Installation Guide for SUNDIALS v2.7.0

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September 26, 2016



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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Chapter 1

SUNDIALS Package Installation Procedure

The installation of any SUNDIALS package is accomplished by installing the SUNDIALS suite as a whole, according to the instructions that follow. The same procedure applies whether or not the downloaded file contains one or all solvers in SUNDIALS.

The SUNDIALS suite (or individual solvers) are distributed as compressed archives (.tar.gz). The name of the distribution archive is of the form <code>solver-x.y.z.tar.gz</code>, where <code>solver</code> is one of: <code>sundials</code>, <code>cvode</code>, <code>cvodes</code>, <code>arkode</code>, <code>ida</code>, <code>idas</code>, or <code>kinsol</code>, and <code>x.y.z</code> represents the version number (of the <code>SUNDIALS</code> suite or of the individual solver). To begin the installation, first uncompress and expand the sources, by issuing

% tar xzf solver-x.y.z.tar.gz

This will extract source files under a directory *solver*-x.y.z.

Starting with version 2.6.0 of SUNDIALS, CMake is the only supported method of installation. The explanations on the installation procedure begins with a few common observations:

• The remainder of this chapter will follow these conventions:

srcdir is the directory solver-x.y.z created above; i.e., the directory containing the SUNDIALS sources.

builddir is the (temporary) directory under which SUNDIALS is built.

- instdir is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory instdir/include while libraries are installed under instdir/lib, with instdir specified at configuration time.
- For sundials CMake-based installation, in-source builds are prohibited; in other words, the build directory *builddir* can **not** be the same as *srcdir* and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.
- The installation directory instdir can **not** be the same as the source directory srcdir.
- By default, only the libraries and header files are exported to the installation directory instdir. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the installed SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as "templates" for your own problems. CMake installs CMakeLists.txt files and also (as an option available only under Unix/Linux) Makefile files. Note this installation



approach also allows the option of building the SUNDIALS examples without having to install them. (This can be used as a sanity check for the freshly built libraries.)

• Even if generation of shared libraries is enabled, only static libraries are created for the FCMIX modules. (Because of the use of fixed names for the Fortran user-provided subroutines, FCMIX shared libraries would result in "undefined symbol" errors at link time.)

1.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Makefiles, as well as KDevelop, Visual Studio, and (Apple) XCode project files from the same configuration file. In addition, CMake also provides a GUI front end and which allows an interactive build and installation process.

The SUNDIALS build process requires CMake version 2.8.1 or higher and a working compiler. On Unix-like operating systems, it also requires Make (and curses, including its development libraries, for the GUI front end to CMake, ccmake), while on Windows it requires Visual Studio. While many Linux distributions offer CMake, the version included is probably out of date. Many new CMake features have been added recently, and you should download the latest version from http://www.cmake.org. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use ccmake, while Windows users will be able to use CMakeSetup.

As previously noted, when using CMake to configure, build and install SUNDIALS, it is always required to use a separate build directory. While in-source builds are possible, they are explicitly prohibited by the SUNDIALS CMake scripts (one of the reasons being that, unlike autotools, CMake does not provide a make distclean procedure and it is therefore difficult to clean-up the source tree after an in-source build). By ensuring a separate build directory, it is an easy task for the user to clean-up all traces of the build by simply removing the build directory. CMake does generate a make clean which will remove files generated by the compiler and linker.

1.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The *installdir* defaults to /usr/local and can be changed by setting the CMAKE_INSTALL_PREFIX variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the cmake command, or from a curses-based GUI by using the ccmake command. Examples for using both methods will be presented. For the examples shown it is assumed that there is a top level SUNDIALS directory with appropriate source, build and install directories:

```
% mkdir (...)sundials/instdir
% mkdir (...)sundials/builddir
% cd (...)sundials/builddir
```

Building with the GUI

Using CMake with the GUI follows this general process:

- Select and modify values, run configure (c key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
 - If it is a boolean (ON/OFF) it will toggle the value
 - If it is string or file, it will allow editing of the string

- For file and directories, the <tab> key can be used to complete
- Repeat until all values are set as desired and the generate option is available (g key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (t key)
- To search for a variable press / key, and to repeat the search, press the n key

To build the default configuration using the GUI, from the *builddir* enter the ccmake command and point to the *srcdir*:

% ccmake ../srcdir

The default configuration screen is shown in Figure 1.1.

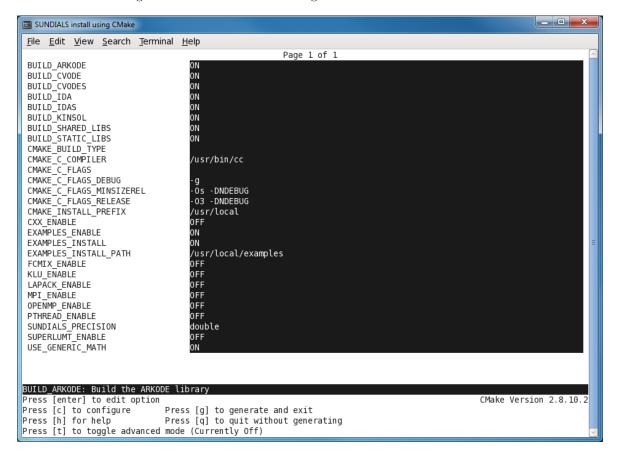


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the CMAKE_INSTALL_PREFIX and the EXAMPLES_INSTALL_PATH as shown in figure 1.2.

Pressing the (g key) will generate makefiles including all dependencies and all rules to build SUN-DIALS on this system. Back at the command prompt, you can now run:

% make

To install SUNDIALS in the installation directory specified in the configuration, simply run:

% make install

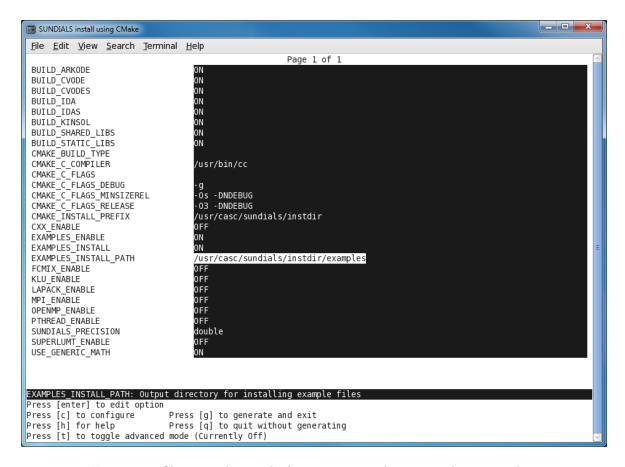


Figure 1.2: Changing the *instdir* for SUNDIALS and corresponding examples

Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the cmake command. The following will build the default configuration:

```
% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../srcdir
% make
% make install
```

1.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

```
BUILD_ARKODE - Build the ARKODE library
Default: ON

BUILD_CVODE - Build the CVODE library
Default: ON

BUILD_CVODES - Build the CVODES library
Default: ON
```

BUILD_IDA - Build the IDA library

Default: ON

BUILD_IDAS - Build the IDAS library

Default: ON

BUILD_KINSOL - Build the KINSOL library

Default: ON

BUILD_SHARED_LIBS - Build shared libraries

Default: OFF

BUILD_STATIC_LIBS - Build static libraries

Default: ON

CMAKE_BUILD_TYPE - Choose the type of build, options are: None (CMAKE_C_FLAGS used) Debug

Release RelWithDebInfo MinSizeRel

Default:

CMAKE_C_COMPILER - C compiler

Default: /usr/bin/cc

CMAKE_C_FLAGS - Flags for C compiler

Default:

CMAKE_C_FLAGS_DEBUG - Flags used by the compiler during debug builds

Default: -g

CMAKE_C_FLAGS_MINSIZEREL - Flags used by the compiler during release minsize builds

Default: -Os -DNDEBUG

 ${\tt CMAKE_C_FLAGS_RELEASE}$ - Flags used by the compiler during release builds

Default: -O3 -DNDEBUG

CMAKE_Fortran_COMPILER - Fortran compiler

Default: /usr/bin/gfortran

Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (FCMIX_ENABLE is ON) or Blas/Lapack support is enabled (LAPACK_ENABLE is ON).

CMAKE_Fortran_FLAGS - Flags for Fortran compiler

Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the compiler during debug builds

Default:

CMAKE_Fortran_FLAGS_MINSIZEREL - Flags used by the compiler during release minsize builds

Default:

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the compiler during release builds

Default:

CMAKE_INSTALL_PREFIX - Install path prefix, prepended onto install directories

Default: /usr/local

Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories <code>include</code> and <code>lib</code> of

CMAKE_INSTALL_PREFIX, respectively.

EXAMPLES_ENABLE - Build the SUNDIALS examples

Default: ON

EXAMPLES_INSTALL - Install example files

Default: ON

Note: This option is triggered only if building example programs is enabled (EXAMPLES_ENABLE ON). If the user requires installation of example programs then the sources and sample output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by EXAMPLES_INSTALL_PATH. A CMake configuration script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by EXAMPLES_INSTALL_PATH.

EXAMPLES_INSTALL_PATH - Output directory for installing example files

Default: /usr/local/examples

Note: The actual default value for this option will an examples subdirectory created under CMAKE_INSTALL_PREFIX.

FCMIX_ENABLE - Enable Fortran-C support

Default: OFF

HYPRE_ENABLE - Enable hypre support

Default: OFF

HYPRE_INCLUDE_DIR - Path to hypre header files

HYPRE_LIBRARY - Path to hypre installed library

KLU_ENABLE - Enable KLU support

Default: OFF

KLU_INCLUDE_DIR - Path to SuiteSparse header files

KLU_LIBRARY_DIR - Path to SuiteSparse installed library files

LAPACK_ENABLE - Enable Lapack support

Default: OFF

Note: Setting this option to ON will trigger the two additional options see below.

LAPACK_LIBRARIES - Lapack (and Blas) libraries

Default: /usr/lib/liblapack.so;/usr/lib/libblas.so

Note: CMake will search for these libraries in your LD_LIBRARY_PATH prior to searching default system paths.

MPI_ENABLE - Enable MPI support

Default: OFF

Note: Setting this option to ON will trigger several additional options related to MPI.

MPI_MPICC - mpicc program

Default:

MPI_RUN_COMMAND - Specify run command for MPI

Default: mpirun

Note: This can either be set to mpirun for OpenMPI or srun if jobs are managed by SLURM - Simple Linux Utility for Resource Management as exists on LLNL's high performance computing clusters.

MPI_MPIF77 - mpif77 program

Default:

Note: This option is triggered only if using MPI compiler scripts (MPI_USE_MPISCRIPTS is ON) and Fortran-C support is enabled (FCMIx_ENABLE is ON).

```
OPENMP_ENABLE - Enable OpenMP support
     Default: OFF
     Turn on support for the OpenMP based nvector.
PETSC_ENABLE - Enable PETSc support
     Default: OFF
PETSC_INCLUDE_DIR - Path to PETSc header files
PETSC_LIBRARY_DIR - Path to PETSc installed library files
PTHREAD_ENABLE - Enable Pthreads support
     Default: OFF
     Turn on support for the Pthreads based nvector.
SUNDIALS_PRECISION - Precision used in SUNDIALS, options are: double, single or extended
     Default: double
SUPERLUMT_ENABLE - Enable SUPERLU_MT support
     Default: OFF
SUPERLUMT_INCLUDE_DIR - Path to SuperLU_MT header files (typically SRC directory)
SUPERLUMT_LIBRARY_DIR - Path to SuperLU_MT installed library files
SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP
USE_GENERIC_MATH - Use generic (stdc) math libraries
     Default: ON
```

1.1.3 Configuration examples

% cmake \

The following examples will help demonstrate usage of the CMake configure options.

> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \

To configure SUNDIALS using the default C and Fortran compilers, and default mpicc and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

1.1.4 Working with external Libraries

The SUNDIALS Suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries.

Building with LAPACK and BLAS

To enable LAPACK and BLAS libraries, set the LAPACK_ENABLE option to ON. If the directory containing the LAPACK and BLAS libraries is in the LD_LIBRARY_PATH environment variable, CMake will set the LAPACK_LIBRARIES variable accordingly, otherwise CMake will attemp to find the LAPACK and BLAS libraries in standard system locations. To explicitly tell CMake what libraries to use, the LAPACK_LIBRARIES variable can be set to the desired libraries. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DLAPACK_LIBRARIES=/mypath/lib/liblapack.so;/mypath/lib/libblas.so \
> /home/myname/sundials/srcdir
%
    make install
%
```

Building with KLU

The KLU libraries are part of SuiteSparse, a suite of sparse matrix software, available from the Texas A&M University website: http://faculty.cse.tamu.edu/davis/suitesparse.html. SUNDIALS has been tested with SuiteSparse version 4.5.3. To enable KLU, set KLU_ENABLE to ON, set KLU_INCLUDE_DIR to the include path of the KLU installation and set KLU_LIBRARY_DIR to the lib path of the KLU installation. The CMake configure will result in populating the following variables: AMD_LIBRARY, AMD_LIBRARY_DIR, BTF_LIBRARY_DIR, COLAMD_LIBRARY, COLAMD_LIBRARY_DIR, and KLU_LIBRARY

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt. SUNDIALS has been tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set SUPERLUMT_ENABLE to ON, set SUPERLUMT_INCLUDE_DIR to the SRC path of the SuperLU_MT installation, and set the variable SUPERLUMT_LIBRARY_DIR to the lib path of the SuperLU_MT installation. At the same time, the variable SUPERLUMT_THREAD_TYPE must be set to either Pthread or OpenMP.



Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either OPENMP_ENABLE or PTHREAD_ENABLE set to ON then SuperLU_MT should be set to use the same threading type.

Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: http://www.mcs.anl.gov/petsc. SUNDIALS has been tested with PETSc version 3.7.2. To enable PETSc, set PETSC_ENABLE to ON, set PETSC_INCLUDE_DIR to the include path of the PETSc installation, and set the variable PETSC_LIBRARY_DIR to the lib path of the PETSc installation.

Building with hypre

The hypre libraries are available for download from the Lawrence Livermore National Laboratory website: http://computation.llnl.gov/projects/hypre-scalable-linear-solvers-multigrid-methods.

SUNDIALS has been tested with hypre version 2.11.1. To enable hypre, set HYPRE_ENABLE to ON, set HYPRE_INCLUDE_DIR to the include path of the hypre installation, and set the variable HYPRE_LIBRARY_DIR to the lib path of the hypre installation.

1.2 Building and Running Examples

Each of the SUNDIALS solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set both EXAMPLES_ENABLE and EXAMPLES_INSTALL to ON. Specify the installation path for the examples with the variable EXAMPLES_INSTALL_PATH. CMake will generate CMakeLists.txt configuration files (and Makefile files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

Either the CMakeLists.txt file or the traditional Makefile may be used to build the examples as well as serve as a template for creating user developed solutions. To use the supplied Makefile simply run make to compile and generate the executables. To use CMake from within the installed example directory, run cmake (or ccmake to use the GUI) followed by make to compile the example code. Note that if CMake is used, it will overwrite the traditional Makefile with a new CMake-generated Makefile. The resulting output from running the examples can be compared with example output bundled in the SUNDIALS distribution.

NOTE: There will potentially be differences in the output due to machine architecture, compiler versions, use of third party libraries etc.



1.3 Configuring, building, and installing on Windows

CMake can also be used to build SUNDIALS on Windows. To build SUNDIALS for use with Visual Studio the following steps should be performed:

- 1. Unzip the downloaded tar file(s) into a directory. This will be the *srcdir*
- 2. Create a separate builddir
- 3. Open a Visual Studio Command Prompt and cd to builddir
- 4. Run cmake-gui ../srcdir
 - (a) Hit Configure
 - (b) Check/Uncheck solvers to be built
 - (c) Change CMAKE_INSTALL_PREFIX to instdir
 - (d) Set other options as desired
 - (e) Hit Generate
- 5. Back in the VS Command Window:
 - (a) Run msbuild ALL_BUILD.vcxproj
 - (b) Run msbuild INSTALL.vcxproj

The resulting libraries will be in the *instdir*. The SUNDIALS project can also now be opened in Visual Studio. Double click on the ALL_BUILD.vcxproj file to open the project. Build the whole *solution* to create the SUNDIALS libraries. To use the SUNDIALS libraries in your own projects, you must set the include directories for your project, add the SUNDIALS libraries to your project solution, and set the SUNDIALS libraries as dependencies for your project.

1.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

% make install

will install the libraries under *libdir* and the public header files under *includedir*. The values for these directories are *instdir*/lib and *instdir*/include, respectively. The location can be changed by setting the CMake variable CMAKE_INSTALL_PREFIX. Although all installed libraries reside under *libdir*/lib, the public header files are further organized into subdirectories under *includedir*/include.

The installed libraries and exported header files are listed for reference in Tables 1.1 and 1.2. The file extension .lib is typically .so for shared libraries and .a for static libraries. Note that, in the Tables, names are relative to libdir for libraries and to includedir for header files.

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

Table 1.1: SUNDIALS libraries and header files

SHARED	Libraries	n/a	
	Header files	sundials/sundials_config.h sundials/sundials_math.h	$sundials/sundials_types.h$
		sundials/sundials_nvector.h	sundials/sundials_fnvector.h
		sundials/sundials_direct.h	sundials/sundials_lapack.h
		sundials/sundials_dense.h	sundials/sundials_band.h
		sundials/sundials_sparse.h	
		sundials/sundials_iterative.h	sundials/sundials_spgmr.h
		sundials/sundials_spbcgs.h	sundials/sundials_sptfqmr.h
		sundials/sundials_pcg.h	sundials/sundials_spfgmr.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.lib	libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h	
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.lib	libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h	<u> </u>
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.lib	libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h	
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.lib	$libsundials_fnvecpthreads.a$
	Header files	nvector/nvector_pthreads.h	
CVODE	Libraries	libsundials_cvode.lib	libsundials_fcvode.a
	Header files	cvode/cvode.h	cvode/cvode_impl.h
		cvode/cvode_direct.h	$cvode/cvode_lapack.h$
		cvode/cvode_dense.h	$cvode/cvode_band.h$
		cvode/cvode_diag.h	
		cvode/cvode_sparse.h	$cvode/cvode_klu.h$
		cvode/cvode_superlumt.h	
		cvode/cvode_spils.h	$cvode/cvode_spgmr.h$
		cvode/cvode_sptfqmr.h	$cvode/cvode_spbcgs.h$
		cvode/cvode_bandpre.h	cvode/cvode_bbdpre.h
CVODES	Libraries	$libsundials_cvodes.lib$	
	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h
		cvodes/cvodes_direct.h	cvodes/cvodes_lapack.h
		cvodes/cvodes_dense.h	$cvodes/cvodes_band.h$
		cvodes/cvodes_diag.h	
		cvodes/cvodes_sparse.h	cvodes_klu.h
		cvodes/cvodes_superlumt.h	
		cvodes/cvodes_spils.h	cvodes/cvodes_spgmr.h
		cvodes/cvodes_sptfqmr.h	cvodes/cvodes_spbcgs.h
	T 11	cvodes/cvodes_bandpre.h	cvodes/cvodes_bbdpre.h
ARKODE	Libraries	libsundials_arkode.lib	libsundials_farkode.a
	Header files	arkode/arkode.h	arkode/arkode_impl.h
		arkode/arkode_direct.h	arkode/arkode_lapack.h
		arkode/arkode_dense.h	arkode/arkode_band.h
		arkode/arkode_sparse.h	arkode/arkode_klu.h
		arkode/arkode_superlumt.h	only do /only do
		arkode/arkode_spils.h	arkode/arkode_spgmr.h
		arkode/arkode_sptfqmr.h	arkode/arkode_spbcgs.h
		arkode/arkode_pcg.h	arkode/arkode_spfgmr.h
		arkode/arkode_bandpre.h	arkode/arkode_bbdpre.h

Table 1.2: SUNDIALS libraries and header files (cont.)

IDA	Libraries	$libsundials_ida.lib$	libsundials_fida.a	
	Header files	ida/ida.h	ida/ida_impl.h	
		$ida/ida_direct.h$	ida/ida_lapack.h	
		ida/ida_dense.h	ida/ida_band.h	
		ida/ida_sparse.h	ida/ida_klu.h	
		ida/ida_superlumt.h	·	
		ida/ida_spils.h	$ida/ida_spgmr.h$	
		ida/ida_spbcgs.h	ida/ida_sptfqmr.h	
		ida/ida_bbdpre.h	·	
IDAS	Libraries	$libsundials_idas.lib$		
	Header files	idas/idas.h	idas/idas_impl.h	
		$idas/idas_direct.h$	idas/idas_lapack.h	
		idas/idas_dense.h	idas/idas_band.h	
		idas/idas_sparse.h	idas/idas_klu.h	
		idas/idas_superlumt.h		
		idas/idas_spils.h	$idas/idas_spgmr.h$	
		$idas/idas_spbcgs.h$	$idas/idas_sptfqmr.h$	
		idas/idas_bbdpre.h		
KINSOL	Libraries	libsundials_kinsol. lib	libsundials_fkinsol.a	
	Header files	kinsol/kinsol.h	kinsol/kinsol_impl.h	
		kinsol/kinsol_direct.h	kinsol/kinsol_lapack.h	
		kinsol/kinsol_dense.h	kinsol/kinsol_band.h	
		kinsol/kinsol_sparse.h	kinsol/kinsol_klu.h	
		kinsol/kinsol_superlumt.h		
		kinsol/kinsol_spils.h	kinsol/kinsol_spgmr.h	
		kinsol/kinsol_spbcgs.h	kinsol/kinsol_sptfqmr.h	
		kinsol/kinsol_bbdpre.h	kinsol/kinsol_spfgmr.h	