# Installation Guide for SUNDIALS v3.0.0

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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 <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 of 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 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. 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.

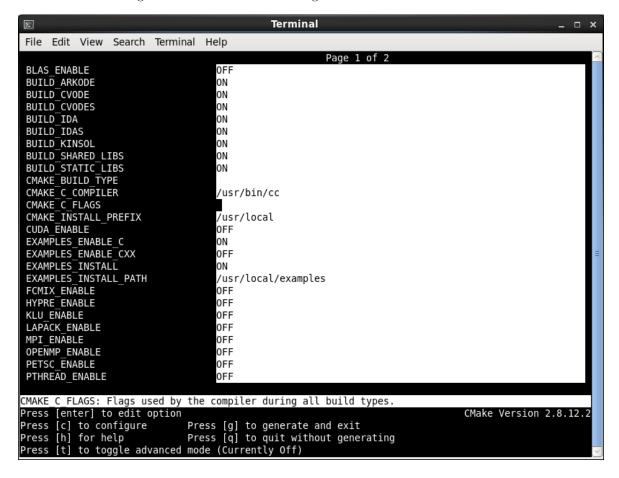


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

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 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

```
Terminal
                                                                                                                 _ 🗆 🗙
 File Edit View Search Terminal Help
 BLAS ENABLE
                                         0FF
 BUILD ARKODE
                                         ON
 BUILD CVODE
                                         ON
 BUILD_CVODES
                                         ON
 BUILD_IDA
BUILD IDAS
                                         ON
 BUILD KINSOL
 BUILD SHARED LIBS
                                         ON
 BUILD STATIC LIBS
 CMAKE BUILD TYPE
 CMAKE C COMPILER
                                         /usr/bin/cc
 CMAKE_C_FLAGS
CMAKE_INSTALL_PREFIX
                                         /usr/casc/sundials/instdir
 CUDA ENABLE
 EXAMPLES ENABLE C
EXAMPLES_ENABLE_CXX
EXAMPLES_INSTALL
EXAMPLES_INSTALL_PATH
                                         0FF
                                         /usr/casc/sundials/instdir/examples
 FCMIX ENABLE
 HYPRE_ENABLE
                                         0FF
 KLU ENABLE
                                         0FF
 LAPACK ENABLE
                                         0FF
 MPI ENABLE
                                         0FF
 OPENMP ENABLE
                                         0FF
 PETSC ENABLE
                                         0FF
 PTHREAD ENABLE
                                         0FF
CMAKE C FLAGS: Flags used by the compiler during all build types.

Press [c] to configure Press [g] to generate and exit
                                                                                              CMake Version 2.8.12.2
Press [h] for help
                                   Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

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.

```
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.

 ${\tt CMAKE\_C\_COMPILER\ -\ C\ compiler}$ 

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

 $\label{eq:cmake_cxx_flags_minsize} \textbf{CMAKE\_CXX\_FLAGS\_MINSIZEREL} \ - \ Flags \ used \ by \ the \ C^{++} \ compiler \ during \ release \ minsize \ builds \\ Default: \ -Os \ -DNDEBUG$ 

 $\label{eq:cmake_cxx_flags_release} \textbf{CMAKE\_CXX\_FLAGS\_RELEASE} \ - \ Flags \ used \ by \ the \ C^{++} \ compiler \ during \ release \ builds \\ Default: \ -O3 \ -DNDEBUG$ 

#### 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).

## ${\tt CMAKE\_Fortran\_FLAGS} \ - \ {\tt Flags} \ \ {\tt for} \ \ {\tt Fortran} \ \ {\tt compiler}$

Default:

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

 $\begin{array}{l} {\tt CMAKE\_Fortran\_FLAGS\_MINSIZEREL\ - Flags\ used\ by\ the\ Fortran\ compiler\ during\ release\ minsize\ builds\ Default:\ -Os \end{array}$ 

## 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 lib of CMAKE\_INSTALL\_PREFIX, respectively.

#### 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 FCMIX\_ENABLE is ON)

#### EXAMPLES\_ENABLE\_F90 - Build the SUNDIALS Fortran90 examples

Default: OFF

## ${\tt EXAMPLES\_INSTALL~Install~example~files}$

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.

## FCMIX\_ENABLE - Enable Fortran-C support

Default: OFF

## ${\tt HYPRE\_ENABLE}$ - ${\tt Enable}$ ${\tt hypre}$ 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.

## ${\tt MPI\_MPICC - mpicc \ program}$

Default:

## MPI\_MPICXX - 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\_MPIF77 - mpif77 program

Default:

Note: This option is triggered only if MPI is enabled (MPI\_ENABLE is ON) and Fortran-C support is enabled (FCMIX\_ENABLE is ON).

MPI\_MPIF90 - mpif90 program

Default:

Note: This option is triggered only if MPI is enabled (MPI\_ENABLE is ON), Fortran-C support is enabled (FCMIX\_ENABLE is ON), and Fortran90 examples are enabled (EXAMPLES\_ENABLE\_F90 is ON).

MPI\_RUN\_COMMAND - Specify run command for MPI

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

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\_INDEX\_TYPE - Integer type used for SUNDIALS indices, options are: int32\_t or int64\_t

Default: int64\_t

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

 ${\tt TPL\_ENABLE\_HYPRE - Enable} \ hypre \ {\tt support}$ 

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

 $\mathtt{TPL\_HYPRE\_INCLUDE\_DIRS}$  - Path to hypre header files

SUNDIALS equivalent: HYPRE\_INCLUDE\_DIR

 ${\tt TPL\_HYPRE\_LIBRARIES} \ - \ hypre \ {\tt library}$ 

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 interface
Default: OFF
SUNDIALS equivalent: FCMIX_ENABLE

XSDK_INDEX_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 32
SUNDIALS equivalent: SUNDIALS_INDEX_TYPE

XSDK_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad
Default: double
SUNDIALS equivalent: SUNDIALS_PRECISION
```

## 1.1.3 Configuration examples

% cmake \

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

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

```
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
   > -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
   > -DMPI_ENABLE=ON \
   > -DFCMIX_ENABLE=ON \
   > /home/myname/sundials/srcdir
  % make install
To disable installation of the examples, use:
   % cmake \
   > -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
   > -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
  > -DMPI_ENABLE=ON \
   > -DFCMIX_ENABLE=ON \
   > -DEXAMPLES_INSTALL=OFF \
   > /home/myname/sundials/srcdir
  % 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 build 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/srcdir
%
make install
%
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.

#### **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/srcdir
%
% make install
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.

## 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. 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 are 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 NVIDIA website: https://developer.nvidia.com/cuda-downloads. To enable CUDA, set CUDA\_ENABLE to ON. If you installed CUDA 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

To build SUNDIALS RAJA modules you need to enable SUNDIALS CUDA support, first. You also need a CUDA-enabled RAJA installation on your system. RAJA is free software, developed by Lawrence Livermore National Laboratory, and can be obtained from https://github.com/LLNL/RAJA. Next you need to set RAJA\_ENABLE to ON, to enable building the RAJA vector module, and EXAMPLES\_ENABLE\_RAJA to ON to build the RAJA examples. If you installed RAJA to a nonstandard location you will be prompted to set the variable RAJA\_DIR with the path to the RAJA CMake configuration file. SUNDIALS was tested with RAJA version 0.3.

## 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 *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 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 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 (<code>e.g.</code>, <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

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_iterative.h sundials/sundials_direct.h		
		sundials/sundials_dense.h sundials/sundials_band.h		
		sundials/sundials_matrix.h sundials/sundials_version.h		
		sundials/sundials_linearsolver.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		
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		
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp.lib		
	Header files	nvector/nvector_parhyp.h		
NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.lib		
	Header files	nvector/nvector_petsc.h		
NVECTOR_CUDA	Libraries	libsundials_nveccuda.lib		
	Header files	nvector/nvector_cuda.h		
		nvector/cuda/ThreadPartitioning.hpp		
		nvector/cuda/Vector.hpp		
		nvector/cuda/VectorKernels.cuh		
NVECTOR_RAJA	Libraries	libsundials_nvecraja.lib		
	Header files	nvector/nvector_raja.h		
		nvector/raja/Vector.hpp		
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.lib libsundials_fsunmatrixband.a		
	Header files	sunmatrix/sunmatrix_band.h		
SUNMATRIX_DENSE	Libraries	$lib sundials\_sunmatrix dense. \\ lib$		
		libsundials_fsunmatrixdense.a		
	Header files	sunmatrix/sunmatrix_dense.h		
SUNMATRIX_SPARSE	Libraries	$libsundials\_sunmatrixsparse.lib$		
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		libsundials_fsunmatrixsparse.a		
	Header files	sunmatrix_sparse.h		
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.lib		
		libsundials_fsunlinsolband.a		
	Header files	sunlinsol/sunlinsol_band.h		
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.lib		
		libsundials_fsunlinsoldense.a		
	Header files	sunlinsol/sunlinsol_dense.h		
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.lib		
		libsundials_fsunlinsolklu.a		
	Header files	sunlinsol/sunlinsol_klu.h		
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.lib		
		libsundials_fsunlinsollapackband.a		
	Header files	sunlinsol/sunlinsol_lapackband.h		
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackde		
		libsundials_fsunlinsollapackdense.a		
	Header files	sunlinsol/sunlinsol_lapackdense.h		
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.lib		
		libsundials_fsunlinsolpcg.a		
	Header files	sunlinsol/sunlinsol_pcg.h		
$SUNLINSOL\_SPBCGS$	Libraries	$libsundials\_sunlinsolspbcgs. \it lib$		
		libsundials_fsunlinsolspbcgs.a		
	Header files	sunlinsol/sunlinsol_spbcgs.h		
SUNLINSOL_SPFGMR	Libraries	$lib sundials\_sunlins olspfgmr. \it lib$		
		libsundials_fsunlinsolspfgmr.a		
	Header files	sunlinsol/sunlinsol_spfgmr.h		
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.lib		
		libsundials_fsunlinsolspgmr.a	ı	
	Header files	sunlinsol/sunlinsol_spgmr.h		
$SUNLINSOL\_SPTFQMR$	Libraries	libsundials_sunlinsolsptfqmr.lib		
		libsundials_fsunlinsolsptfqmr.a		
	Header files	sunlinsol/sunlinsol_sptfqmr.h		
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlur		
		libsundials_fsunlinsolsuperlumt.a		
Header fi		, 1		
CVODE	Libraries	libsundials_cvode.lib	libsundials_fcvode.a	
	Header files	cvode/cvode.h	cvode/cvode_impl.h	
		cvode/cvode_direct.h	cvode/cvode_spils.h	
		cvode/cvode_bandpre.h	cvode/cvode_bbdpre.h	
CVODES	Libraries	libsundials_cvodes.lib		
	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h	
			continued on next page	

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		cvodes/cvodes_direct.h	cvodes/cvodes_spils.h	
		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	$arkode/arkode\_spils.h$	
		arkode/arkode_bandpre.h	$arkode/arkode\_bbdpre.h$	
IDA	Libraries	libsundials_ida.lib	libsundials_fida.a	
	Header files	ida/ida.h	ida/ida_impl.h	
		ida/ida_direct.h	$ida/ida\_spils.h$	
		ida/ida_bbdpre.h		
IDAS	Libraries	libsundials_idas.lib		
	Header files	idas/idas.h	idas/idas_impl.h	
		idas/idas_direct.h	$idas/idas\_spils.h$	
		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_spils.h	
		kinsol/kinsol_bbdpre.h		