsLS);`

Description   The function `KINDenseGetNumFuncEvals` returns the number of calls to the user system function due to the finite difference dense Jacobian approximation.

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

KINDENSE_SUCCESS   The optional output value has been successfully set.

KINDENSE_MEM_NULL   The `kin_mem` pointer is NULL.

KINDENSE_LMEM_NULL The KINDENSE linear solver has not been initialized.

Notes   The value nfevalsLS is incremented only if the default KINDenseDQJac difference quotient function is used.

| KINDenseGetLastFlag |

Call   flag = KINDenseGetLastFlag(kin_mem, &lsflag);

Description The function KINDenseGetLastFlag returns the last return value from a KINDENSE routine.

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

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

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

             KINDENSE_SUCCESS   The optional output value has been successfully set.

             KINDENSE_MEM_NULL   The kin_mem pointer is NULL.

             KINDENSE_LMEM_NULL The KINDENSE linear solver has not been initialized.

Notes   If the KINDENSE setup function failed (KINSol returned KIN_LSETUP_FAIL), then 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 Jacobian matrix.

5.5.5.3 Band linear solver

The following optional outputs are available from the KINBAND module: workspace requirements, number of calls to the Jacobian routine, number of calls to the right-hand side routine for finite-difference Jacobian approximation, and last return value from a KINBAND function.

| KINBandGetWorkSpace |

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

Description The function KINBandGetWorkSpace returns the KINBAND real and integer workspace sizes.

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

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

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

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

             KINBAND_SUCCESS   The optional output value has been successfully set.

             KINBAND_MEM_NULL   The kin_mem pointer is NULL.

             KINBAND_LMEM_NULL The KINBAND linear solver has not been initialized.

Notes   In terms of the problem size N and Jacobian half-bandwidths, the actual size of the real workspace is $(2\,\texttt{mupper}+3\,\texttt{mlower}+2)\,N$ realtype words, and the actual size of the integer workspace is N integer words.

| KINBandGetNumJacEvals |

Call   flag = KINBandGetNumJacEvals(kin_mem, &njevals);

Description The function KINBandGetNumJacEvals returns the number of calls to the banded Jacobian approximation function.

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

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

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

> KINBAND_SUCCESS   The optional output value has been successfully set.
>
> KINBAND_MEM_NULL   The kin_mem pointer is NULL.
>
> KINBAND_LMEM_NULL The KINBAND linear solver has not been initialized.

KINBandGetNumRhsEvals

Call	`flag = KINBandGetNumFuncEvals(kin_mem, &nfevalsLS);`
Description	The function `KINBandGetNumFuncEvals` returns the number of calls to the user system function due to the finite difference banded Jacobian approximation.
Arguments	`kin_mem` (`void *`) pointer to the CVODE 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

> KINBAND_SUCCESS   The optional output value has been successfully set.
>
> KINBAND_MEM_NULL   The kin_mem pointer is NULL.
>
> KINBAND_LMEM_NULL The KINBAND linear solver has not been initialized.

Notes	The value `nfevalsLS` is incremented only if the default `KINBandDQJac` difference quotient function is used.

KINBandGetLastFlag

Call	`flag = KINBandGetLastFlag(kin_mem, &lsflag);`
Description	The function `KINBandGetLastFlag` returns the last return value from a KINBAND routine.
Arguments	`kin_mem` (`void *`) pointer to the CVODE memory block.
	`lsflag` (`int`) the value of the last return flag from a KINBAND function.
Return value	The return value `flag` (of type `int`) is one of

> KINBAND_SUCCESS   The optional output value has been successfully set.
>
> KINBAND_MEM_NULL   The kin_mem pointer is NULL.
>
> KINBAND_LMEM_NULL The KINBAND linear solver has not been initialized.

Notes	If the KINBAND setup sunction failed (`KINSol` returned `KIN_LSETUP_FAIL`), the value `lsflag` is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the banded Jacobian matrix.

5.5.5.4   SPILS linear solvers

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

KINSpilsGetWorkSpace

Call	`flag = KINSpilsGetWorkSpace(kin_mem, &lenrwLS, &leniwLS);`
Description	The function `KINSpilsGetWorkSpace` returns the global sizes of the linear solver real and integer workspaces.
Arguments	`kin_mem` (`void *`) pointer to the KINSOL memory block.
	`lenrwSG` (`long int`) the number of `realtype` values in the linear solver workspace.
	`leniwSG` (`long int`) the number of integer values in the linear solver workspace.

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

KINSPILS_SUCCESS   The optional output values have been successfully set.

KINSPILS_MEM_NULL   The kin_mem pointer is NULL.

KINSPILS_LMEM_NULL   The KINSPGMR linear solver has not been initialized.

Notes   In terms of the problem size N and maximum subspace size maxl, the actual size of the real workspace is roughly:

$(\text{maxl}+3) * N + \text{maxl} * (\text{maxl}+4) + 1$ realtype words for KINSPGMR,

$7 * N$ realtype words for KINSPBCG,

and $11 * N$ realtype words for KINSPTFQMR.

In a parallel setting, this value is global — summed over all processes.

| KINSpilsGetNumLinIters |

Call   flag = KINSpilsGetNumLinIters(kin_mem, &nliters);

Description   The function KINSpilsGetNumLinIters 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:

KINSPILS_SUCCESS   The optional output value has been successfully set.

KINSPILS_MEM_NULL   The kin_mem pointer is NULL.

KINSPLIS_LMEM_NULL   The linear solver module has not been initialized.

| KINSpilsGetNumConvFails |

Call   flag = KINSpilsGetNumConvFails(kin_mem, &nlcfails);

Description   The function KINSpilsGetNumConvFails returns the cumulative number of linear convergence 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:

KINSPILS_SUCCESS   The optional output value has been successfully set.

KINSPILS_MEM_NULL   The kin_mem pointer is NULL.

KINSPILS_LMEM_NULL   The linear solver module has not been initialized.

| KINSpilsGetNumPrecEvals |

Call   flag = KINSpilsGetNumPrecEvals(kin_mem, &npevals);

Description   The function KINSpilsGetNumPrecEvals returns the 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:

KINSPILS_SUCCESS   The optional output value has been successfully set.

KINSPILS_MEM_NULL   The kin_mem pointer is NULL.

KINSPILS_LMEM_NULL   The linear solver module has not been initialized.

KINSpilsGetNumPrecSolves

Call   `flag = KINSpilsGetNumPrecSolves(kin_mem, &npsolves);`

Description   The function `KINSpilsGetNumPrecSolves` 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:

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

             `KINSPILS_MEM_NULL`   The `kin_mem` pointer is NULL.

             `KINSPILS_LMEM_NULL` The linear solver module has not been initialized.

KINSpilsGetNumJtimesEvals

Call   `flag = KINSpilsGetNumJtimesEvals(kin_mem, &njvevals);`

Description   The function `KINSpilsGetNumJtimesEvals` returns the cumulative number made to the Jacobian-vector product function, `jtimes`.

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

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

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

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

             `KINSPILS_MEM_NULL`   The `kin_mem` pointer is NULL.

             `KINSPILS_LMEM_NULL` The linear solver module has not been initialized.

KINSpilsGetNumFuncEvals

Call   `flag = KINSpilsGetNumFuncEvals(kin_mem, &nfevalsLS);`

Description   The function `KINSpilsGetNumFuncEvals` returns the number of calls to the user system function for finite difference Jacobian-vector product approximations.

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:

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

             `KINSPILS_MEM_NULL`   The `kin_mem` pointer is NULL.

             `KINSPILS_LMEM_NULL` The linear solver module has not been initialized.

Notes   The value `nfevalsLS` is incremented only if the default `KINSpilsDQJtimes` difference quotient function is used.

KINSpilsGetLastFlag

Call   `flag = KINSpilsGetLastFlag(kin_mem, &lsflag);`

Description   The function `KINSpilsGetLastFlag` returns the last return value from a KINSPILS routine.

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

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

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

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

             `KINSPILS_MEM_NULL`   The `kin_mem` pointer is NULL.

KINSPILS␣LMEM␣NULL The linear solver module has not been initialized.

Notes   If the KINSPILS setup function failed (KINSOL returned KIN␣LSETUP␣FAIL), lsflag will be SPGMR␣PSET␣FAIL␣UNREC, SPBCG␣PSET␣FAIL␣UNREC, or SPTFQMR␣PSET␣FAIL␣UNREC.

If the KINSPGMR solve function failed (KINSol returned KIN␣LSOLVE␣FAIL), lsflag contains the error return flag from SpgmrSolve and will be one of: SPGMR␣MEM␣NULL, indicating that the SPGMR memory is NULL; SPGMR␣ATIMES␣FAIL␣UNREC, indicating an unrecoverable failure in the Jacobian-times-vector function; SPGMR␣PSOLVE␣FAIL␣UNREC, indicating that the preconditioner solve function psolve failed unrecoverably; SPGMR␣GS␣FAIL, indicating a failure in the Gram-Schmidt procedure; or SPGMR␣QRSOL␣FAIL, indicating that the matrix R was found to be singular during the QR solve phase.

If the KINSPBCG solve function failed (KINSol returned KIN␣LSOLVE␣FAIL), lsflag contains the error return flag from SpbcgSolve and will be one of: SPBCG␣MEM␣NULL, indicating that the SPBCG memory is NULL; SPBCG␣ATIMES␣FAIL␣UNREC, indicating an unrecoverable failure in the Jacobian-times-vector function; or SPBCG␣PSOLVE␣FAIL␣UNREC, indicating that the preconditioner solve function psolve failed unrecoverably.

If the KINSPTFQMR solve function failed (KINSol returned KIN␣LSOLVE␣FAIL), lsflag contains the error return flag from SptfqmrSolve and will be one of: SPTFQMR␣MEM␣NULL, indicating that the SPTFQMR memory is NULL; SPTFQMR␣ATIMES␣FAIL␣UNREC, indicating an unrecoverable failure in the Jacobian-times-vector function; or SPTFQMR␣PSOLVE␣FAIL␣UNREC, indicating that the preconditioner solve function psolve failed unrecoverably.

5.6 User-supplied functions

The user-supplied functions consist of one function defining the nonlinear system, (optionally) a function that handles error and warning messages, (optionally) a function that handles informational messages, (optionally) a function that provides Jacobian-related information for the linear solver, and (optionally) one or two functions that define the preconditioner for use in any of the Krylov iterative algorithms.

5.6.1 Problem-defining function

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

KINSysFn

Definition   `typedef void (*KINSysFn)(N␣Vector u, N␣Vector fval, void *f␣data);`

Purpose   This function computes $F(u)$ for a given value of the vector u.

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

fval   is the output vector $F(u)$.

f␣data is a pointer to user data, same as the pointer f␣data passed to KINSetFdata.

Return value A KINSysFn function should return 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 and KIN␣SYSFUNC␣FAIL is returned).

Notes   Allocation of memory for fval is handled within KINSOL.

5.6.2 Error message handler function

As an alternative to the default behavior of directing error and warning messages to the file pointed to by errfp (see KINSetErrFile), the user may provide a function of type 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 returning a pointer to memory (*e.g.*, `KINBBDPrecAlloc`) encounters an error, it sets `error_code` to 0 before returning `NULL`.

5.6.3 Informational message handler function

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

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 `KINSetInfoHandlerFn`.
Return value	A `KINInfoHandlerFn` function has no return value.

5.6.4 Jacobian information (direct method with dense Jacobian)

If the direct linear solver with dense treatment of the Jacobian is used (i.e. `KINDense` is called in Step 7 of §5.4), the user may provide a function of type `KINDenseJacFn` defined by

---

KINDenseJacFn

Definition	`typedef int (*KINDenseJacFn)(long int N, DenseMat J,`
	`N_Vector u, N_Vector fu, void *jac_data,`
	`N_Vector tmp1, N_Vector tmp2);`
Purpose	This function computes the dense Jacobian $J(u)$ (or an approximation to it).
Arguments	`N` is the problem size.
	`J` is the output Jacobian matrix.
	`u` is the current (unscaled) iterate.
	`fu` is the current value of the vector $F(u)$.

jac_data is a pointer to user data — the same as the jac_data parameter passed to KINDenseSetJacData.

tmp1

tmp2   are pointers to memory allocated for variables of type N_Vector which can be used by KINDenseJacFn as temporary storage or work space.

Return value   A function of type KINDenseJacFn should return 0 if successful or a non-zero value otherwise.

Notes   A user-supplied dense Jacobian function must load the N by N dense matrix J with an approximation to the Jacobian matrix J at u. Only nonzero elements need to be loaded into J because J is set to the zero matrix before the call to the Jacobian function. The type of J is DenseMat.

The accessor macros DENSE_ELEM and DENSE_COL allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the DenseMat type. DENSE_ELEM(J, i, j) references the (i, j)-th element of the dense matrix J (i, $j = 0 \ldots N-1$). This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to N, the Jacobian element $J_{m,n}$ can be loaded with the statement DENSE_ELEM(J, m-1, n-1) = $J_{m,n}$. Alternatively, DENSE_COL(J, j) returns a pointer to the storage for the jth column of J ($j = 0 \ldots N-1$), and the elements of the jth column are then accessed via ordinary array indexing. Thus $J_{m,n}$ can be loaded with the statements col_n = DENSE_COL(J, n-1); col_n[m-1] = $J_{m,n}$. For large problems, it is more efficient to use DENSE_COL than to use DENSE_ELEM. Note that both of these macros number rows and columns starting from 0, not 1.

The DenseMat type and the accessor macros DENSE_ELEM and DENSE_COL are documented in §9.1.

If the user's KINDenseJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. To obtain these, use the KINGet* functions described in §5.5.5.1. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

5.6.5   Jacobian information (direct method with banded Jacobian)

If the direct linear solver with banded treatment of the Jacobian is used (*i.e.*, KINBand is called in Step 7 of §5.4), the user may provide a function of type KINBandJacFn defined as follows:

KINBandJacFn

Definition
```
typedef int (*KINBandJacFn)(long int N, long int mupper,
                            long int mlower, BandMat J,
                            N_Vector u, N_Vector fu, void *jac_data,
                            N_Vector tmp1, N_Vector tmp2);
```

Purpose   This function computes the banded Jacobian $J(u)$ (or a banded approximation to it).

Arguments   N   is the problem size.

mlower

mupper   are the lower and upper half-bandwidths of the Jacobian.

J   is the output Jacobian matrix.

u   is the current (unscaled) iterate.

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

jac_data is a pointer to user data — the same as the jac_data parameter passed to KINBandSetJacData.

tmp1

| | tmp2 | are pointers to memory allocated for variables of type N_Vector which can be used by KINBandJacFn as temporary storage or work space. |

Return value   A function of type KINBandJacFn should return 0 if successful or a non-zero value otherwise.

Notes   A user-supplied band Jacobian function must load the band matrix J of type BandMat with the elements of the Jacobian J at u. Only nonzero elements need to be loaded into J because J is preset to zero before the call to the Jacobian function.

The accessor macros BAND_ELEM, BAND_COL, and BAND_COL_ELEM allow the user to read and write band matrix elements without making specific references to the underlying representation of the BandMat type. BAND_ELEM(J, i, j) references the (i, j)th element of the band matrix J, counting from 0. This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to N with (m, n) within the band defined by mupper and mlower, the Jacobian element $J_{m,n}$ can be loaded with the statement BAND_ELEM(J, m-1, n-1) = $J_{m,n}$. The elements within the band are those with -mupper $\leq$ m-n $\leq$ mlower. Alternatively, BAND_COL(J, j) returns a pointer to the diagonal element of the jth column of J, and if we assign this address to realtype *col_j, then the ith element of the jth column is given by BAND_COL_ELEM(col_j, i, j), counting from 0. Thus for (m, n) within the band, $J_{m,n}$ can be loaded by setting col_n = BAND_COL(J, n-1); BAND_COL_ELEM(col_n, m-1, n-1) = $J_{m,n}$. The elements of the jth column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type BandMat. The array col_n can be indexed from −mupper to mlower. For large problems, it is more efficient to use the combination of BAND_COL and BAND_COL_ELEM than to use the BAND_ELEM. As in the dense case, these macros all number rows and columns starting from 0, not 1.

The BandMat type and the accessor macros BAND_ELEM, BAND_COL, and BAND_COL_ELEM are documented in §9.2.

If the user's KINBandJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. To obtain these, use the KINGet* functions described in §5.5.5.1. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

5.6.6   Jacobian information (matrix-vector product)

If one of the Krylov iterative linear solvers SPGMR, SPBCG, or SPTFQMR is selected (KINSp* is called in step 7 of §5.4), the user may provide a function of type KINSpilsJacTimesVecFn in the following form:

KINSpilsJacTimesVecFn

Definition   typedef int (*KINSpilsJacTimesVecFn)(N_Vector v, N_Vector Jv,
                                                      N_Vector u, booleantype new_u,
                                                      void *jac_data);

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

Arguments   v   is the vector by which the Jacobian must be multiplied to the right.

               Jv   is the output vector computed.

               u   is the current value of the dependent variable vector.

               new_u   is a flag (reset by user) indicating if the iterate has been updated in the interim — Jacobian needs to be updated/reevaluated, if appropriate, unless new_u = FALSE.

               jac_data is a pointer to user data — the same as the jac_data parameter passed to KINSp*SetJacTimesVecFn.

Return value   The value to be returned by the Jacobian-times-vector function should be 0 if successful. If a recoverable failure occured, the return value should be positive. In this case, KINSOL will attempt to correct by calling the preconditioner setup function if the preconditioner information. 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 KINSPGMR function, using difference quotient approximations, is used.

If the user-provided KINSpilsJacTimesVecFn function needs the unit roundoff, this can be accessed as UNIT_ROUNDOFF defined in sundialstypes.h.

The user is responsible for resetting the value of new_u to FALSE.

5.6.7   Preconditioning (linear system solution)

If preconditioning is used, then the user must provide a C function to solve the linear system $Pz = r$ where P is the preconditioner matrix. This function must be of type KINSpilsPrecSolveFn, defined as follows:

KINSpilsPrecSolveFn

Definition
```
typedef int (*KINSpilsPrecSolveFn)(N_Vector u, N_Vector uscale,
                                   N_Vector fval, N_Vector fscale,
                                   N_Vector v, void *prec_data,
                                   N_Vector tmp);
```

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

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

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

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

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

v   on input, v is set to the right-hand side vector of the linear system, r. On output, v must contain the solution z of the linear system $Pz = r$.

prec_data is a pointer to user data - the same as the prec_data parameter passed to the function KINSpilsSetPreconditioner.

tmp   is a pointer to memory allocated for a variable of type N_Vector which can be used for work space.

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

5.6.8   Preconditioning (Jacobian data)

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 C function of type KINSpilsPrecSetupFn, defined as follows:

KINSpilsPrecSetupFn

Definition   typedef int (*KINSpilsPrecSetupFn)(N_Vector u, N_Vector uscale,
                                                   N_Vector fval, N_Vector fscale,
                                                   void *prec_data, N_Vector tmp1,
                                                   N_Vector tmp2);

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

Arguments   The arguments of a KINSpilsPrecSetupFn are as follows:

               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.
               prec_data is a pointer to user data - the same as the prec_data parameter passed to
                          the function KINSpilsSetPreconditioner.
               tmp1
               tmp2   are pointers to memory allocated for variables of type N_Vector which can
                          be used by KINSpilsPrecSetupFn as temporary storage or work space.

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 precondi-
               tioner matrix P (stored in the memory block referenced by the prec_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 preconditioner solve routine requires no preparation, then a preconditioner setup
               function need not be given.

5.7   A parallel band-block-diagonal preconditioner module

The efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced
through preconditioning. For problems in which the user cannot define a more effective, problem-
specific preconditioner, KINSOL provides a band-block-diagonal preconditioner module KINBBDPRE, to
be used with the parallel N_Vector module described in §7.2.

   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 mu + ml +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 `mu` and `ml` 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 `KINLocalFn`) which approximates the nonlinear system function function $G(u) \approx F(u)$ and which is computed locally, and an optional function `Gcomm` (of type `KINCommFn`) 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 `f_data` as that passed by the user to `KINSetFdata` and passed to the user's function `func`, and neither function has a return value. The user is responsible for providing space (presumably within `f_data`) for components of `u` that are communicated by `Gcomm` from the other processes, and that are then used by `Gloc`, which is not expected to do any communication.

`KINLocalFn`

Definition	`typedef void (*KINLocalFn)(long int Nlocal, N_Vector u,` `N_Vector gval, void *f_data);`
Purpose	This 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.
	`f_data` is a pointer to user data - the same as the `f_data` parameter passed to `KINSetFdata`.
Return value	A `KINLocalFn` function type does not have a return value.
Notes	This function assumes that all interprocess communication of data needed to calculate `gval` has already been done, and this data is accessible within `f_data`.
	Memory for `u` and `gval` is handled within the preconditioner module.
	The case where G is mathematically identical to F is allowed.

`KINCommFn`

Definition	`typedef void (*KINCommFn)(long int Nlocal, N_Vector u, void *f_data);`
Purpose	This function performs all interprocess communications necessary for the execution 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.
	`f_data` is a pointer to user data - the same as the `f_data` parameter passed to `KINSetFdata`.
Return value	A `KINCommFn` function type does not have a return value.
Notes	The `Gcomm` function is expected to save communicated data in space defined within the structure `f_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 `KINBBDPrecAlloc` (see below).

Besides the header files required for the solution of a nonlinear problem (see §5.3), 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 §5.4 are grayed out.

1. **Initialize MPI**

2. **Set problem dimensions**

3. **Set vector with initial guess**

4. **Create** KINSOL **object**

5. **Set optional inputs**

6. **Allocate internal memory**

7. **Initialize the** KINBBDPRE **preconditioner module**

   Specify the upper and lower half-bandwidth pairs `mu,ml` and `mukeep,mlkeep`, and call

   ```
   bbd_data = KINBBDPrecAlloc(kin_mem, Nlocal, mudq, mldq,
                              mukeep, mlkeep, dq_rel_u, Gloc, Gcomm);
   ```

   to allocate memory for and initialize a data structure `bbd_data` to be passed to the appropriate KINSPILS linear solver. The last two arguments of `KINBBDPrecAlloc` are the two user-supplied functions described above.

8. **Attach the Kyrlov linear solver, one of:**

   ```
   flag = KINBBDSpgmr(kin_mem, maxl, bbd_data);
   ```

   ```
   flag = KINBBDSpbcg(kin_mem, maxl, bbd_data);
   ```

   ```
   flag = KINBBDSptfqmr(kin_mem, maxl, bbd_data);
   ```

   Each function `KINBBDSp*` is a wrapper around the corresponding specification function `KINSp*` and performs the following actions:

   - Attaches the KINSPILS linear solver to the main KINSOL solver memory;
   - Sets the preconditioner data structure for KINBBDPRE;
   - Sets the preconditioner setup function for KINBBDPRE;
   - Sets the preconditioner solve function for KINBBDPRE;

   The argument `maxl` is described below. The last argument of `KINBBDSp*` is the pointer to the KINBBDPRE data returned by `KINBBDPrecAlloc`.

9. **Set linear solver optional inputs**

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

10. **Solve problem**

11. **Get optional output**

12. **Deallocate memory for solution vector**

13. **Free the** KINBBDPRE **data structure**

    ```
    KINBBDPrecFree(&bbd_data);
    ```

14. **Free solver memory**

15. **Finalize MPI**

The user-callable functions that initialize, attach, and deallocate the KINBBDPRE preconditioner module (steps 7, 8, and 13 above) are described in more detail below.

KINBBDPrecAlloc

Call   `bbd_data = KINBBDPrecAlloc(kin_mem, Nlocal, mudq, mldq,`
                                                `mukeep, mlkeep, dq_rel_u, Gloc, Gcomm);`

Description   The function `KINBBDPrecAlloc` initializes and allocates memory for the KINBBDPRE preconditioner.

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

                     `Nlocal`   (`long int`) local vector length.

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

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

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

                     `mlkeep`   (`long int`) lower half-bandwidth of the retained banded approximate Jacobian block.

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

                     `Gloc`   (`KINLocalFn`) the C function which computes the approximation $G(u) \approx F(u)$.

                     `Gcomm`   (`KINCommFn`) the optional C function which performs all interprocess communication required for the computation of $G(u)$.

Return value   If successful, `KINBBDPrecAlloc` returns a pointer to the newly created KINBBDPRE memory block (of type `void *`). If an error occurred, `KINBBDPrecAlloc` returns `NULL`.

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.

KINBBDSpgmr

Call   `flag = KINBBDSpgmr(kin_mem, maxl, bbd_data);`

Description   The function `KINBBDSpgmr` links the KINBBDPRE data to the KINSPGMR linear solver and attaches the latter to the KINSOL memory block.

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

                     `maxl`   (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL`$= 5$.

                     `bbd_data` (`void *`) pointer to the KINBBDPRE data structure.

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

               `KINSPILS_SUCCESS`   The KINSPGMR initialization was successful.

               `KINSPILS_MEM_NULL`   The `kin_mem` pointer is `NULL`.

               `KINSPILS_ILL_INPUT`   The NVECTOR module used does not implement a required operation.

               `KINSPILS_MEM_FAIL`   A memory allocation request failed.

               `KINBBDPRE_PDATA_NULL` The KINBBDPRE preconditioner has not been initialized.

KINBBDSpbcg

Call   `flag = KINBBDSpbcg(kin_mem, maxl, bbd_data);`

Description   The function `KINBBDSpbcg` links the KINBBDPRE data to the KINSPBCG linear solver and attaches the latter to the KINSOL memory block.

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

              `maxl`   (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL`= 5.

              `bbd_data` (`void *`) pointer to the KINBBDPRE data structure.

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

              `KINSPILS_SUCCESS`   The KINSPGMR initialization was successful.

              `KINSPILS_MEM_NULL`   The `kin_mem` pointer is `NULL`.

              `KINSPILS_ILL_INPUT`   The NVECTOR module used does not implement a required operation.

              `KINSPILS_MEM_FAIL`   A memory allocation request failed.

              `KINBBDPRE_PDATA_NULL`   The KINBBDPRE preconditioner has not been initialized.

KINBBDSptfqmr

Call   `flag = KINBBDSptfqmr(kin_mem, maxl, bbd_data);`

Description   The function `KINBBDSptfqmr` links the KINBBDPRE data to the KINSPTFQMR linear solver and attaches the latter to the KINSOL memory block.

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

              `maxl`   (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `KINSPILS_MAXL`= 5.

              `bbd_data` (`void *`) pointer to the KINBBDPRE data structure.

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

              `KINSPILS_SUCCESS`   The KINSPGMR initialization was successful.

              `KINSPILS_MEM_NULL`   The `kin_mem` pointer is `NULL`.

              `KINSPILS_ILL_INPUT`   The NVECTOR module used does not implement a required operation.

              `KINSPILS_MEM_FAIL`   A memory allocation request failed.

              `KINBBDPRE_PDATA_NULL`   The KINBBDPRE preconditioner has not been initialized.

KINBBDPrecFree

Call   `KINBBDPrecFree(&bbd_data);`

Description   The function `KINBBDPrecFree` frees the pointer allocated by `KINBBDPrecAlloc`.

Arguments   The only argument of `KINBBDPrecFree` is the pointer to the KINBBDPRE data structure (of type `void *`).

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

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

KINBBDPrecGetWorkSpace

Call   `flag = KINBBDPrecGetWorkSpace(bbd_data, &lenrwBBDP, &leniwBBDP);`

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

Arguments   `bbd_data`   (`void *`) pointer to the KINBBDPRE data structure.

lenrwBBDP (`long int`) local number of `realtype` values in the KINBBDPRE 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:

KINBBDPRE_SUCCESS The optional output values have been successfully set.

KINBBDPRE_PDATA_NULL The KINBBDPRE preconditioner has not been initialized.

Notes In terms of the local vector dimension `Nlocal` and $\text{smu} = \min(N_l - 1, \text{mukeep} + \text{mlkeep})$, the actual size of the real workspace is $(2\,\text{mlkeep} + \text{mukeep} + \text{smu} + 2)\,\text{Nlocal}$ `realtype` words, and the actual size of the integer workspace is `Nlocal` integer words. These values are local to the current processor.

The workspaces referred to here exist in addition to those given by the corresponding `KINSp*GetWorkSpace` function.

 KINBBDPrecGetNumGfnEvals

Call `flag = KINBBDPrecGetNumGfnEvals(bbd_data, &ngevalsBBDP);`

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

Arguments bbd_data (`void *`) pointer to the KINBBDPRE data structure.

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

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

KINBBDPRE_SUCCESS The optional output value has been successfully set.

KINBBDPRE_PDATA_NULL The KINBBDPRE preconditioner has not been initialized.

 KINBBDPrecGetReturnFlagName

Call `name = KINBBDPrecGetReturnFlagName(flag);`

Description The function `KINBBDPrecGetReturnFlagName` returns the name of the KINBBDPRE constant corresponding to `flag`.

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

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

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 §5.5.5).

Chapter 6

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 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 both the serial and the parallel NVECTOR implementations.

6.1   Important note on portability

In this package, the names of the interface functions, and the names of the FORTRAN user routines called by them, appear as dummy names which are mapped to actual values by a series of definitions in the header files `fkinsol.h`and `fkinbbd.h`. By default, those mapping definitions depend in turn on the C macro `F77_FUNC` defined in the header file `sundials_config.h` by `configure`. However, the set of flags `SUNDIALS_CASE_UPPER`, `SUNDIALS_CASE_LOWER`, `SUNDIALS_UNDERSCORE_NONE`, `SUNDIALS_UNDERSCORE_ONE`, and `SUNDIALS_UNDERSCORE_TWO` can be explicitly defined in the header file `sundials_config.h` when configuring SUNDIALS via the options `--with-f77underscore` and `--with-f77case` to override the default behavior if necessary (see Chapter 2). Either way, the names into which the dummy names are mapped are in upper or lower case and have up to two underscores appended.

The user must also ensure that variables in the user FORTRAN code are declared in a manner consistent with their counterparts in KINSOL. All real variables must be declared as `REAL`, `DOUBLE PRECISION`, or perhaps as `REAL*`n, where n denotes the number of bytes, depending on whether KINSOL was built in single, double or extended precision (see Chapter 2). Moreover, some of the FORTRAN integer variables must be declared as `INTEGER*4` or `INTEGER*8` according to the C type `long int`. These integer variables include: the array of integer optional inputs and outputs (`IOUT`), problem dimensions (`NEQ`, `NLOCAL`, `NGLOBAL`), and Jacobian half-bandwidths (`MU` and `ML`). This is particularly important when using KINSOL and the FKINSOL package on 64-bit architectures.

6.2   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`.

- Interface to the main KINSOL module

– FKINMALLOC interfaces to KINCreate, KINSetFdata, and KINMalloc.

– FKINSETIIN and FKINSETRIN interface to KINSet* functions.

– 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 linear solver modules

– FKINDENSE interfaces to KINDense.

– FKINDENSESETJAC interfaces to KINDenseSetJacFn.

– FKINBAND interfaces to KINBand.

– FKINBANDSETJAC interfaces to KINBandSetJacFn.

– FKINSPGMR interfaces to KINSpgmr and SPGMR optional input functions.

– FKINSPBCG interfaces to KINSpbcg and SPBCG optional input functions.

– FKINSPTFQMR interfaces to KINSptfqmr and SPTFQMR optional input functions.

– FKINSPILSSETJAC interfaces to KINSpilsSetJacTimesVecFn.

– FKINSPILSSETPREC interfaces to KINSpilsSetPreconditioner.

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

FKINSOL routine (FORTRAN)	KINSOL function (C)	KINSOL function type
FKFUN	FKINfunc	KINSysFn
FKDJAC	FKINDenseJac	KINDenseJacFn
FKBJAC	FKINBandJac	KINBandJacFn
FKPSET	FKINPSet	KINSpilsPrecSetupFn
FKPSOL	FKINPSol	KINSpilsPrecSolveFn
FKJTIMES	FKINJtimes	KINSpilsJacTimesVecFn

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.

6.3   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.

Steps marked with [**S**] in the instructions below apply to the serial NVECTOR implementation (NVECTOR_SERIAL) only, while those marked with [**P**] apply to NVECTOR_PARALLEL.

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 corret), or a negative value if it failed unrecoverably (in which case the the solution process is halted).

2. NVECTOR **module initialization**

   [**S**] To initialize the serial NVECTOR module, the user must make the following call:

   ```
   CALL FNVINITS (KEY, NEQ, IER)
   ```

   where `KEY` is the solver id (`KEY` = 3 for KINSOL), `NEQ` is the size of vectors, and `IER` is a return completion flag which is 0 on success and -1 if a failure occurred.

   [**P**] To initialize the parallel vector module, the user must make the following call:

   ```
   CALL FNVINITP (COMM, KEY, NLOCAL, NGLOBAL, IER)
   ```

   in which the arguments are: `COMM` = MPI communicator, `KEY` = 3, `NLOCAL` = the local size of vectors on this processor, and `NGLOBAL` = the system size (and the global size of all vectors, equal to the sum of all values of `NLOCAL`). The return flag `IER` is set to 0 on a successful return and to -1 otherwise.

   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.

3. **Problem specification**

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

   | FKINMALLOC |

Call	`CALL FKINMALLOC (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 otherwise. 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 6.2.

4. **Linear solver specification**

   The solution method in KINSOL involves the solution of linear systems related to the Jacobian of the nonlinear system. KINSOL presently includes five choices for the treatment of these systems, and the user of FKINSOL must call a routine with a specific name to make the desired choice.

   [**S**] **Dense treatment of the linear system**

   The user must make the call:

   ```
   CALL FKINDENSE (NEQ, IER)
   ```

where NEQ is the size of the nonlinear system. The argument IER is an error return flag which is 0 for success , −1 if a memory allocation failure occurred, or −2 for illegal input. As an option when using the DENSE linear solver, the user may supply a routine that computes a dense approximation of the system Jacobian $J = \partial F/\partial u$. 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).

If the FKDJAC routine is provided, then, following the call to FKINDENSE, 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.

Optional outputs specific to the DENSE case are listed in Table 6.2.

[S] **Band treatment of the linear system**

The user must make the call:

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

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

As an option when using the BAND linear solver, the user may supply a routine that computes a band approximation of the system Jacobian $J = \partial F/\partial u$. 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).

If the FKBJAC routine is provided, then, following the call to FKINBAND, 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.

Optional outputs specific to the BAND case are listed in Table 6.2.

[S][P] SPGMR treatment of the linear systems

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

```
CALL FKINSPGMR (MAXL, MAXLRST, IER)
```

The arguments are as follows. MAXL is the maximum Krylov subspace dimension. MAXLRST is the maximum number of restarts. IER is an error return flag which is 0 to indicate success, -1 if a memory allocation failure occurred, or -2 to indicate an illegal input.

Optional outputs specific to the SPGMR case are listed in Table 6.2.

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

[S][P] SPBCG treatment of the linear systems

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

```
CALL FKINSPBCG (MAXL, IER)
```

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

Optional outputs specific to the SPBCG case are listed in Table 6.2.

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

[S][P] SPTFQMR treatment of the linear systems

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

```
CALL FKINSPTFQMR (MAXL, IER)
```

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

Optional outputs specific to the SPTFQMR case are listed in Table 6.2.

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

[S][P] Functions used by SPGMR/SPBCG/SPTFQMR

An optional user-supplied routine, FKINJTIMES (see below), can be provided for Jacobian-vector products. If it is, then, following the call to FKINSPGMR, FKINSPBCG, or FKINSPTFQMR, the user must make the call:

```
CALL FKINSPILSSETJAC (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.

If preconditioning is to be done, then the user must call

```
CALL FKINSPILSSETPREC (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).

[S][P] User-supplied routines for SPGMR/SPBCG/SPTFQMR

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

As an option when using the SPGMR, SPBCG, or SPTFQMR linear solvers, the user may supply a routine that computes the product of the system Jacobian $J = \partial F/\partial u$ and a given vector v. 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 NEQ, 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.

If 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, FTEM, IER)
DIMENSION U(*), USCALE(*), FVAL(*), FSCALE(*), VTEM(*), FTEM(*)
```

Typically this routine will use only U, FVAL, VTEM and FTEM. 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, VTEMP1, VTEMP2, IER)
DIMENSION U(*), USCALE(*), FVAL(*), FSCALE(*), VTEMP1(*), VTEMP2(*)
```

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. The arrays VTEMP1 and VTEMP2 are available for work space. If scaling is being used, USCALE and FSCALE are available for those operations requiring scaling. NEQ is the problem size.

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

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

5. **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 (1 specifies Inexact Newton, while 2 indicates line search). 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 KINSol returns (see §5.5.3 and §10.2). The values of the optional outputs are available in IOPT and ROPT (see Table 6.2).

6. **Memory deallocation**

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

```
CALL FKINFREE
```

6.4   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 two routines: FKINSETIIN for integer optional inputs and FKINSETRIN for real optional inputs. These functions should be called as follows:

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

where KEY is a quoted string indicating which optional input is set (see Table 6.1), IVAL is the integer input value to the used, RVAL is the real input value to be used, and IER is an integer return flag which is set to 0 on success and a negative value if a filure occurred.

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 FKINMALLOC. Table 6.2 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 §5.5.4 and §5.5.5.

6.5   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 §5.7), 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 KINBBDPrecAlloc.

- FKINBBDSPGMR interfaces to KINBBDSpgmr and SPGMR optional input functions.

- FKINBBDSPBCG interfaces to KINBBDSpbcg and SPBCG optional input functions.

- FKINBBDSPTFQMR interfaces to KINBBDSptfmqr and SPTFQMR optional input functions.

- FKINBBDOPT interfaces to KINBBDPRE optional output functions.

- FKINBBDFREE interfaces to KINBBDPrecFree.

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):

Table 6.1: Keys for setting FKINSOL optional inputs

Integer optional inputs FKINSETIIN

Key	Optional input	Default value
PRNT_LEVEL	Verbosity level of output	0
MAX_NITER	Maximum no. of nonlinear iterations	200
ETA_FORM	Form of η coefficient	1 (KIN_ETACHOICE1)
MAX_SETUPS	Maximum no. of iterations without prec. setup	10
MAX_SP_SETUPS	Maximum no. of iterations without residual check	5
NO_INIT_SETUP	No initial preconditioner setup	FALSE
NO_MIN_EPS	Lower bound on ϵ	FALSE
NO_RES_MON	No residual monitoring	FALSE

Real optional inputs (FKINSETRIN)

Key	Optional input	Default value
FNORM_TOL	Function-norm stopping tolerance	$\sqrt[3]{\text{uround}}$
SSTEP_TOL	Scaled-step stopping tolerance	u$round^{2/3}$
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

FKINBBD routine (FORTRAN)	KINSOL function (C)	KINSOL function type
FKLOCFN	FKINgloc	KINLocalFn
FKCOMMF	FKINgcomm	KINCommFn
FKJTIMES	FKINJtimes	KINSpilsJacTimesVecFn

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 §6.2, 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 §6.3 are grayed-out.

1. **Nonlinear system function specification**

2. NVECTOR **module initialization**

3. **Problem specification**

4. **Linear solver specification**

   To initialize the KINBBDPRE preconditioner, make the following call:

   ```
   CALL FKINBBDINIT (NLOCAL, MUDQ, MLDQ, MU, ML, IER)
   ```

   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

Table 6.2: Description of the FKINSOL optional output arrays IOUT and ROUT

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
KINDENSE linear solver		
7	LENRWLS	KINDenseGetWorkSpace
8	LENIWLS	KINDenseGetWorkSpace
9	LS_FLAG	KINDenseGetLastFlag
10	NFELS	KINDenseGetNumFuncEvals
11	NJE	KINDenseGetNumJacEvals
KINBAND linear solver		
7	LENRWLS	KINBandGetWorkSpace
8	LENIWLS	KINBandGetWorkSpace
9	LS_FLAG	KINBandGetLastFlag
10	NFELS	KINBandGetNumFuncEvals
11	NJE	KINBandGetNumJacEvals
KINSPGMR, KINSPBCG, KINSPTFQMR linear solvers		
7	LENRWLS	KINSpilsGetWorkSpace
8	LENIWLS	KINSpilsGetWorkSpace
9	LS_FLAG	KINSpilsGetLastFlag
10	NFELS	KINSpilsGetNumFuncEvals
11	NJTV	KINSpilsGetNumJacEvals
12	NPE	KINSpilsGetNumPrecEvals
13	NPS	KINSpilsGetNumPrecSolves
14	NLI	KINSpilsGetNumLinIters
15	NCFL	KINSpilsGetNumConvFails

Real output array ROUT

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

value of 0 indicates success, while a value of -1 indicates that a memory failure occurred or that an input had an illegal value.

To specify the SPGMR linear system solver and use the KINBBDPRE preconditioner, make the following call:

```
CALL FKINBBDSPGMR (MAXL, MAXLRST, IER)
```

Its arguments are the same as those of FKINSPGMR (see step 4 in §6.3).

To specify the SPBCG linear system solver and use the KINBBDPRE preconditioner, make the following call:

```
CALL FKINBBDSPBCG (MAXL, IER)
```

Its arguments are the same as those of FKINSPGMR (see step 4 in §6.3).

To specify the SPTFQMR linear system solver and use the KINBBDPRE preconditioner, make the following call:

```
CALL FKINBBDSPTFQMR (MAXL, IER)
```

Its arguments are the same as those of FKINSPGMR (see step 4 in §6.3).

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

```
CALL FKINSPILSSETJAC (FLAG, IER)
```

with FLAG $\neq 0$. (see step 4 in §6.3).

5. **Problem solution**

6. KINBBDPRE **Optional outputs**

   Optional outputs specific to the SPGMR, SPBCG, or SPTFQMR solver are listed in Table 6.2. To obtain the optional outputs associated with the KINBBDPRE module, make the following call:

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

   The arguments returned 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.

7. **Memory deallocation**

   To free the internal memory created by the call to FKINBBDINIT, before calling FKINFREE and FNVFREEP, the user must call

   ```
   CALL FKINBBDFREE
   ```

8. **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 4 in §6.3.

Chapter 7

Description of the NVECTOR module

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

The generic `N_Vector` type is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the vector, and an *ops* field pointing to a structure with generic vector operations. The type `N_Vector` is defined as

```
typedef struct _generic_N_Vector *N_Vector;

struct _generic_N_Vector {
    void *content;
    struct _generic_N_Vector_Ops *ops;
};
```

The `_generic_N_Vector_Ops` structure is essentially a list of pointers to the various actual vector operations, and is defined as

```
struct _generic_N_Vector_Ops {
  N_Vector    (*nvclone)(N_Vector);
  N_Vector    (*nvcloneempty)(N_Vector);
  void        (*nvdestroy)(N_Vector);
  void        (*nvspace)(N_Vector, long int *, long int *);
  realtype*   (*nvgetarraypointer)(N_Vector);
  void        (*nvsetarraypointer)(realtype *, N_Vector);
  void        (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
  void        (*nvconst)(realtype, N_Vector);
  void        (*nvprod)(N_Vector, N_Vector, N_Vector);
  void        (*nvdiv)(N_Vector, N_Vector, N_Vector);
  void        (*nvscale)(realtype, N_Vector, N_Vector);
  void        (*nvabs)(N_Vector, N_Vector);
  void        (*nvinv)(N_Vector, N_Vector);
  void        (*nvaddconst)(N_Vector, realtype, N_Vector);
  realtype    (*nvdotprod)(N_Vector, N_Vector);
  realtype    (*nvmaxnorm)(N_Vector);
  realtype    (*nvwrmsnorm)(N_Vector, N_Vector);
  realtype    (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
  realtype    (*nvmin)(N_Vector);
```

```
   realtype    (*nvwl2norm)(N_Vector, N_Vector);
   realtype    (*nvl1norm)(N_Vector);
   void        (*nvcompare)(realtype, N_Vector, N_Vector);
   booleantype (*nvinvtest)(N_Vector, N_Vector);
   booleantype (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
   realtype    (*nvminquotient)(N_Vector, N_Vector);
};
```

The generic NVECTOR module defines and implements the vector operations acting on N_Vector. These routines are nothing but wrappers for the vector operations defined by a particular NVECTOR implementation, which are accessed through the *ops* field of the N_Vector structure. To illustrate this point we show below the implementation of a typical vector operation from the generic NVECTOR module, namely N_VScale, which performs the scaling of a vector x by a scalar c:

```
void N_VScale(realtype c, N_Vector x, N_Vector z)
{
   z->ops->nvscale(c, x, z);
}
```

Table 7.1 contains a complete list of all vector operations defined by the generic NVECTOR module.

Finally, note that the generic NVECTOR module defines the functions N_VCloneVectorArray and N_VCloneEmptyVectorArray. Both functions create (by cloning) an array of count variables of type N_Vector, each of the same type as an existing N_Vector. Their prototypes are

```
N_Vector *N_VCloneVectorArray(int count, N_Vector w);
N_Vector *N_VCloneEmptyVectorArray(int count, N_Vector w);
```

and their definitions are based on the implementation-specific N_VClone and N_VCloneEmpty operations, respectively.

An array of variables of type N_Vector can be destroyed by calling N_VDestroyVectorArray, whose prototype is

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

and whose definition is based on the implementation-specific N_VDestroy operation.

A particular implementation of the NVECTOR module must:

- Specify the *content* field of N_Vector.

- Define and implement the vector operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one NVECTOR module (each with different N_Vector internal data representations) in the same code.

- Define and implement user-callable constructor and destructor routines to create and free an N_Vector with the new *content* field and with *ops* pointing to the new vector operations.

- Optionally, define and implement additional user-callable routines acting on the newly defined N_Vector (e.g., a routine to print the content for debugging purposes).

- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the *content* field of the newly defined N_Vector.

Table 7.1: Description of the NVECTOR operations

Name	Usage and Description
N_VClone	`v = N_VClone(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not copy the vector, but rather allocates storage for the new vector.
N_VCloneEmpty	`v = N_VCloneEmpty(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not allocate storage for the data array.
N_VDestroy	`N_VDestroy(v);` Destroys the `N_Vector` `v` and frees memory allocated for its internal data.
N_VSpace	`N_VSpace(nvSpec, &lrw, &liw);` Returns storage requirements for one `N_Vector`. `lrw` contains the number of realtype words and `liw` contains the number of integer words.
N_VGetArrayPointer	`vdata = N_VGetArrayPointer(v);` 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 linear solvers, as well as the interfaces to the banded preconditioners provided with SUNDIALS.
N_VSetArrayPointer	`N_VSetArrayPointer(vdata, v);` Overwrites the data in an `N_Vector` with a given array of `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 linear solver.
N_VLinearSum	`N_VLinearSum(a, x, b, y, z);` Performs the operation $z = ax + by$, where a and b are scalars and x and y are of type `N_Vector`: $z_i = ax_i + by_i$, $i = 0, \ldots, n-1$.
N_VConst	`N_VConst(c, z);` Sets all components of the `N_Vector` `z` to c: $z_i = c$, $i = 0, \ldots, n-1$.
N_VProd	`N_VProd(x, y, z);` Sets the `N_Vector` `z` to be the component-wise product of the `N_Vector` inputs `x` and `y`: $z_i = x_i y_i$, $i = 0, \ldots, n-1$.
N_VDiv	`N_VDiv(x, y, z);` Sets the `N_Vector` `z` to be the component-wise ratio of the `N_Vector` inputs `x` and `y`: $z_i = x_i/y_i$, $i = 0, \ldots, n-1$. The y_i may not be tested for 0 values. It should only be called with an `x` that is guaranteed to have all nonzero components.

	continued from last page
Name	**Usage and Description**
N_VScale	N_VScale(c, x, z); Scales the N_Vector x by the scalar c and returns the result in z: $z_i = cx_i$, $i = 0, \ldots, n-1$.
N_VAbs	N_VAbs(x, z); Sets the components of the N_Vector z to be the absolute values of the components of the N_Vector x: $y_i = |x_i|$, $i = 0, \ldots, n-1$.
N_VInv	N_VInv(x, z); Sets the components of the N_Vector z to be the inverses of the components of the N_Vector x: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine may not check for division by 0. It should be called only with an x which is guaranteed to have all nonzero components.
N_VAddConst	N_VAddConst(x, b, z); Adds the scalar b to all components of x and returns the result in the N_Vector z: $z_i = x_i + b$, $i = 0, \ldots, n-1$.
N_VDotProd	d = N_VDotProd(x, y); Returns the value of the ordinary dot product of x and y: $d = \sum_{i=0}^{n-1} x_i y_i$.
N_VMaxNorm	m = N_VMaxNorm(x); Returns the maximum norm of the N_Vector x: $m = \max_i |x_i|$.
N_VWrmsNorm	m = N_VWrmsNorm(x, w) Returns the weighted root-mean-square norm of the N_Vector x with weight vector w: $m = \sqrt{\left(\sum_{i=0}^{n-1}(x_i w_i)^2\right)/n}$.
N_VWrmsNormMask	m = N_VWrmsNormMask(x, w, id); Returns the weighted root mean square norm of the N_Vector x with weight vector w built using only the elements of x corresponding to nonzero elements of the N_Vector id: $m = \sqrt{\left(\sum_{i=0}^{n-1}(x_i w_i \mathrm{sign}(id_i))^2\right)/n}$.
N_VMin	m = N_VMin(x); Returns the smallest element of the N_Vector x: $m = \min_i x_i$.
N_VWL2Norm	m = N_VWL2Norm(x, w); Returns the weighted Euclidean ℓ_2 norm of the N_Vector x with weight vector w: $m = \sqrt{\sum_{i=0}^{n-1}(x_i w_i)^2}$.
N_VL1Norm	m = N_VL1Norm(x); Returns the ℓ_1 norm of the N_Vector x: $m = \sum_{i=0}^{n-1}|x_i|$.
N_VCompare	N_VCompare(c, x, z); Compares the components of the N_Vector x to the scalar c and returns an N_Vector z such that: $z_i = 1.0$ if $|x_i| \geq c$ and $z_i = 0.0$ otherwise.

	continued from last page
Name	**Usage and Description**
N_VInvTest	t = N_VInvTest(x, z); Sets the components of the N_Vector z to be the inverses of the components of the N_Vector x, with prior testing for zero values: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine returns TRUE if all components of x are nonzero (successful inversion) and returns FALSE otherwise.
N_VConstrMask	t = N_VConstrMask(c, x, m); Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \geq 0$ if $c_i = 1$, $x_i \leq 0$ if $c_i = -1$, $x_i < 0$ if $c_i = -2$. There is no constraint on x_i if $c_i = 0$. This routine returns FALSE if any element failed the constraint test, TRUE if all passed. It also sets a mask vector m, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.
N_VMinQuotient	minq = N_VMinQuotient(num, denom); This routine returns the minimum of the quotients obtained by termwise 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.

7.1 The NVECTOR_SERIAL implementation

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

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

The following five macros are provided to access the content of an NVECTOR_SERIAL vector. The suffix _S in the names denotes serial version.

- NV_CONTENT_S

  This routine gives access to the contents of the serial vector N_Vector.

  The assignment v_cont = NV_CONTENT_S(v) sets v_cont to be a pointer to the serial N_Vector content structure.

  Implementation:

  ```
  #define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
  ```

- NV_OWN_DATA_S, NV_DATA_S, NV_LENGTH_S

  These macros give individual access to the parts of the content of a serial N_Vector.

  The assignment v_data = NV_DATA_S(v) sets v_data to be a pointer to the first component of the data for the N_Vector v. The assignment NV_DATA_S(v) = v_data sets the component array of v to be v_data by storing the pointer v_data.

  The assignment v_len = NV_LENGTH_S(v) sets v_len to be the length of v. On the other hand, the call NV_LENGTH_S(v) = len_v sets the length of v to be len_v.

Implementation:

```
#define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )

#define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )

#define NV_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
```

- NV_Ith_S

  This macro gives access to the individual components of the data array of an N_Vector.

  The assignment `r = NV_Ith_S(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_S(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n - 1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_S(v,i) ( NV_DATA_S(v)[i] )
  ```

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Table 7.1. Their names are obtained from those in Table 7.1 by appending the suffix _Serial. The module NVECTOR_SERIAL provides the following additional user-callable routines:

- N_VNew_Serial

  This function creates and allocates memory for a serial N_Vector. Its only argument is the vector length.

  ```
  N_Vector N_VNew_Serial(long int vec_length);
  ```

- N_VNewEmpty_Serial

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

  ```
  N_Vector N_VNewEmpty_Serial(long int vec_length);
  ```

- N_VMake_Serial

  This function creates and allocates memory for a serial vector with user-provided data array.

  ```
  N_Vector N_VMake_Serial(long int vec_length, realtype *v_data);
  ```

- N_VCloneVectorArray_Serial

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

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

- N_VCloneVectorArrayEmpty_Serial

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

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

- N_VDestroyVectorArray_Serial

  This function frees memory allocated for the array of count variables of type N_Vector created with N_VCloneVectorArray_Serial or with N_VCloneVectorArrayEmpty_Serial.

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

- N_VPrint_Serial

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

  ```
  void N_VPrint_Serial(N_Vector v);
  ```

Notes

- When looping over the components of an N_Vector v, it is more efficient to first obtain the component array via v_data = NV_DATA_S(v) and then access v_data[i] within the loop than it is to use NV_Ith_S(v,i) within the loop.

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

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

7.2   The NVECTOR_PARALLEL implementation

The parallel implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_PARALLEL, 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, an a boolean flag *own_data* indicating ownership of the data array *data*.

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

The following seven macros are provided to access the content of a NVECTOR_PARALLEL vector. The suffix _P in the names denotes 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_VectorParallelContent.

  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_Ith_P

  This macro gives access to the individual components of the local data array of an N_Vector.

  The assignment `r = NV_Ith_P(v,i)` sets `r` to be the value of the `i`-th component of the local part of `v`. The assignment `NV_Ith_P(v,i) = r` sets the value of the `i`-th component of the local part of `v` to be `r`.

  Here i ranges from 0 to $n - 1$, where n is the local length.

  Implementation:

  ```
  #define NV_Ith_P(v,i) ( NV_DATA_P(v)[i] )
  ```

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Table 7.1 Their names are obtained from those in Table 7.1 by appending the suffix _Parallel. The module NVECTOR_PARALLEL provides the following additional user-callable routines:

- N_VNew_Parallel

  This function creates and allocates memory for a parallel vector.

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

- N_VNewEmpty_Parallel

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

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

- N_VMake_Parallel

  This function creates and allocates memory for a parallel vector with user-provided data array.

  ```
  N_Vector N_VMake_Parallel(MPI_Comm comm,
                            long int local_length,
                            long int global_length,
                            realtype *v_data);
  ```

- N_VCloneVectorArray_Parallel

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

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

- N_VCloneVectorArrayEmpty_Parallel

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

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

- N_VDestroyVectorArray_Parallel

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

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

- N_VPrint_Parallel

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

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

Notes

- When looping over the components of an N_Vector v, it is more efficient to first obtain the local
    component array via v_data = NV_DATA_P(v) and then access v_data[i] within the loop than
    it is to use NV_Ith_P(v,i) within the loop.

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

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

7.3   NVECTOR functions used by KINSOL

In Table 7.2 below, we list the vector functions in the NVECTOR module 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 four KINSOL linear solvers (KINSPILS stands for any of KINSPGMR,
KINSPBCG, or KINSPTFQMR), the KINBBDPRE preconditioner module, and the FKINSOL module.

There is one subtlety in the KINSPILS column hidden by the table explained here for the case of the
KINSPGMR module. The dot product function N_VDotProd is called both within the implementation file
kinsol_spgmr.c for the KINSPGMR solver and within the implementation files sundials_spgmr.c and
sundials_iterative.c for the generic SPGMR solver upon which the KINSPGMR solver is implemented.
Also, although N_VDiv is not called within the implementation file kinsol_spgmr.c, it is called within
the implementation file sundials_spgmr.c and so is required by the KINSPGMR solver module. This
issue does not arise for the other two KINSOL linear solvers because the generic DENSE and BAND solvers
(used in the implementation of KINDENSE and KINBAND) do not make calls to any vector functions.

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.

The vector functions listed in Table 7.1 that are *not* used by KINSOL are: N_VAddConst, N_VWrmsNorm,
N_VWrmsNormMask, N_VCompare, and N_VInvTest. Therefore a user-supplied NVECTOR module for KIN-
SOL could omit these five functions.

Table 7.2: List of vector functions usage by KINSOL code modules

	KINSOL	KINDENSE	KINBAND	KINSPILS	KINBBDPRE	FKINSOL
N_VClone	✓			✓	✓	
N_VCloneEmpty						✓
N_VDestroy	✓			✓	✓	✓
N_VSpace	✓					
N_VGetArrayPointer		✓	✓		✓	✓
N_VSetArrayPointer		✓				✓
N_VLinearSum	✓	✓		✓		
N_VConst				✓		
N_VProd	✓	✓	✓	✓		
N_VDiv	✓			✓		
N_VScale	✓	✓	✓	✓	✓	
N_VAbs	✓					
N_VInv	✓					
N_VDotProd		✓	✓	✓		
N_VMaxNorm	✓					
N_VMin	✓					
N_VWL2Norm	✓	✓	✓	✓		
N_VL1Norm				✓		
N_VConstrMask	✓					
N_VMinQuotient	✓					

Chapter 8

Providing Alternate Linear Solver Modules

The central KINSOL module interfaces with the linear solver module to be used by way of calls to four routines. These are denoted here by `linit`, `lsetup`, `lsolve`, and `lfree`. Briefly, their purposes are as follows:

- `linit`: initialize and allocate memory specific to the linear solver;

- `lsetup`: evaluate and preprocess the Jacobian or preconditioner;

- `lsolve`: solve the linear system;

- `lfree`: free the linear solver memory.

A linear solver module must also provide a user-callable specification routine (like that described in §5.5.2) which will attach the above four routines to the main KINSOL memory block. The KINSOL memory block is a structure defined in the header file `kinsol_impl.h`. A pointer to such a structure is defined as the type `KINMem`. The four fields in a `KINMem` structure that must point to the linear solver's functions are `kin_linit`, `kin_lsetup`, `kin_lsolve`, and `kin_lfree`, respectively. Note that of the four interface routines, only the `lsolve` routine is required. The `lfree` routine must be provided only if the solver specification routine makes any memory allocation. For consistency with the existing KINSOL linear solver modules, we recommend that the return value of the specification function be 0 for a successful return or a negative value if an error occurs (the pointer to the main KINSOL memory block is `NULL`, an input is illegal, the NVECTOR implementation is not compatible, a memory allocation fails, etc.)

To facilitate data exchange between the four interface functions, the field `kin_lmem` in the KINSOL memory block can be used to attach a linear solver-specific memory block.

These four routines that interface between KINSOL and the linear solver module necessarily have fixed call sequences. Thus, a user wishing to implement another linear solver within the KINSOL package must adhere to this set of interfaces. The following is a complete description of the call list for each of these routines. Note that the call list of each routine includes a pointer to the main KINSOL memory block, by which the routine can access various data related to the KINSOL solution. The contents of this memory block are given in the file `kinsol_impl.h` (but not reproduced here, for the sake of space).

8.1 Initialization function

The type definition of `linit` is

`linit`

Definition   `int (*linit)(KINMem kin_mem);`

Purpose   The purpose of `linit` is to complete initializations for a specific linear solver, such as counters and statistics.

Arguments   `kin_mem` is the KINSOL memory pointer of type `KINMem`.

Return value   An `linit` function should return 0 if it has successfully initialized the KINSOL linear solver and -1 otherwise.

8.2   Setup function

The type definition of `lsetup` is

`lsetup`

Definition   `int (*lsetup)(KINMem kin_mem);`

Purpose   The job of `lsetup` is to prepare the linear solver for subsequent calls to `lsolve`. It may recompute Jacobian-related data if it deems necessary.

Arguments   `kin_mem` is the KINSOL memory pointer of type `KINMem`.

Return value   The `lsetup` routine should return 0 if successful and a non-zero value otherwise.

8.3   Solve function

The type definition of `lsolve` is

`lsolve`

Definition   `int (*lsolve)(KINMem kin_mem, N_Vector x,`
               `                  N_Vector b, realtype *res_norm);`

Purpose   The routine `lsolve` must solve the linear equation $Jx = b$, where $J = \partial F/\partial u$ is evaluated at the current iterate and the right-hand side vector b is input.

Arguments   `kin_mem`   is the KINSOL memory pointer of type `KINMem`.
               `x`   is a vector set to an initial guess prior to calling `lsolve`. On return it should contain the solution to $Jx = b$.
               `b`   is the right-hand side vector b, set to $-F(u)$, evaluated at the current iterate.
               `res_norm` holds the value of the L_2 norm of the residual vector upon return.

Return value   `lsolve` should return 0 if successful. If an error occurs and recovery could be possible by calling again the `lsetup` function, then it should return a positive value. Otherwise, `lsolve` should return a negative value.

8.4   Memory deallocation function

The type definition of `lfree` is

`lfree`

Definition   `void (*lfree)(KINMem kin_mem);`

Purpose   The routine `lfree` should free any linear solver memory allocated by the `linit` routine.

Arguments   `kin_mem` is the KINSOL memory pointer of type `KINMem`.

Return value   This routine has no return value.

Notes   This routine is called once a problem has been completed and the linear solver is no longer needed.

Chapter 9

Generic Linear Solvers in SUNDIALS

In this chapter, we describe five generic linear solver code modules that are included in SUNDIALS, but which are of potential use as generic packages in themselves, either in conjunction with the use of KINSOL or separately. These modules are:

- The DENSE matrix package, which includes functions for small dense matrices treated as simple array types.

- The BAND matrix package, which includes the matrix type `BandMat`, macros and functions for `BandMat` matrices.

- The SPGMR package, which includes a solver for the scaled preconditioned GMRES method.

- The SPBCG package, which includes a solver for the scaled preconditioned Bi-CGStab method.

- The SPTFQMR package, which includes a solver for the scaled preconditioned TFQMR method.

For reasons related to installation, the names of the files involved in these generic solvers begin with the prefix `sundials_`. But despite this, each of the solvers is in fact generic, in that it is usable completely independently of SUNDIALS.

For the sake of space, the functions for `DenseMat` and `BandMat` matrices and the functions in SPGMR, SPBCG, and SPTFQMR are only summarized briefly, since they are less likely to be of direct use in connection with KINSOL. The functions for small dense matrices are fully described, because we expect that they will be useful in the implementation of preconditioners used with the combination of KINSOL and the KINSPGMR, KINSPBCG, or KINSPTFQMR solver.

9.1 The DENSE module

Relative to the SUNDIALS *source_tree*, the files comprising the DENSE generic linear solver are as follows:

- header files (located in *source_tree*/`shared/include`)
  `sundials_dense.h sundials_smalldense.h`
  `sundials_types.h sundials_math.h sundials_config.h`

- source files (located in *source_tree*/`shared/source`)
  `sundials_dense.c sundials_smalldense.c sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are relevant to the DENSE package by itself (see §2.5 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```

- (optional) use of generic math functions: `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro RCONST, while the `sundials_math.h` header file is needed for the `ABS` macro and `RAbs` function.

   The eight files listed above can be extracted from the SUNDIALS *source_tree* and compiled by themselves into a DENSE library or into a larger user code.

9.1.1   Type DenseMat

The type `DenseMat` is defined to be a pointer to a structure with a size and a data field:

```
typedef struct {
  long int size;
  realtype  **data;
} *DenseMat;
```

The *size* field indicates the number of columns (which is the same as the number of rows) of a dense matrix, while the *data* field is a two dimensional array used for component storage. The elements of a dense matrix are stored columnwise (i.e columns are stored one on top of the other in memory). If A is of type `DenseMat`, then the (i,j)-th element of A (with $0 \le i, j \le \texttt{size}-1$) is given by the expression `(A->data)[j][i]` or by the expression `(A->data)[0][j*size+i]`. The macros below allow a user to efficiently access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer to the j-th column of elements can be obtained via the `DENSE_COL` macro. Users should use these macros whenever possible.

9.1.2   Accessor Macros

The following two macros are defined by the DENSE module to provide access to data in the `DenseMat` type:

- `DENSE_ELEM`

  Usage : `DENSE_ELEM(A,i,j) = a_ij;` or `a_ij = DENSE_ELEM(A,i,j);`

  `DENSE_ELEM` references the (i,j)-th element of the $N \times N$ `DenseMat` A, $0 \le i, j \le N - 1$.

- `DENSE_COL`

  Usage : `col_j = DENSE_COL(A,j);`

  `DENSE_COL` references the j-th column of the $N \times N$ `DenseMat` A, $0 \le j \le N - 1$. The type of the expression `DENSE_COL(A,j)` is `realtype *`. After the assignment in the usage above, `col_j` may be treated as an array indexed from 0 to $N - 1$. The (i, j)-th element of A is referenced by `col_j[i]`.

9.1.3   Functions

The following functions for `DenseMat` matrices are available in the DENSE package. For full details, see the header file `sundials_dense.h`.

- `DenseAllocMat`: allocation of a `DenseMat` matrix;

- `DenseAllocPiv`: allocation of a pivot array for use with `DenseFactor`/`DenseBacksolve`;

- `DenseFactor`: LU factorization with partial pivoting;

- `DenseBacksolve`: solution of $Ax = b$ using LU factorization;

- `DenseZero`: load a matrix with zeros;

- `DenseCopy`: copy one matrix to another;

- `DenseScale`: scale a matrix by a scalar;

- `DenseAddI`: increment a matrix by the identity matrix;

- `DenseFreeMat`: free memory for a `DenseMat` matrix;

- `DenseFreePiv`: free memory for a pivot array;

- `DensePrint`: print a `DenseMat` matrix to standard output.

9.1.4 Small Dense Matrix Functions

The following functions for small dense matrices are available in the DENSE package:

- `denalloc`

  `denalloc(n)` allocates storage for an `n` by `n` dense matrix. It returns a pointer to the newly allocated storage if successful. If the memory request cannot be satisfied, then `denalloc` returns `NULL`. The underlying type of the dense matrix returned is `realtype**`. If we allocate a dense matrix `realtype** a` by `a = denalloc(n)`, then `a[j][i]` references the (i,j)-th element of the matrix `a`, $0 \leq$ `i`, `j` $\leq$ `n`-1, and `a[j]` is a pointer to the first element in the j-th column of `a`. The location `a[0]` contains a pointer to `n`^{2} contiguous locations which contain the elements of `a`.

- `denallocpiv`

  `denallocpiv(n)` allocates an array of `n` integers. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `gefa`

  `gefa(a,n,p)` factors the `n` by `n` dense matrix `a`. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.

  A successful LU factorization leaves the matrix `a` and the pivot array `p` with the following information:

  1. `p[k]` contains the row number of the pivot element chosen at the beginning of elimination step `k`, `k` $= 0, 1, ...,$`n`-1.

  2. If the unique LU factorization of `a` is given by $Pa = LU$, where P is a permutation matrix, L is a lower triangular matrix with all 1's on the diagonal, and U is an upper triangular matrix, then the upper triangular part of `a` (including its diagonal) contains U and the strictly lower triangular part of `a` contains the multipliers, $I - L$.

     `gefa` returns 0 if successful. Otherwise it encountered a zero diagonal element during the factorization. In this case it returns the column index (numbered from one) at which it encountered the zero.

- `gesl`

  `gesl(a,n,p,b)` solves the `n` by `n` linear system $ax = b$. It assumes that `a` has been LU-factored and the pivot array `p` has been set by a successful call to `gefa(a,n,p)`. The solution x is written into the `b` array.

- `denzero`

  `denzero(a,n)` sets all the elements of the `n` by `n` dense matrix `a` to be 0.0;

- `dencopy`

  `dencopy(a,b,n)` copies the `n` by `n` dense matrix `a` into the `n` by `n` dense matrix `b`;

- `denscale`

  `denscale(c,a,n)` scales every element in the `n` by `n` dense matrix `a` by `c`;

- `denaddI`

  `denaddI(a,n)` increments the `n` by `n` dense matrix `a` by the identity matrix;

- `denfreepiv`

  `denfreepiv(p)` frees the pivot array `p` allocated by `denallocpiv`;

- `denfree`

  `denfree(a)` frees the dense matrix `a` allocated by `denalloc`;

- `denprint`

  `denprint(a,n)` prints the `n` by `n` dense matrix `a` to standard output as it would normally appear on paper. It is intended as a debugging tool with small values of `n`. The elements are printed using the `%g` option. A blank line is printed before and after the matrix.

9.2 The BAND module

Relative to the SUNDIALS *source_tree*, the files comprising the BAND generic linear solver are as follows:

- header files (located in *source_tree*/`shared/include`)
  `sundials_band.h`
  `sundials_types.h` `sundials_math.h` `sundials_config.h`

- source files (located in *source_tree*/`shared/source`)
  `sundials_band.c` `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are required to use the BAND package by itself (see §2.5 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  `#define SUNDIALS_DOUBLE_PRECISION 1`
  `#define SUNDIALS_SINGLE_PRECISION 1`
  `#define SUNDIALS_EXTENDED_PRECISION 1`

- (optional) use of generic math functions:
  `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines of the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the `MIN`, `MAX`, and `ABS` macros and `RAbs` function.

The six files listed above can be extracted from the SUNDIALS *source_tree* and compiled by themselves into a BAND library or into a larger user code.

9.2.1 Type BandMat

The type `BandMat` is the type of a large band matrix A (possibly distributed). It is defined to be a pointer to a structure defined by:

```
typedef struct {
  long int size;
  long int mu, ml, smu;
  realtype **data;
} *BandMat;
```

The fields in the above structure are:

- *size* is the number of columns (which is the same as the number of rows);

- *mu* is the upper half-bandwidth, $0 \leq mu \leq size-1$;

- *ml* is the lower half-bandwidth, $0 \leq ml \leq size-1$;

- *smu* is the storage upper half-bandwidth, $mu \leq smu \leq size-1$. The `BandFactor` routine writes the LU factors into the storage for A. The upper triangular factor U, however, may have an upper half-bandwidth as big as $\min(size-1, mu+ml)$ because of partial pivoting. The *smu* field holds the upper half-bandwidth allocated for A.

- *data* is a two dimensional array used for component storage. The elements of a band matrix of type `BandMat` 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.

  If we number rows and columns in the band matrix starting from 0, then

  - *data[0]* is a pointer to $(smu+ml+1)*size$ contiguous locations which hold the elements within the band of A

  - *data[j]* is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from $smu-mu$ (to access the uppermost element within the band in the j-th column) to $smu+ml$ (to access the lowest element within the band in the j-th column). Indices from 0 to $smu-mu-1$ give access to extra storage elements required by `BandFactor`.

  - *data[j][i-j+smu]* is the (i,j)-th element, $j-mu \leq i \leq j+ml$.

The macros below allow a user to access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer into the j-th column of elements can be obtained via the `BAND_COL` macro. Users should use these macros whenever possible.

See Figure 9.1 for a diagram of the `BandMat` type.

9.2.2 Accessor Macros

The following three macros are defined by the BAND module to provide access to data in the `BandMat` type:

- `BAND_ELEM`

  Usage : `BAND_ELEM(A,i,j) = a_ij;` or `a_ij = BAND_ELEM(A,i,j);`

  `BAND_ELEM` references the (i,j)-th element of the $N \times N$ band matrix A, where $0 \leq$ i, j $\leq N-1$. The location (i,j) should further satisfy $j-($A->mu$) \leq$ i $\leq$ j$+($A->ml$)$.
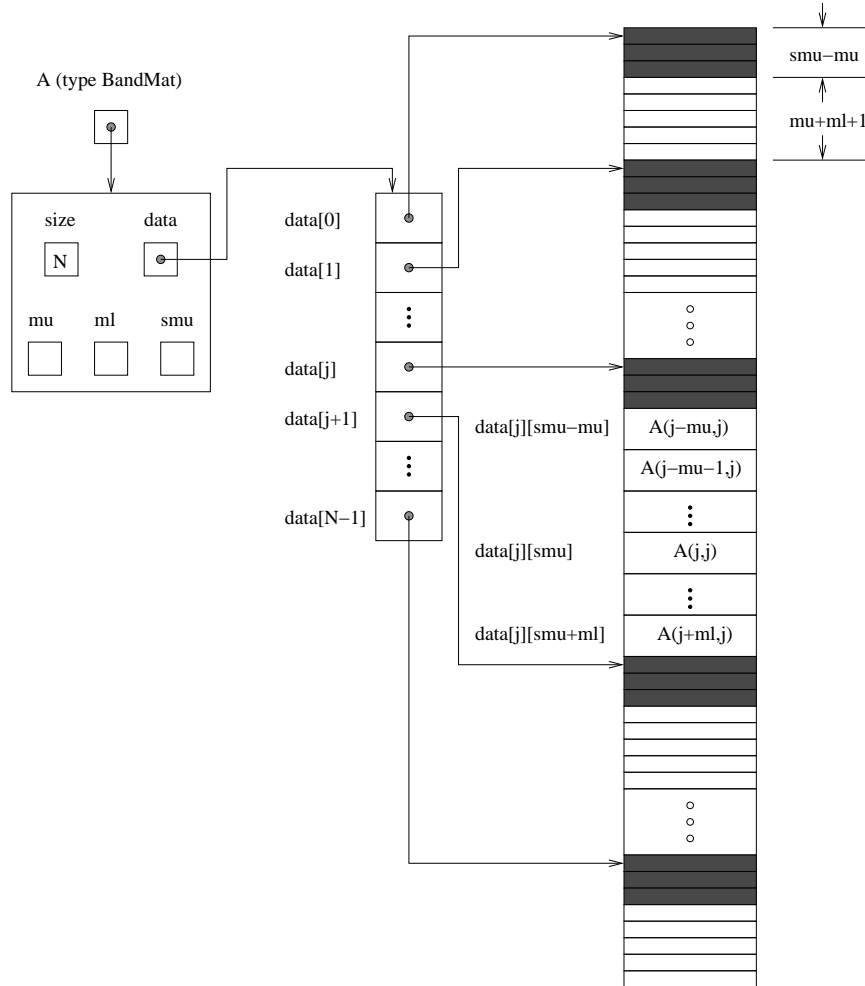
Figure 9.1: Diagram of the storage for a band matrix of type `BandMat`. Here `A` is an $N \times N$ band matrix of type `BandMat` with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to $N - 1$ and the (i, j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the `BandFactor` and `BandBacksolve` routines.

- BAND_COL

  Usage : `col_j = BAND_COL(A,j);`

  BAND_COL references the diagonal element of the j-th column of the $N \times N$ band matrix A, $0 \leq j \leq N - 1$. The type of the expression BAND_COL(A,j) is realtype *. The pointer returned by the call BAND_COL(A,j) can be treated as an array which is indexed from $-(\texttt{A->mu})$ to $(\texttt{A->ml})$.

- BAND_COL_ELEM

  Usage : `BAND_COL_ELEM(col_j,i,j) = a_ij;` or `a_ij = BAND_COL_ELEM(col_j,i,j);`

  This macro references the (i,j)-th entry of the band matrix A when used in conjunction with BAND_COL to reference the j-th column through col_j. The index (i,j) should satisfy $\texttt{j} - (\texttt{A->mu}) \leq \texttt{i} \leq \texttt{j} + (\texttt{A->ml})$.

9.2.3 Functions

The following functions for `BandMat` matrices are available in the BAND package. For full details, see the header file `sundials_band.h`.

- `BandAllocMat`: allocation of a `BandMat` matrix;

- `BandAllocPiv`: allocation of a pivot array for use with `BandFactor`/`BandBacksolve`;

- `BandFactor`: LU factorization with partial pivoting;

- `BandBacksolve`: solution of $Ax = b$ using LU factorization;

- `BandZero`: load a matrix with zeros;

- `BandCopy`: copy one matrix to another;

- `BandScale`: scale a matrix by a scalar;

- `BandAddI`: increment a matrix by the identity matrix;

- `BandFreeMat`: free memory for a `BandMat` matrix;

- `BandFreePiv`: free memory for a pivot array;

- `BandPrint`: print a `BandMat` matrix to standard output.

9.3 The SPGMR module

The SPGMR package, in the files `sundials_spgmr.h` and `sundials_spgmr.c`, includes an implementation of the scaled preconditioned GMRES method. A separate code module, implemented in `sundials_iterative.(h,c)`, contains auxiliary functions that support SPGMR, as well as the other Krylov solvers in SUNDIALS (SPBCG and SPTFQMR). For full details, including usage instructions, see the header files `sundials_spgmr.h` and `sundials_iterative.h`.

Relative to the SUNDIALS *source_tree*, the files comprising the SPGMR generic linear solver are as follows:

- header files (located in *source_tree*/`shared/include`)
  `sundials_spgmr.h sundials_iterative.h sundials_nvector.h`
  `sundials_types.h sundials_math.h sundials_config.h`

- source files (located in *source_tree*/`shared/source`)
  `sundials_spgmr.c sundials_iterative.c sundials_nvector.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are required to use the SPGMR package by itself (see §2.5 for details):

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```

- (optional) use of generic math functions:
  ```
  #define SUNDIALS_USE_GENERIC_MATH 1
  ```

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro RCONST, while the `sundials_math.h` header file is needed for the MAX and ABS macros and RAbs and RSqrt functions.

The generic NVECTOR files, `sundials_nvector.(h,c)` are needed for the definition of the generic `N_Vector` type and functions. The NVECTOR functions used by the SPGMR module are: N_VDotProd, N_VLinearSum, N_VScale, N_VProd, N_VDiv, N_VConst, N_VClone, N_VCloneVectorArray, N_VDestroy, and N_VDestroyVectorArray.

The SPGMR package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The nine files listed above can be extracted from the SUNDIALS *source_tree* and compiled by themselves into an SPGMR library or into a larger user code.

9.3.1   Functions

The following functions are available in the SPGMR package:

- `SpgmrMalloc`: allocation of memory for `SpgmrSolve`;

- `SpgmrSolve`: solution of $Ax = b$ by the SPGMR method;

- `SpgmrFree`: free memory allocated by `SpgmrMalloc`.

The following functions are available in the support package `sundials_iterative.(h,c)`:

- `ModifiedGS`: performs modified Gram-Schmidt procedure;

- `ClassicalGS`: performs classical Gram-Schmidt procedure;

- `QRfact`: performs QR factorization of Hessenberg matrix;

- `QRsol`: solves a least squares problem with a Hessenberg matrix factored by `QRfact`.

9.4   The SPBCG module

The SPBCG package, in the files `sundials_spbcgs.h` and `sundials_spbcgs.c`, includes an implementation of the scaled preconditioned Bi-CGStab method. For full details, including usage instructions, see the file `sundials_spbcgs.h`.

The SPBCG package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The files needed to use the SPBCG module by itself are the same as for the SPGMR module, with `sundials_spbcgs.(h,c)` replacing `sundials_spgmr.(h,c)`.

9.4.1 Functions

The following functions are available in the SPBCG package:

- `SpbcgMalloc`: allocation of memory for `SpbcgSolve`;

- `SpbcgSolve`: solution of $Ax = b$ by the SPBCG method;

- `SpbcgFree`: free memory allocated by `SpbcgMalloc`.

9.5 The SPTFQMR module

The SPTFQMR package, in the files `sundials_sptfqmr.h` and `sundials_sptfqmr.c`, includes an implementation of the scaled preconditioned TFQMR method. For full details, including usage instructions, see the file `sundials_sptfqmr.h`.

The SPTFQMR package can only be used in conjunction with an actual NVECTOR implementation library, such as the NVECTOR_SERIAL or NVECTOR_PARALLEL provided with SUNDIALS.

The files needed to use the SPTFQMR module by itself are the same as for the SPGMR module, with `sundials_sptfqmr.(h,c)` replacing `sundials_spgmr.(h,c)`.

9.5.1 Functions

The following functions are available in the SPTFQMR package:

- `SptfqmrMalloc`: allocation of memory for `SptfqmrSolve`;

- `SptfqmrSolve`: solution of $Ax = b$ by the SPTFQMR method;

- `SptfqmrFree`: free memory allocated by `SptfqmrMalloc`.

Chapter 10

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.

10.1 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	3	Use constant value for η.
KIN_NONE	0	Use inexact Newton globalization.
KIN_LINESEARCH	1	Use line search globalization.

Iterative linear solver module		
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.

10.2 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_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.
KIN_LINESEARCH_NONCONV	-5	The line search algorithm was unable to find an iterate sufficiently distinct from the current iterate.

KIN_MAXITER_REACHED	-6	The maximum number of nonlinear iterations has been reached.
KIN_MXNEWT_5X_EXCEEDED	-7	Five consecutive steps have been taken that satisfy a scaled step length test.
KIN_LINESEARCH_BCFAIL	-8	The line search algorithm was unable to satisfy the β-condition for `nbcfails` iterations.
KIN_LINSOLV_NO_RECOVERY	-9	The user-supplied routine preconditioner slve function failed recoverably, but the preconditioner is already current.
KIN_LINIT_FAIL	-10	The linear solver's initialization function failed.
KIN_LSETUP_FAIL	-11	The linear solver's setup function failed in an unrecoverable manner.
KIN_LSOLVE_FAIL	-12	The linear solver's solve function failed in an unrecoverable manner.
KIN_SYSFUNC_FAIL	-13	The system function failed in an unrecoverable manner.
KIN_FIRST_SYSFUNC_ERR	-14	The system function failed recoverably at the first call.
KIN_REPTD_SYSFUNC_ERR	-15	The system function had repeated recoverable errors.

KINDENSE **linear solver module**		
KINDENSE_SUCCESS	0	Successful function return.
KINDENSE_MEM_NULL	-1	The `kin_mem` argument was NULL.
KINDENSE_LMEM_NULL	-2	The KINDENSE linear solver has not been initialized.
KINDENSE_ILL_INPUT	-3	The KINDENSE solver is not compatible with the current NVECTOR module.
KINDENSE_MEM_FAIL	-4	A memory allocation request failed.

KINBAND **linear solver module**		
KINBAND_SUCCESS	0	Successful function return.
KINBAND_MEM_NULL	-1	The `kin_mem` argument was NULL.
KINBAND_LMEM_NULL	-2	The KINBAND linear solver has not been initialized.
KINBAND_ILL_INPUT	-3	The KINBAND solver is not compatible with the current NVECTOR module, or an input value was illegal.
KINBAND_MEM_FAIL	-4	A memory allocation request failed.

KINSPILS **linear solver modules**		
KINSPILS_SUCCESS	0	Successful function return.
KINSPILS_MEM_NULL	-1	The `kin_mem` argument was NULL.
KINSPILS_LMEM_NULL	-2	The linear solver has not been initialized.
KINSPILS_ILL_INPUT	-3	The solver is not compatible with the current NVECTOR module, or an input value was illegal.
KINSPILS_MEM_FAIL	-4	A memory allocation request failed.

SPGMR **generic linear solver module**		
SPGMR_SUCCESS	0	Converged.
SPGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.

SPGMR_CONV_FAIL	2	Failure to converge.
SPGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPGMR_MEM_NULL	-1	The SPGMR memory is NULL
SPGMR_ATIMES_FAIL	-2	The Jacobian tims vector function failed.
SPGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPGMR_QRSOL_FAIL	-5	The matrix R was found to be singular during the QR solve phase.

SPBCG **generic linear solver module**		
SPBCG_SUCCESS	0	Converged.
SPBCG_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPBCG_CONV_FAIL	2	Failure to converge.
SPBCG_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPBCG_MEM_NULL	-1	The SPBCG memory is NULL
SPBCG_ATIMES_FAIL	-2	The Jacobian tims vector function failed.
SPBCG_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.

SPTFQMR **generic linear solver module**		
SPTFQMR_SUCCESS	0	Converged.
SPTFQMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPTFQMR_CONV_FAIL	2	Failure to converge.
SPTFQMR_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPTFQMR_MEM_NULL	-1	The SPTFQMR memory is NULL
SPTFQMR_ATIMES_FAIL	-2	The Jacobian tims vector function failed.
SPTFQMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.

KINBBDPRE **preconditioner module**		
KINBBDPRE_SUCCESS	0	Successful function return.
KINBBDPRE_PDATA_NULL	-11	The preconditioner module has not been initialized.

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