

# Installation Guide for SUNDIALS v4.0.0

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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 `solver-x.y.z.tar.gz`, where *solver* is one of: `sundials`, `cvode`, `cvodes`, `arkode`, `ida`, `idas`, or `kinsol`, and `x.y.z` represents the version number (of the SUNDIALS suite or of the individual solver). To begin the installation, first uncompress and expand the sources, by issuing

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

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

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

- The remainder of this chapter will follow these conventions:

***solverdir*** is the directory `solver-x.y.z` created above; i.e., the directory containing the 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/CMAKE_INSTALL_LIBDIR`, with *instdir* and `CMAKE_INSTALL_LIBDIR` specified at configuration time.

- For SUNDIALS CMake-based installation, in-source builds are prohibited; in other words, the build directory *builddir* can **not** be the same as *solverdir* and such an attempt will lead to an error. This prevents “polluting” the source tree and allows efficient builds for different configurations and/or options.
- The installation directory *instdir* can **not** be the same as the source directory *solverdir*.
- By default, only the libraries and header files are exported to the installation directory *instdir*. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the *installed* SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as “templates” for your own problems. CMake installs `CMakeLists.txt` files



and also (as an option available only under Unix/Linux) **Makefile** files. Note this installation approach also allows the option of building the SUNDIALS examples without having to install them. (This can be used as a sanity check for the freshly built libraries.)

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

## 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 3.1.3 or higher and a working C compiler. On Unix-like operating systems, it also requires Make (and **curses**, including its development libraries, for the GUI front end to CMake, **ccmake**), while on Windows it requires Visual Studio. CMake is continually adding new features, and the latest version can be downloaded from <http://www.cmake.org>. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use **ccmake**, while Windows users will be able to use **CMakeSetup**.

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

### 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 *instdir* defaults to */usr/local* and can be changed by setting the **CMAKE\_INSTALL\_PREFIX** variable. Support for FORTRAN and all other options are disabled.

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

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

#### Building with the GUI

Using CMake with the GUI follows this general process:

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

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

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

```
% ccmake ../solverdir
```

The default configuration screen is shown in Figure 1.1.

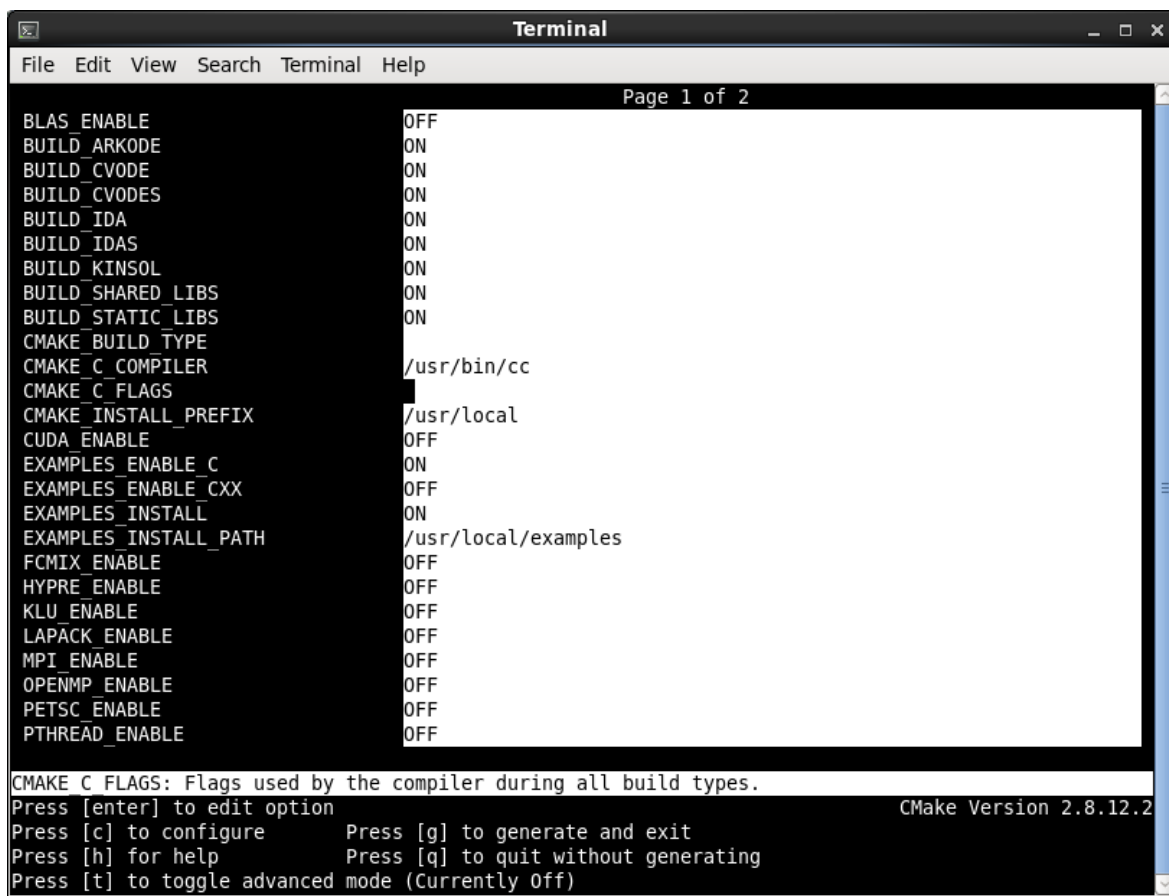


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instldir* 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 SUNDIALS 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
```

```

CMake
File Edit View Search Terminal Help
Page 1 of 2
BLAS_ENABLE OFF
BUILD_ARKODE ON
BUILD_CVODE ON
BUILD_CVODES ON
BUILD_IDA ON
BUILD_IDAS ON
BUILD_KINSOL ON
BUILD_SHARED_LIBS ON
BUILD_STATIC_LIBS ON
CMAKE_BUILD_TYPE
CMAKE_C_COMPILER /usr/bin/cc
CMAKE_C_FLAGS
CMAKE_INSTALL_PREFIX /usr/casc/sundials/instdir
CUDA_ENABLE OFF
EXAMPLES_ENABLE_C ON
EXAMPLES_ENABLE_CXX OFF
EXAMPLES_INSTALL ON
EXAMPLES_INSTALL_PATH /usr/casc/sundials/instdir/examples
FCMIX_ENABLE OFF
HYPRE_ENABLE OFF
KLU_ENABLE OFF
LAPACK_ENABLE OFF
MPI_ENABLE OFF
OPENMP_ENABLE OFF
PETSC_ENABLE OFF
PTHREAD_ENABLE OFF
CMAKE C FLAGS: Flags used by the compiler during all build types.
Press [enter] to edit option
Press [c] to configure Press [g] to generate and exit
Press [h] for help Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
CMake Version 2.8.12.2

```

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 \
> ../solverdir
% 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.

**BLAS\_ENABLE** - Enable BLAS support

Default: OFF

Note: Setting this option to ON will trigger additional CMake options. See additional information on building with BLAS enabled in [1.1.4](#).

**BLAS\_LIBRARIES** - BLAS library

Default: `/usr/lib/libblas.so`



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

`BUILD_ARKODE` - Build the ARKODE library  
Default: ON

`BUILD_CVODE` - Build the CVODE library  
Default: ON

`BUILD_CVODES` - Build the CVODES library  
Default: ON

`BUILD_IDA` - Build the IDA library  
Default: ON

`BUILD_IDAS` - Build the IDAS library  
Default: ON

`BUILD_KINSOL` - Build the KINSOL library  
Default: ON

`BUILD_SHARED_LIBS` - Build shared libraries  
Default: ON

`BUILD_STATIC_LIBS` - Build static libraries  
Default: ON

`CMAKE_BUILD_TYPE` - Choose the type of build, options are: `None` (`CMAKE_C_FLAGS` used), `Debug`, `Release`, `RelWithDebInfo`, and `MinSizeRel`  
Default:  
Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by `CMAKE_<language>_FLAGS`.

`CMAKE_C_COMPILER` - C compiler  
Default: `/usr/bin/cc`

`CMAKE_C_FLAGS` - Flags for C compiler  
Default:

`CMAKE_C_FLAGS_DEBUG` - Flags used by the C compiler during debug builds  
Default: `-g`

`CMAKE_C_FLAGS_MINSIZEREL` - Flags used by the C compiler during release minsize builds  
Default: `-Os -DNDEBUG`

`CMAKE_C_FLAGS_RELEASE` - Flags used by the C compiler during release builds  
Default: `-O3 -DNDEBUG`

`CMAKE_CXX_COMPILER` - C++ compiler  
Default: `/usr/bin/c++`  
Note: A C++ compiler (and all related options) are only triggered if C++ examples are enabled (`EXAMPLES_ENABLE_CXX` is ON). All SUNDIALS solvers can be used from C++ applications by default without setting any additional configuration options.

`CMAKE_CXX_FLAGS` - Flags for C++ compiler  
Default:

`CMAKE_CXX_FLAGS_DEBUG` - Flags used by the C++ compiler during debug builds  
Default: `-g`

**CMAKE\_CXX\_FLAGS\_MINSIZEREL** - Flags used by the C++ compiler during release minsize builds  
Default: -Os -DNDEBUG

**CMAKE\_CXX\_FLAGS\_RELEASE** - Flags used by the C++ compiler during release builds  
Default: -O3 -DNDEBUG

**CMAKE\_Fortran\_COMPILER** - Fortran compiler  
Default: /usr/bin/gfortran  
Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (**FCMIX\_ENABLE** is ON) or BLAS/LAPACK support is enabled (**BLAS\_ENABLE** or **LAPACK\_ENABLE** is ON).

**CMAKE\_Fortran\_FLAGS** - Flags for Fortran compiler  
Default:

**CMAKE\_Fortran\_FLAGS\_DEBUG** - Flags used by the Fortran compiler during debug builds  
Default: -g

**CMAKE\_Fortran\_FLAGS\_MINSIZEREL** - Flags used by the Fortran compiler during release minsize builds  
Default: -Os

**CMAKE\_Fortran\_FLAGS\_RELEASE** - Flags used by the Fortran compiler during release builds  
Default: -O3

**CMAKE\_INSTALL\_PREFIX** - Install path prefix, prepended onto install directories  
Default: /usr/local  
Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories **include** and **CMAKE\_INSTALL\_LIBDIR** of **CMAKE\_INSTALL\_PREFIX**, respectively.

**CMAKE\_INSTALL\_LIBDIR** - Library installation directory  
Default:  
Note: This is the directory within **CMAKE\_INSTALL\_PREFIX** that the SUNDIALS libraries will be installed under. The default is automatically set based on the operating system using the GNUInstallDirs CMake module.

**Fortran\_INSTALL\_MODDIR** - Fortran module installation directory  
Default: fortran

**CUDA\_ENABLE** - Build the SUNDIALS CUDA vector module.  
Default: OFF

**EXAMPLES\_ENABLE\_C** - Build the SUNDIALS C examples  
Default: ON

**EXAMPLES\_ENABLE\_CUDA** - Build the SUNDIALS CUDA examples  
Default: OFF  
Note: You need to enable CUDA support to build these examples.

**EXAMPLES\_ENABLE\_CXX** - Build the SUNDIALS C++ examples  
Default: OFF

**EXAMPLES\_ENABLE\_RAJA** - Build the SUNDIALS RAJA examples  
Default: OFF  
Note: You need to enable CUDA and RAJA support to build these examples.

**EXAMPLES\_ENABLE\_F77** - Build the SUNDIALS Fortran77 examples  
Default: ON (if **F77\_INTERFACE\_ENABLE** is ON)

**EXAMPLES\_ENABLE\_F90** - Build the SUNDIALS Fortran90/Fortran2003 examples  
Default: ON (if **F77\_INTERFACE\_ENABLE** or **F2003\_INTERFACE\_ENABLE** is ON)

**EXAMPLES\_INSTALL** - Install example files

Default: ON

Note: This option is triggered when any of the SUNDIALS example programs are enabled (**EXAMPLES\_ENABLE\_<language>** is ON). If the user requires installation of example programs then the sources and sample output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by **EXAMPLES\_INSTALL\_PATH**. A CMake configuration script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by **EXAMPLES\_INSTALL\_PATH**.

**EXAMPLES\_INSTALL\_PATH** - Output directory for installing example files

Default: /usr/local/examples

Note: The actual default value for this option will be an **examples** subdirectory created under **CMAKE\_INSTALL\_PREFIX**.

**F77\_INTERFACE\_ENABLE** - Enable Fortran-C support via the Fortran 77 interfaces

Default: OFF

**F2003\_INTERFACE\_ENABLE** - Enable Fortran-C support via the Fortran 2003 interfaces

Default: OFF

**HYPRE\_ENABLE** - Enable *hypre* support

Default: OFF

Note: See additional information on building with *hypre* enabled in [1.1.4](#).

**HYPRE\_INCLUDE\_DIR** - Path to *hypre* header files

**HYPRE\_LIBRARY\_DIR** - Path to *hypre* installed library files

**KLU\_ENABLE** - Enable KLU support

Default: OFF

Note: See additional information on building with KLU enabled in [1.1.4](#).

**KLU\_INCLUDE\_DIR** - Path to SuiteSparse header files

**KLU\_LIBRARY\_DIR** - Path to SuiteSparse installed library files

**LAPACK\_ENABLE** - Enable LAPACK support

Default: OFF

Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in [1.1.4](#).

**LAPACK\_LIBRARIES** - LAPACK (and BLAS) libraries

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

Note: CMake will search for libraries in your **LD\_LIBRARY\_PATH** prior to searching default system paths.

**MPI\_ENABLE** - Enable MPI support (build the parallel nvector).

Default: OFF

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

**MPI\_C\_COMPILER** - mpicc program

Default:

**MPI\_CXX\_COMPILER** - mpicxx program

Default:

Note: This option is triggered only if MPI is enabled (**MPI\_ENABLE** is ON) and C++ examples are enabled (**EXAMPLES\_ENABLE\_CXX** is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than **MPI\_ENABLE**.

**MPI\_Fortran\_COMPILER** - mpif77 or mpif90 program

Default:

Note: This option is triggered only if MPI is enabled (**MPI\_ENABLE** is ON) and Fortran-C support is enabled (**F77\_INTERFACE\_ENABLE** or **F2003\_INTERFACE\_ENABLE** is ON).

**MPIEXEC\_EXECUTABLE** - Specify the executable for running MPI programs

Default: **mpirun**

Note: This option is triggered only if MPI is enabled (**MPI\_ENABLE** is ON).

**OPENMP\_ENABLE** - Enable OpenMP support (build the OpenMP nvector).

Default: OFF

**OPENMP\_DEVICE\_ENABLE** - Enable OpenMP device offloading (build the OpenMPDEV nvector) if supported by the provided compiler.

Default: OFF

**SKIP\_OPENMP\_DEVICE\_CHECK** - **advanced option** - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.

Default: OFF

**PETSC\_ENABLE** - Enable PETSc support

Default: OFF

Note: See additional information on building with PETSc enabled in [1.1.4](#).

**PETSC\_INCLUDE\_DIR** - Path to PETSc header files

**PETSC\_LIBRARY\_DIR** - Path to PETSc installed library files

**PTHREAD\_ENABLE** - Enable Pthreads support (build the Pthreads nvector).

Default: OFF

**RAJA\_ENABLE** - Enable RAJA support (build the RAJA nvector).

Default: OFF

Note: You need to enable CUDA in order to build the RAJA vector module.

**SUNDIALS\_F77\_FUNC\_CASE** - **advanced option** - Specify the case to use in the Fortran name-mangling scheme, options are: **lower** or **upper**

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (**lower**) scheme if one can not be determined. If used, **SUNDIALS\_F77\_FUNC\_UNDERSCORES** must also be set.

**SUNDIALS\_F77\_FUNC\_UNDERSCORES** - **advanced option** - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: **none**, **one**, or **two**

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (**one**) scheme if one can not be determined. If used, **SUNDIALS\_F77\_FUNC\_CASE** must also be set.

**SUNDIALS\_INDEX\_TYPE** - **advanced option** - Integer type used for SUNDIALS indices. The size must match the size provided for the **SUNDIALS\_INDEX\_SIZE** option.

Default:

Note: In past SUNDIALS versions, a user could set this option to **INT64\_T** to use 64-bit integers, or **INT32\_T** to use 32-bit integers. Starting in SUNDIALS 3.2.0, these special values are deprecated. For SUNDIALS 3.2.0 and up, a user will only need to use the **SUNDIALS\_INDEX\_SIZE** option in most cases.

**SUNDIALS\_INDEX\_SIZE** - Integer size (in bits) used for indices in SUNDIALS, options are: 32 or 64

Default: 64

Note: The build system tries to find an integer type of appropriate size. Candidate 64-bit integer types are (in order of preference): **int64\_t**, **\_int64**, **long long**, and **long**. Candidate 32-bit integers are (in order of preference): **int32\_t**, **int**, and **long**. The advanced option, **SUNDIALS\_INDEX\_TYPE** can be used to provide a type not listed here.

**SUNDIALS\_PRECISION** - Precision used in SUNDIALS, options are: **double**, **single**, or **extended**

Default: **double**

**SUPERLUMT\_ENABLE** - Enable SuperLU\_MT support

Default: OFF

Note: See additional information on building with SuperLU\_MT enabled in [1.1.4](#).

**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

Default: Pthread

**USE\_GENERIC\_MATH** - Use generic (stdc) math libraries

Default: ON

### xSDK Configuration Options

SUNDIALS supports CMake configuration options defined by the Extreme-scale Scientific Software Development Kit (xSDK) community policies (see <https://xsdk.info> for more information). xSDK CMake options are unused by default but may be activated by setting **USE\_XSDK\_DEFAULTS** to ON.

When xSDK options are active, they will overwrite the corresponding SUNDIALS option and may have different default values (see details below). As such the equivalent SUNDIALS options should not be used when configuring with xSDK options. In the GUI front end to CMake (**ccmake**), setting **USE\_XSDK\_DEFAULTS** to ON will hide the corresponding SUNDIALS options as advanced CMake variables. During configuration, messages are output detailing which xSDK flags are active and the equivalent SUNDIALS options that are replaced. Below is a complete list xSDK options and the corresponding SUNDIALS options if applicable.



**TPL\_BLAS\_LIBRARIES** - BLAS library

Default: /usr/lib/libblas.so

SUNDIALS equivalent: **BLAS\_LIBRARIES**

Note: CMake will search for libraries in your **LD\_LIBRARY\_PATH** prior to searching default system paths.

**TPL\_ENABLE\_BLAS** - Enable BLAS support

Default: OFF

SUNDIALS equivalent: **BLAS\_ENABLE**

**TPL\_ENABLE\_HYPRE** - Enable *hypre* support

Default: OFF

SUNDIALS equivalent: **HYPRE\_ENABLE**

**TPL\_ENABLE\_KLU** - Enable KLU support  
 Default: OFF  
 SUNDIALS equivalent: **KLU\_ENABLE**

**TPL\_ENABLE\_PETSC** - Enable PETSc support  
 Default: OFF  
 SUNDIALS equivalent: **PETSC\_ENABLE**

**TPL\_ENABLE\_LAPACK** - Enable LAPACK support  
 Default: OFF  
 SUNDIALS equivalent: **LAPACK\_ENABLE**

**TPL\_ENABLE\_SUPERLUMT** - Enable SuperLU-MT support  
 Default: OFF  
 SUNDIALS equivalent: **SUPERLUMT\_ENABLE**

**TPL\_HYPRE\_INCLUDE\_DIRS** - Path to *hypre* header files  
 SUNDIALS equivalent: **HYPRE\_INCLUDE\_DIR**

**TPL\_HYPRE\_LIBRARIES** - *hypre* library  
 SUNDIALS equivalent: N/A

**TPL\_KLU\_INCLUDE\_DIRS** - Path to KLU header files  
 SUNDIALS equivalent: **KLU\_INCLUDE\_DIR**

**TPL\_KLU\_LIBRARIES** - KLU library  
 SUNDIALS equivalent: N/A

**TPL\_LAPACK\_LIBRARIES** - LAPACK (and BLAS) libraries  
 Default: /usr/lib/liblapack.so;/usr/lib/libblas.so  
 SUNDIALS equivalent: **LAPACK\_LIBRARIES**  
 Note: CMake will search for libraries in your **LD\_LIBRARY\_PATH** prior to searching default system paths.

**TPL\_PETSC\_INCLUDE\_DIRS** - Path to PETSc header files  
 SUNDIALS equivalent: **PETSC\_INCLUDE\_DIR**

**TPL\_PETSC\_LIBRARIES** - PETSc library  
 SUNDIALS equivalent: N/A

**TPL\_SUPERLUMT\_INCLUDE\_DIRS** - Path to SuperLU-MT header files  
 SUNDIALS equivalent: **SUPERLUMT\_INCLUDE\_DIR**

**TPL\_SUPERLUMT\_LIBRARIES** - SuperLU-MT library  
 SUNDIALS equivalent: N/A

**TPL\_SUPERLUMT\_THREAD\_TYPE** - SuperLU-MT library thread type  
 SUNDIALS equivalent: **SUPERLUMT\_THREAD\_TYPE**

**USE\_XSDK\_DEFAULTS** - Enable xSDK default configuration settings  
 Default: OFF  
 SUNDIALS equivalent: N/A  
 Note: Enabling xSDK defaults also sets **CMAKE\_BUILD\_TYPE** to Debug

**XSDK\_ENABLE\_FORTRAN** - Enable SUNDIALS Fortran interfaces  
 Default: OFF  
 SUNDIALS equivalent: **F77\_INTERFACE\_ENABLE/F2003\_INTERFACE\_ENABLE**

XSDK\_INDEX\_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64

Default: 32

SUNDIALS equivalent: SUNDIALS\_INDEX\_SIZE

XSDK\_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad

Default: double

SUNDIALS equivalent: SUNDIALS\_PRECISION

### 1.1.3 Configuration examples

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

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

```
% cmake \  
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \  
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \  
> -DMPI_ENABLE=ON \  
> -DFCMIX_ENABLE=ON \  
> /home/myname/sundials/solverdir  
%  
% make install  
%
```

To disable installation of the examples, use:

```
% cmake \  
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \  
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \  
> -DMPI_ENABLE=ON \  
> -DFCMIX_ENABLE=ON \  
> -DEXAMPLES_INSTALL=OFF \  
> /home/myname/sundials/solverdir  
%  
% make install  
%
```

### 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. When building SUNDIALS as a shared library external libraries any used with SUNDIALS must also be build as a shared library or as a static library compiled with the -fPIC flag.



#### Building with BLAS

SUNDIALS does not utilize BLAS directly but it may be needed by other external libraries that SUNDIALS can be built with (e.g. LAPACK, PETSc, SuperLU\_MT, etc.). To enable BLAS, set the BLAS\_ENABLE option to ON. If the directory containing the BLAS library is in the LD\_LIBRARY\_PATH environment variable, CMake will set the BLAS\_LIBRARIES variable accordingly, otherwise CMake will attempt to find the BLAS library in standard system locations. To explicitly tell CMake what libraries to use, the BLAS\_LIBRARIES variable can be set to the desired library. Example:

```
% cmake \  
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \  

```

```

> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/myblaspath/lib/libblas.so \
> -DSUPERLUMT_ENABLE=ON \
> -DSUPERLUMT_INCLUDE_DIR=/mysuperlumtpath/SRC
> -DSUPERLUMT_LIBRARY_DIR=/mysuperlumtpath/lib
> /home/myname/sundials/solverdir
%
% make install
%

```



When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options `SUNDIALS_F77_FUNC.CASE` and `SUNDIALS_F77_FUNC.UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

## Building with LAPACK

To enable LAPACK, set the `LAPACK_ENABLE` option to `ON`. If the directory containing the LAPACK library is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `LAPACK_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the `LAPACK_LIBRARIES` variable can be set to the desired libraries. When setting the LAPACK location explicitly the location of the corresponding BLAS library will also need to be set. Example:



```

% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/mylapackpath/lib/libblas.so \
> -DLAPACK_ENABLE=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/solverdir
%
% make install
%

```



When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options `SUNDIALS_F77_FUNC.CASE` and `SUNDIALS_F77_FUNC.UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

## Building with KLU

The KLU libraries are part of SuiteSparse, a suite of sparse matrix software, available from the Texas A&M University website: <http://faculty.cse.tamu.edu/davis/suitesparse.html>. SUNDIALS has been tested with SuiteSparse version 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`, `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](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>. 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.

## Building with CUDA

SUNDIALS CUDA modules and examples have been tested with version 8.0 of the CUDA toolkit. To build them, you need to install the Toolkit and compatible NVIDIA drivers. Both are available for download from the NVIDIA website: <https://developer.nvidia.com/cuda-downloads>. To enable CUDA, set `CUDA_ENABLE` to `ON`. If CUDA is installed in a nonstandard location, you may be prompted to set the variable `CUDA_TOOLKIT_ROOT_DIR` with your CUDA Toolkit installation path. To enable CUDA examples, set `EXAMPLES_ENABLE_CUDA` to `ON`.

## Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from <https://github.com/LLNL/RAJA>. SUNDIALS RAJA modules and examples have been tested with RAJA version 0.3. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set `CUDA_ENABLE` and `RAJA_ENABLE` to `ON`. If RAJA is installed in a nonstandard location you will be prompted to set the variable `RAJA_DIR` with the path to the RAJA CMake configuration file. To enable building the RAJA examples set `EXAMPLES_ENABLE_RAJA` to `ON`.

### 1.1.5 Testing the build and installation

If SUNDIALS was configured with `EXAMPLES_ENABLE_<language>` options to `ON`, then a set of regression tests can be run after building with the `make` command by running:

```
% make test
```

Additionally, if `EXAMPLES_INSTALL` was also set to `ON`, then a set of smoke tests can be run after installing with the `make install` command by running:

```
% make test_install
```

## 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 at least of the `EXAMPLES_ENABLE_<language>` options to `ON`, and set `EXAMPLES_INSTALL` to `ON`. Specify the installation path for the examples with the variable `EXAMPLES_INSTALL_PATH`. CMake will generate `CMakeLists.txt` configuration files (and `Makefile` files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

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



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

## 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 *solverdir*
2. Create a separate *builddir*
3. Open a Visual Studio Command Prompt and cd to *builddir*
4. Run `cmake-gui ../solverdir`
  - (a) Hit Configure
  - (b) Check/Uncheck solvers to be built
  - (c) Change `CMAKE_INSTALL_PREFIX` to *instdir*
  - (d) Set other options as desired
  - (e) Hit Generate
5. Back in the VS Command Window:
  - (a) Run `msbuild ALL_BUILD.vcxproj`
  - (b) Run `msbuild INSTALL.vcxproj`

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

## 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*/`CMAKE_INSTALL_LIBDIR` and *instdir*/`include`, respectively. The location can be changed by setting the CMake variable `CMAKE_INSTALL_PREFIX`. Although all installed libraries reside under *libdir*/`CMAKE_INSTALL_LIBDIR`, the public header files are further organized into subdirectories under *includedir*/`include`.

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

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the *includedir*/`include/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, and would be useful, for example, if the functions declared in `sundials_dense.h` 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_fconfig.h sundials/sundials_types.h sundials/sundials_math.h sundials/sundials_nvector.h sundials/sundials_fnvector.h sundials/sundials_matrix.h sundials/sundials_linearsolver.h sundials/sundials_iterative.h sundials/sundials_direct.h sundials/sundials_dense.h sundials/sundials_band.h sundials/sundials_nonlinearsolver.h sundials/sundials_version.h sundials/sundials_mpi_types.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial. <i>lib</i> libsundials_fnvecserial_mod. <i>lib</i> libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module files	fnvector_serial_mod.mod
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel. <i>lib</i> libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp. <i>lib</i> libsundials_fnvecopenmp_mod. <i>lib</i> libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h
	Module files	fnvector_openmp_mod.mod
NVECTOR_OPENMPDEV	Libraries	libsundials_nvecopenmpdev. <i>lib</i>
	Header files	nvector/nvector_openmpdev.h
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads. <i>lib</i> libsundials_fnvecpthreads_mod. <i>lib</i> libsundials_fnvecpthreads.a
	Header files	nvector/nvector_pthreads.h
	Module files	fnvector_pthreads_mod.mod
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp. <i>lib</i>
	Header files	nvector/nvector_parhyp.h
continued on next page		

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NVECTOR_PETSC	Libraries	libsundials_nvecpetsc. <i>lib</i>
	Header files	nvector/nvector_petsc.h
NVECTOR_CUDA	Libraries	libsundials_nveccuda. <i>lib</i>
	Libraries	libsundials_nvecmpicuda. <i>lib</i>
	Header files	nvector/nvector_cuda.h
		nvector/nvector_mpicuda.h nvector/cuda/ThreadPartitioning.hpp nvector/cuda/Vector.hpp nvector/cuda/VectorKernels.cuh
NVECTOR_RAJA	Libraries	libsundials_nveccudaraja. <i>lib</i>
	Libraries	libsundials_nveccudampiraja. <i>lib</i>
	Header files	nvector/nvector_raja.h nvector/nvector_mpiraja.h nvector/raja/Vector.hpp
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband. <i>lib</i>
		libsundials_fsunmatrixband_mod. <i>lib</i> libsundials_fsunmatrixband.a
	Header files	sunmatrix/sunmatrix_band.h
	Module files	fsunmatrix_band_mod.mod
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense. <i>lib</i>
		libsundials_fsunmatrixdense_mod. <i>lib</i> libsundials_fsunmatrixdense.a
	Header files	sunmatrix/sunmatrix_dense.h
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse. <i>lib</i>
		libsundials_fsunmatrixsparse_mod. <i>lib</i> libsundials_fsunmatrixsparse.a
	Header files	sunmatrix/sunmatrix_sparse.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband. <i>lib</i>
		libsundials_fsunlinsolband_mod. <i>lib</i> libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense. <i>lib</i>
		libsundials_fsunlinsoldense_mod. <i>lib</i> libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
<i>continued on next page</i>		

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	Module files	fsunlinsol_dense_mod.mod
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu. <i>lib</i> libsundials_fsunlinsolklu_mod. <i>lib</i> libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module files	fsunlinsol_klu_mod.mod
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband. <i>lib</i> libsundials_fsunlinsollapackband.a
	Header files	sunlinsol/sunlinsol_lapackband.h
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense. <i>lib</i> libsundials_fsunlinsollapackdense.a
	Header files	sunlinsol/sunlinsol_lapackdense.h
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg. <i>lib</i> libsundials_fsunlinsolpcg_mod. <i>lib</i> libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module files	fsunlinsol_pcg_mod.mod
SUNLINSOL_SPCGGS	Libraries	libsundials_sunlinsolspbcgs. <i>lib</i> libsundials_fsunlinsolspbcgs_mod. <i>lib</i> libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module files	fsunlinsol_spbcgs_mod.mod
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr. <i>lib</i> libsundials_fsunlinsolspfgmr_mod. <i>lib</i> libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module files	fsunlinsol_spfgmr_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr. <i>lib</i> libsundials_fsunlinsolspgmr_mod. <i>lib</i> libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr. <i>lib</i> libsundials_fsunlinsolsptfqmr_mod. <i>lib</i> libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
<i>continued on next page</i>		

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	Module files	fsunlinsol_sptfqmr_mod.mod	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt. <i>lib</i> libsundials_fsunlinsolsuperlumt.a	
	Header files	sunlinsol/sunlinsol_superlumt.h	
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnewton. <i>lib</i> libsundials_fsunnonlinsolnewton_mod. <i>lib</i> libsundials_fsunnonlinsolnewton.a	
	Header files	sunnonlinsol/sunnonlinsol_newton.h	
	Module files	fsunnonlinsol_newton_mod.mod	
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint. <i>lib</i> libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod. <i>lib</i>	
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h	
	Module files	fsunnonlinsol_fixedpoint_mod.mod	
CVODE	Libraries	libsundials_cvode. <i>lib</i>	libsundials_fcvcde.a
	Header files	cvcde/cvcde.h	cvcde/cvcde_impl.h
		cvcde/cvcde_direct.h	cvcde/cvcde_ls.h
		cvcde/cvcde_spils.h	cvcde/cvcde_bandpre.h
	Module files	fcvcde_mod.mod	
CVODES	Libraries	libsundials_cvodes. <i>lib</i>	
	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h
		cvodes/cvodes_direct.h	cvodes/cvodes_ls.h
		cvodes/cvodes_spils.h	cvodes/cvodes_bandpre.h
		cvodes/cvodes_bbdpre.h	
ARKODE	Libraries	libsundials_arkode. <i>lib</i>	libsundials_farkode.a
	Header files	arkode/arkode.h	arkode/arkode_impl.h
		arkode/arkode_ls.h	arkode/arkode_bandpre.h
		arkode/arkode_bbdpre.h	
IDA	Libraries	libsundials_ida. <i>lib</i>	libsundials_fida.a
	Header files	ida/ida.h	ida/ida_impl.h
		ida/ida_direct.h	ida/ida_ls.h
		ida/ida_spils.h	ida/ida_bbdpre.h
IDAS	Libraries	libsundials_idas. <i>lib</i>	
	Header files	idas/idas.h	idas/idas_impl.h
		idas/idas_direct.h	idas/idas_ls.h
		idas/idas_spils.h	idas/idas_bbdpre.h
KINSOL	Libraries	libsundials_kinsol. <i>lib</i>	libsundials_fkinsol.a
<i>continued on next page</i>			

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	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_spils.h	kinsol/kinsol_impl.h kinsol/kinsol_ls.h kinsol/kinsol_bbdpre.h