Installation Guide for SUNDIALS v4.1.0

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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 SUNDI-ALS sources.

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

instdir is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory instdir/include while libraries are installed under instdir/CMAKE_INSTALL_LIBDIR, with instdir and CMAKE_INSTALL_LIBDIR specified at configuration time.

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



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

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

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.

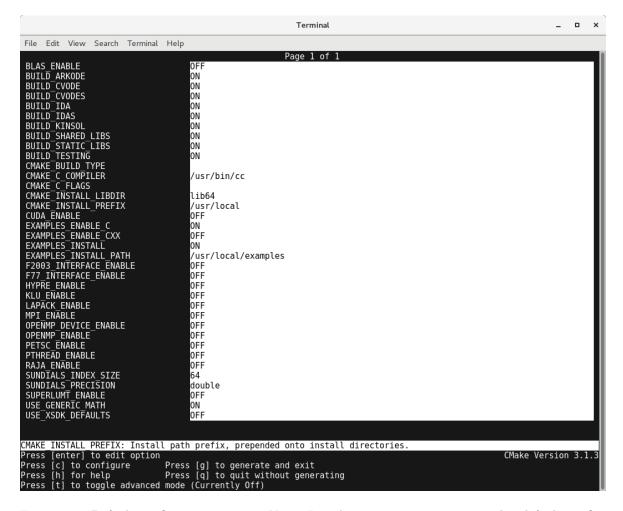


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *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:

```
Terminal
File Edit View Search Terminal Help
 BLAS ENABLE
BLAS ENABLE
BUILD_ARKODE
BUILD_CVODE
BUILD_CVODES
BUILD_IDA
BUILD_IDAS
BUILD_KINSOL
BUILD_SHARED_LIBS
BUILD_STATIC_LIBS
BUILD_TESTING
                                                                              ON
ON
ON
ON
ON
ON
 BUTLD TESTING
  CMAKE_BUILD_TYPE
 CMAKE_C_COMPILER
CMAKE_C_FLAGS
CMAKE_INSTALL_LIBDIR
                                                                              /usr/bin/cc
                                                                              lib64
CMAKE INSTALL LIBDIR
CMAKE INSTALL PREFIX
CUDA ENABLE
EXAMPLES ENABLE C
EXAMPLES ENABLE CXX
EXAMPLES INSTALL
EXAMPLES INSTALL
FATH
F2003 INTERFACE ENABLE
F77 INTERFACE ENABLE
HYPRE ENABLE
LAPACK FNABLE
                                                                              /usr/casc/sundials/instdir
OFF
                                                                              ON
                                                                              0FF
                                                                              /usr/casc/sundials/instdir/examples
OFF
                                                                              0FF
  LAPĀCK_ENABLE
LAPĀCK ENABLE
MPI ENĀBLE
OPENMP DEVICE ENABLE
OPENMP ENABLE
PETSC ĒNABLE
PTHREĀD ENABLE
RAJA ENĀBLE
SUNDĪALS INDEX SIZE
SUNDĪALS INDEX SIZE
SUNDĪALS PRECIŠION
SUPERLUMT ENABLE
USE GENERĪC MATH
ISF XSDR DFFAIITS
                                                                              OFF
OFF
                                                                              double
                                                                              0FF
                                                                              ON
  USE XSDK DEFAULTS
                                                                              0FF
CMAKE_INSTALL_PREFIX: Install path prefix, prepended onto install directories.
             [enter] to edit option
[c] to configure
                                                                                                                                                                                                                               CMake Version 3.1.3
                                                                  Press [g] to generate and exit
Press [q] to quit without generating
                      for help
```

Figure 1.2: Changing the instdir for SUNDIALS and corresponding examples

% make

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

% make install

Building from the command line

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

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

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

${\tt CMAKE_C_FLAGS}$ - Flags for C compiler

Default:

${\tt CMAKE_C_FLAGS_DEBUG}$ - Flags used by the C compiler during debug builds

Default: -g

CMAKE_C_FLAGS_MINSIZEREL - Flags used by the C compiler during release minsize builds

Default: -Os -DNDEBUG

CMAKE_C_FLAGS_RELEASE - Flags used by the C compiler during release builds

Default: -O3 -DNDEBUG

${\tt CMAKE_CXX_COMPILER}$ - C^{++} compiler

Default: /usr/bin/c++

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

CMAKE_CXX_FLAGS - Flags for C++ compiler

Default:

CMAKE_CXX_FLAGS_DEBUG - Flags used by the C++ compiler during debug builds

Default: -g

CMAKE_CXX_FLAGS_MINSIZEREL - Flags used by the C++ compiler during release minsize builds

Default: -Os -DNDEBUG

CMAKE_CXX_FLAGS_RELEASE - Flags used by the C++ compiler during release builds

Default: -O3 -DNDEBUG

CMAKE_Fortran_COMPILER - Fortran compiler

Default: /usr/bin/gfortran

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

CMAKE_Fortran_FLAGS - Flags for Fortran compiler

Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the Fortran compiler during debug builds

Default: -g

CMAKE_Fortran_FLAGS_MINSIZEREL - Flags used by the Fortran compiler during release minsize builds

Default: -Os

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the Fortran compiler during release builds

Default: -O3

CMAKE_INSTALL_PREFIX - Install path prefix, prepended onto install directories

Default: /usr/local

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

 ${\bf GNUInstall Dirs\ CMake\ module.}$

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

 $\label{eq:Default:off} Default: \ OFF \ unless \ \mbox{\tt Trilinos_ENABLE} \ is \ ON.$

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples

Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90/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/libblapack.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

Trilinos_ENABLE - Enable Trilinos support (build the Tpetra NVECTOR).

Default: OFF

Trilinos_DIR - Path to the Trilinos install directory.

Default:

TRILINOS_INTERFACE_C_COMPILER - advanced option - Set the C compiler for building the Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_COMPILER or MPI_C_COMPILER if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_C_COMPILER_FLAGS - advanced option - Set the C compiler flags for Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_FLAGS if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same flags that were used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER - advanced option - Set the C++ compiler for builing Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C++ compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_CXX_COMPILER or MPI_CXX_COMPILER if USE_XSDK_DEFAULTS=ON.

Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER_FLAGS - advanced option - Set the C++ compiler flags for Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).

Default: The C^{++} compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=0FF. CMAKE_CXX_FLAGS if USE_XSDK_DEFAULTS=0N.

Note: Is is recommended to use the same flags that were used to build the Trilinos library.

USE_GENERIC_MATH - Use generic (stdc) math libraries

Default: ON

xSDK Configuration Options

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

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

TPL_BLAS_LIBRARIES - BLAS library

Default: /usr/lib/libblas.so

SUNDIALS equivalent: BLAS_LIBRARIES

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

paths.

TPL_ENABLE_BLAS - Enable BLAS support

Default: OFF

SUNDIALS equivalent: BLAS_ENABLE

 ${\tt TPL_ENABLE_HYPRE - Enable} \ hypre \ {\tt support}$

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

 ${\tt TPL_ENABLE_SUPERLUMT - Enable \ SuperLU_MT \ support}$

Default: OFF

SUNDIALS equivalent: SUPERLUMT_ENABLE

TPL_HYPRE_INCLUDE_DIRS - Path to hypre header files

SUNDIALS equivalent: HYPRE_INCLUDE_DIR

 ${\tt TPL_HYPRE_LIBRARIES} \ - \ hypre \ {\tt library}$

SUNDIALS equivalent: N/A

 ${\tt TPL_KLU_INCLUDE_DIRS}$ - Path to KLU header files

SUNDIALS equivalent: KLU_INCLUDE_DIR

TPL_KLU_LIBRARIES - KLU library

SUNDIALS equivalent: N/A

```
TPL_LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
     Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
     SUNDIALS equivalent: LAPACK_LIBRARIES
     Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system
     paths.
TPL_PETSC_INCLUDE_DIRS - Path to PETSc header files
     SUNDIALS equivalent: PETSC_INCLUDE_DIR
TPL_PETSC_LIBRARIES - PETSc library
     SUNDIALS equivalent: N/A
TPL_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
```

1.1.3 Configuration examples

SUNDIALS equivalent: SUNDIALS_PRECISION

Default: double

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

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

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

To disable installation of the examples, use:

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

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_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/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_CUDA to ON.

Building with Trilinos

Trilinos is a suite of numerical libraries developed by Sandia National Laboratories. It can be obtained at https://github.com/trilinos/Trilinos. SUNDIALS Trilinos modules and examples have been tested with Trilinos version 12.14. To enable Trilinos, set Trilinos_ENABLE to ON. If Trilinos is installed in a nonstandard location you will be prompted to set the variable Trilinos_DIR with the path to the Trilinos CMake configuration file. It is desireable to build the Trilinos vector interface with same compiler and options that were used to build Trilinos. CMake will try to find the correct compiler settings automatically from the Trilinos configuration file. If that is not successful, the compilers and options can be manually set with the following CMake variables:

- Trilinos_INTERFACE_C_COMPILER
- Trilinos_INTERFACE_C_COMPILER_FLAGS
- Trilinos_INTERFACE_CXX_COMPILER
- Trilinos_INTERFACE_CXX_COMPILER_FLAGS

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 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	<u>: 1.1 (</u>	SUNDL	ALS	libraries	and	header	files	
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	.,, 20101011111111111	Header files	nvector/nvector_parhyp.h		
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NVECTOR_PETSC	Libraries	$libsundials_nvecpetsc.lib$		
	Header files	nvector/nvector_petsc.h		
NVECTOR_CUDA	Libraries	libsundials_nveccuda. lib		
	Libraries	libsundials_nvecmpicuda.lib		
	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.lib		
	Libraries	libsundials_nveccudampiraja.lib		
	Header files	nvector/nvector_raja.h		
		nvector/nvector_mpiraja.h		
		nvector/raja/Vector.hpp		
NVECTOR_TRILINOS	Libraries	libsundials_nvectrilinos.lib		
WECTORETHEINOS	Header files	nvector/nvector_trilinos.h		
	Treader mes	nvector/trilinos/SundialsTpetraVectorInterface.hpp		
		nvector/trilinos/SundialsTpetraVectorKernels.hpp		
CHNMATDIY DAND	Libraries	libsundials_sunmatrixband.lib		
SUNMATRIX_BAND	Libraries	libsundials_fsunmatrixband_mod.lib		
	Header files	libsundials_fsunmatrixband.a		
		sunmatrix/sunmatrix_band.h		
	Module	fsunmatrix_band_mod.mod		
	files			
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.lib		
		$libsundials_fsunmatrix dense_mod. \it lib$		
		libsundials_fsunmatrixdense.a		
	Header files	sunmatrix/sunmatrix_dense.h		
	Module	fsunmatrix_dense_mod.mod		
	files			
SUNMATRIX_SPARSE	Libraries	$libsundials_sunmatrixsparse.lib$		
		libsundials_fsunmatrixsparse_mod.lib		
		libsundials_fsunmatrixsparse.a		
	Header files	sunmatrix/sunmatrix_sparse.h		
	Module	fsunmatrix_sparse_mod.mod		
	files	•		
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.lib		
		$libsundials_fsunlinsolband_mod.lib$		
		libsundials_fsunlinsolband.a		
	Header files	sunlinsol/sunlinsol_band.h		
	Module	fsunlinsol_band_mod.mod		
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	files			

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SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.lib
		$libsundials_fsunlinsoldense_mod. \it lib$
		libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	Module	fsunlinsol_dense_mod.mod
	files	
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.lib
		libsundials_fsunlinsolklu_mod. lib
		libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module	fsunlinsol_klu_mod.mod
	files	
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.lib
		libsundials_fsunlinsollapackband.a
	Header files	sunlinsol/sunlinsol_lapackband.h
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.lib
		libsundials_fsunlinsollapackdense.a
	Header files	sunlinsol/sunlinsol_lapackdense.h
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.lib
		libsundials_fsunlinsolpcg_mod.lib
		libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module	fsunlinsol_pcg_mod.mod
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SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.lib
		libsundials_fsunlinsolspbcgs_mod.lib
		libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module	fsunlinsol_spbcgs_mod.mod
	files	The state of the s
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.lib
		libsundials_fsunlinsolspfgmr_mod.lib
		libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module	fsunlinsol_spfgmr_mod.mod
	files	T O
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.lib
		libsundials_fsunlinsolspgmr_mod.lib
		libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module	fsunlinsol_spgmr_mod.mod
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SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqm	r.lib	
		libsundials_fsunlinsolsptfqmr_mod.lib		
		libsundials_fsunlinsolsptfqn	ar.a	
	Header files	sunlinsol/sunlinsol_sptfqmr.h		
	Module	fsunlinsol_sptfqmr_mod.mod		
	files			
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlu	$\mathrm{imt}.lib$	
		libsundials_fsunlinsolsuperlumt.a		
	Header files	sunlinsol/sunlinsol_superlu	mt.h	
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnev	vton.lib	
		libsundials_fsunnonlinsolne	$\operatorname{wton_mod}.lib$	
		libsundials_fsunnonlinsolne	wton.a	
	Header files	sunnonlinsol/sunnonlinsol_	newton.h	
	Module	fsunnonlinsol_newton_mod.	mod	
	files			
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixe	edpoint. lib	
		libsundials_fsunnonlinsolfix		
		libsundials_fsunnonlinsolfix	$edpoint_mod.lib$	
	Header files	sunnonlinsol/sunnonlinsol_	fixedpoint.h	
	Module	fsunnonlinsol_fixedpoint_me	od.mod	
	files	-		
CVODE	Libraries	libsundials_cvode.lib	libsundials_fcvode.a	
	Header files	cvode/cvode.h	cvode/cvode_impl.h	
		cvode/cvode_direct.h	cvode/cvode_ls.h	
		cvode/cvode_spils.h	cvode/cvode_bandpre.h	
		cvode/cvode_bbdpre.h		
	Module	fcvode_mod.mod		
	files			
CVODES	Libraries	libsundials_cvodes.lib		
	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	$libsundials_arkode.lib$	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.lib	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. lib		
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	Header files idas		$idas/idas_impl.h$		
	ida		$idas/idas_ls.h$		
	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_ls.h		
		kinsol/kinsol_spils.h	$kinsol/kinsol_bbdpre.h$		