

# Installation Guide for SUNDIALS v3.1.0

Eddy Banks, Aaron M. Collier, David J. Gardner, Alan C. Hindmarsh,  
Radu Serban, and Carol S. Woodward  
*Center for Applied Scientific Computing  
Lawrence Livermore National Laboratory*

November 7, 2017



UCRL-SM-208116

## **DISCLAIMER**

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

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

# Contents

<b>1</b>	<b>SUNDIALS Package Installation Procedure</b>	<b>1</b>
1.1	CMake-based installation	2
1.1.1	Configuring, building, and installing on Unix-like systems	2
1.1.2	Configuration options (Unix/Linux)	4
1.1.3	Configuration examples	10
1.1.4	Working with external Libraries	10
1.1.5	Testing the build and installation	12
1.2	Building and Running Examples	13
1.3	Configuring, building, and installing on Windows	13
1.4	Installed libraries and exported header files	14



# 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:

*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.

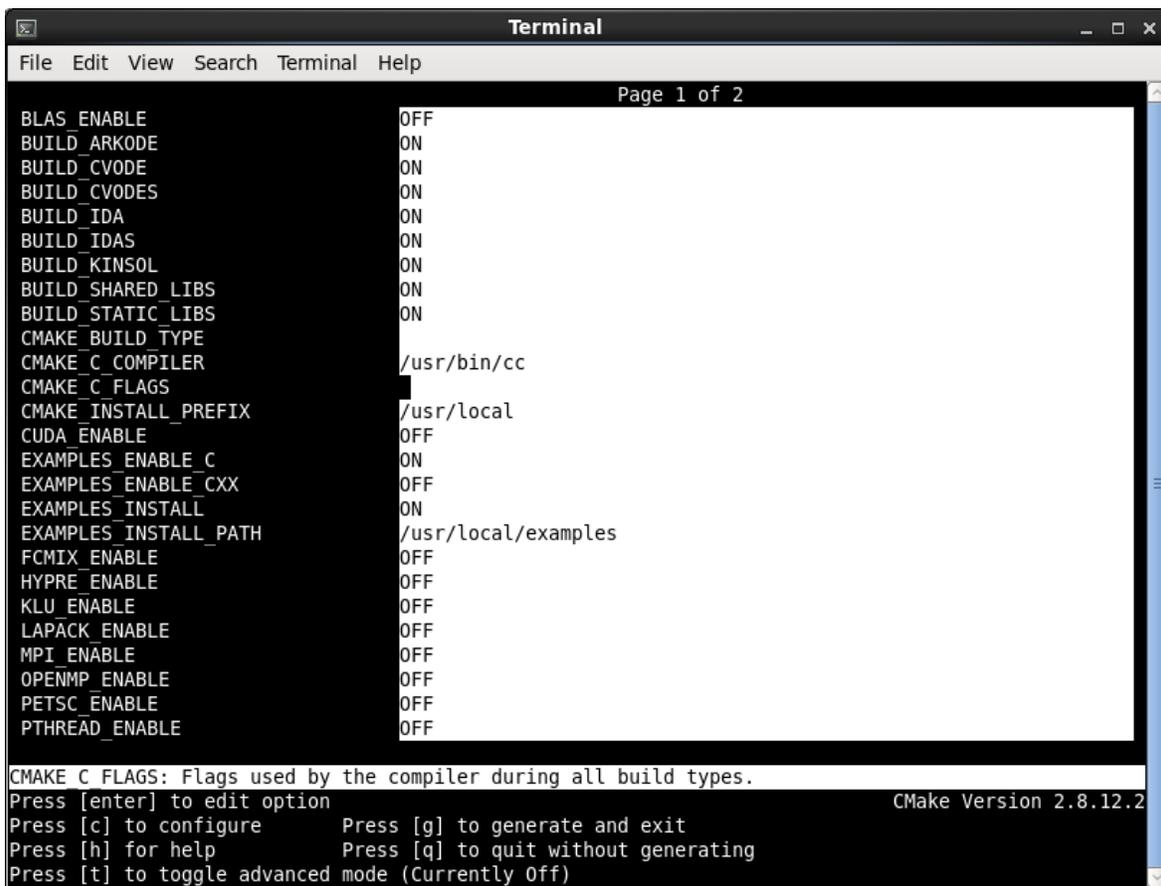


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

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
```

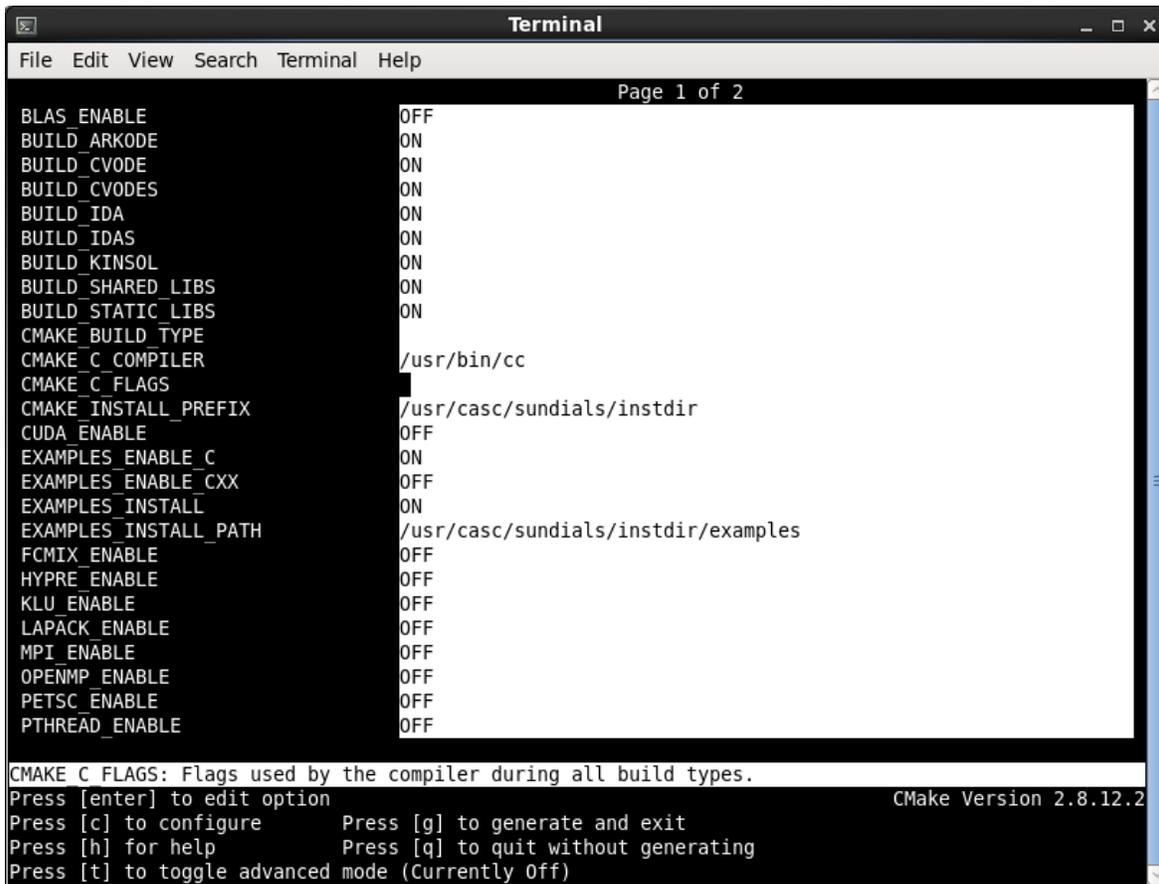


Figure 1.2: Changing the *instdir* for SUNDIALS and corresponding examples

## 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.

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 **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

**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`

`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_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

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 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

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/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`, `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 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.

## 1.1.5 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 *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 *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_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	

*continued on next page*

<i>continued from last page</i>		
NVECTOR_RAJA	Libraries	libsundials_nvecraja. <i>lib</i>
	Header files	nvector/nvector_raj.h nvector/raja/Vector.hpp
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband. <i>lib</i> libsundials_fsunmatrixband.a
	Header files	sunmatrix/sunmatrix_band.h
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense. <i>lib</i> libsundials_fsunmatrixdense.a
	Header files	sunmatrix/sunmatrix_dense.h
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse. <i>lib</i> libsundials_fsunmatrixsparse.a
	Header files	sunmatrix/sunmatrix_sparse.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband. <i>lib</i> libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense. <i>lib</i> libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu. <i>lib</i> libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
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.a
	Header files	sunlinsol/sunlinsol_pcg.h
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs. <i>lib</i> libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr. <i>lib</i> libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr. <i>lib</i> libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqr. <i>lib</i> libsundials_fsunlinsolsptfqr.a

*continued on next page*

<i>continued from last page</i>			
	Header files	sunlinsol/sunlinsol_sptfqmr.h	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt. <i>lib</i> libsundials_fsunlinsolsuperlumt.a	
	Header files	sunlinsol/sunlinsol_superlumt.h	
CVODE	Libraries	libsundials_cvode. <i>lib</i>	libsundials_fcvode.a
	Header files	cvode/cvode.h	cvode/cvode_impl.h
		cvode/cvode_direct.h cvode/cvode_bandpre.h	cvode/cvode_spils.h cvode/cvode_bbdpre.h
CVODES	Libraries	libsundials_cvodes. <i>lib</i>	
	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h
		cvodes/cvodes_direct.h cvodes/cvodes_bandpre.h	cvodes/cvodes_spils.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_direct.h arkode/arkode_bandpre.h	arkode/arkode_spils.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_bbdpre.h	ida/ida_spils.h
IDAS	Libraries	libsundials_idas. <i>lib</i>	
	Header files	idas/idas.h	idas/idas_impl.h
		idas/idas_direct.h idas/idas_bbdpre.h	idas/idas_spils.h
KINSOL	Libraries	libsundials_kinsol. <i>lib</i>	libsundials_fkinsol.a
	Header files	kinsol/kinsol.h	kinsol/kinsol_impl.h
		kinsol/kinsol_direct.h kinsol/kinsol_bbdpre.h	kinsol/kinsol_spils.h