Installation Guide for SUNDIALS v4.0.0

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Chapter 1

SUNDIALS Package Installation Procedure

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

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

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

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

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

- The remainder of this chapter will follow these conventions:

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

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

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

- For SUNDIALS CMake-based installation, in-source builds are prohibited; in other words, the build directory *builddir* can **not** be the same as *solverdir* and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.

- The installation directory *instdir* can **not** be the same as the source directory *solverdir*.

- By default, only the libraries and header files are exported to the installation directory *instdir*. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the *installed* SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as "templates" for your own problems. CMake installs `CMakeLists.txt` files

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

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

1.1 CMake-based installation

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

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

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

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

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

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

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

Building with the GUI

Using CMake with the GUI follows this general process:

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

  - For file and directories, the `<tab>` key can be used to complete

- Repeat until all values are set as desired and the generate option is available (`g` key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (`t` key)
- To search for a variable press `/` key, and to repeat the search, press the `n` key

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

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

The default configuration screen is shown in Figure 1.1.

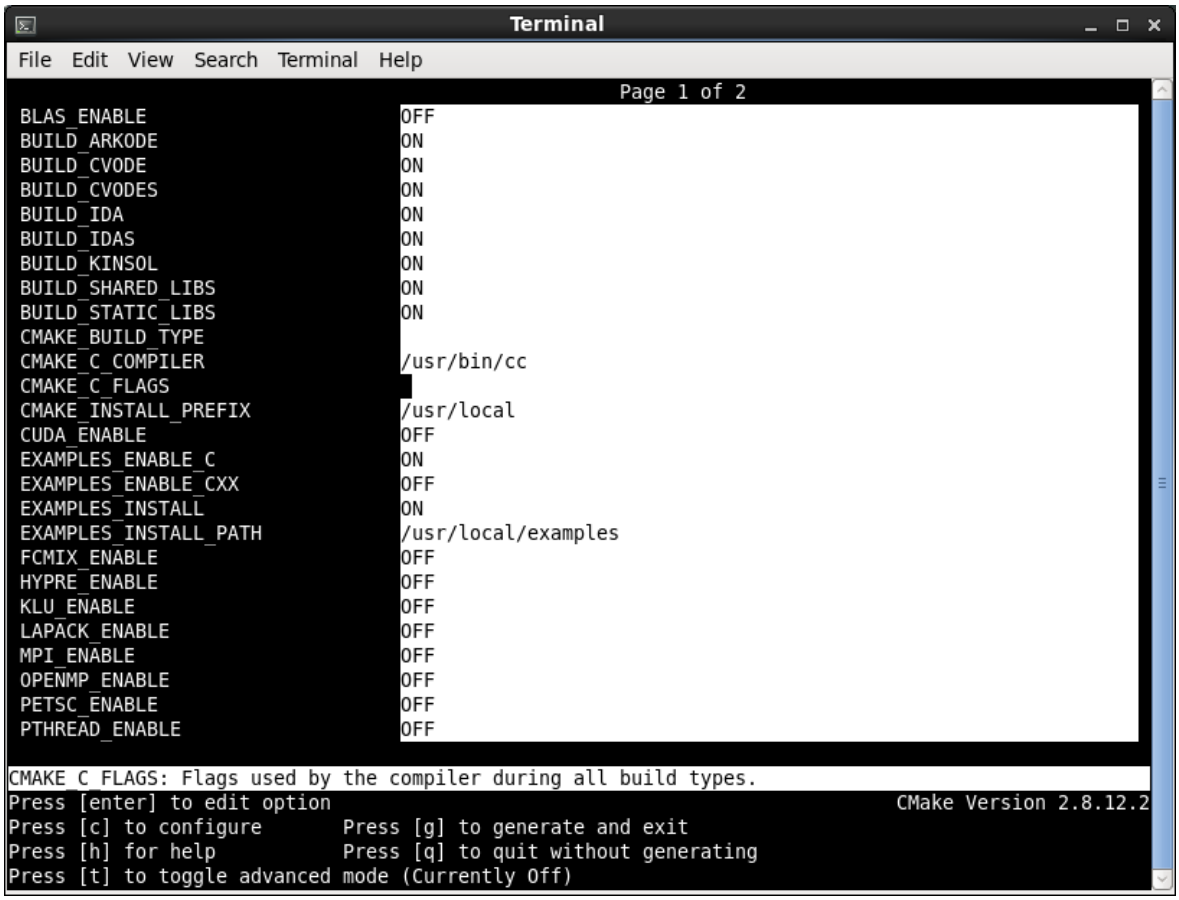

Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *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
```

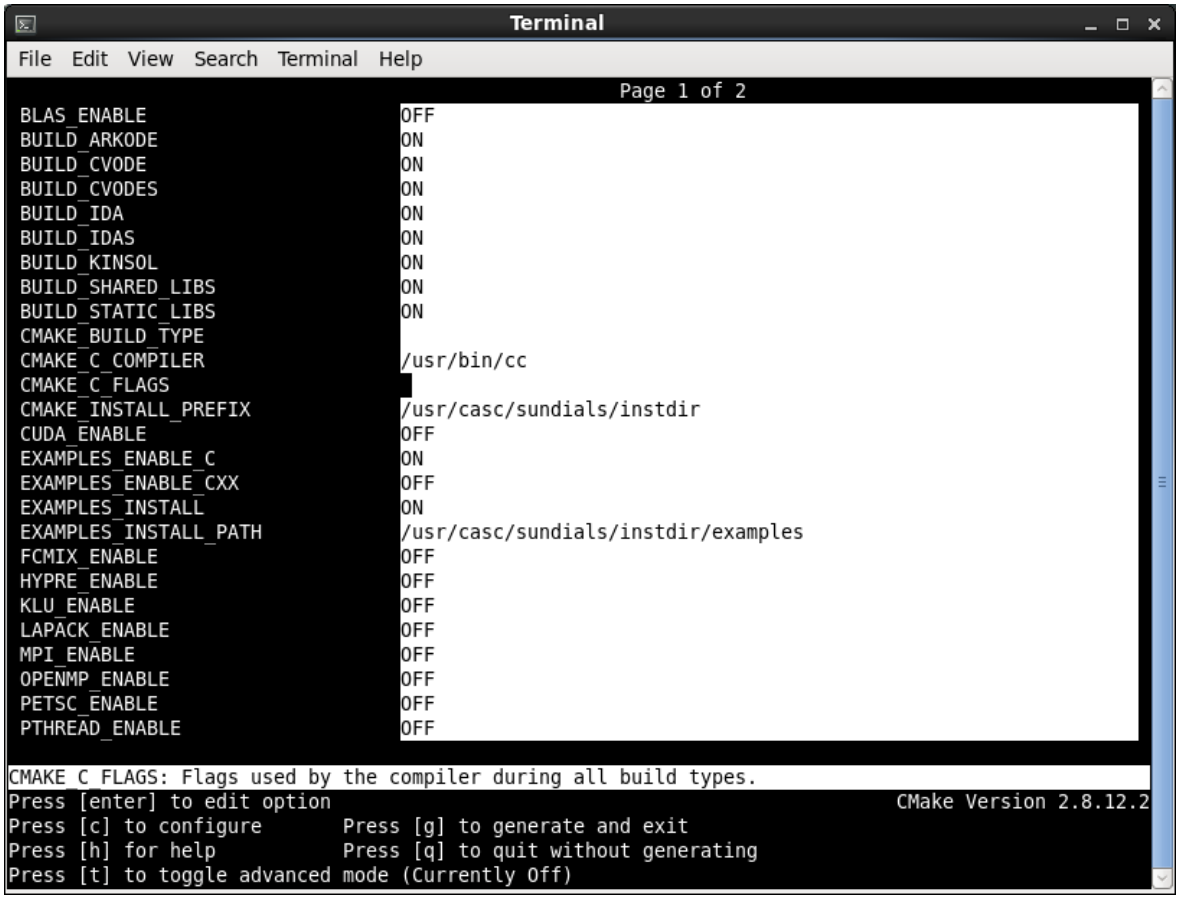

Figure 1.2: Changing the *instdir* for SUNDIALS and corresponding `examples`

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 \
> ../solverdir
% make
% make install
```

1.1.2 Configuration options (Unix/Linux)

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

`BLAS_ENABLE` - Enable BLAS support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with BLAS enabled in 1.1.4.

`BLAS_LIBRARIES` - BLAS library
Default: /usr/lib/libblas.so

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

BUILD_ARKODE - Build the ARKODE library
Default: ON

BUILD_CVODE - Build the CVODE library
Default: ON

BUILD_CVODES - Build the CVODES library
Default: ON

BUILD_IDA - Build the IDA library
Default: ON

BUILD_IDAS - Build the IDAS library
Default: ON

BUILD_KINSOL - Build the KINSOL library
Default: ON

BUILD_SHARED_LIBS - Build shared libraries
Default: ON

BUILD_STATIC_LIBS - Build static libraries
Default: ON

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

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

CMAKE_C_FLAGS - Flags for C compiler
Default:

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

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

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

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

CMAKE_CXX_FLAGS - Flags for C++ compiler
Default:

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

CMAKE_CXX_FLAGS_MINSIZEREL - Flags used by the C++ compiler during release minsize builds
Default: -Os -DNDEBUG

CMAKE_CXX_FLAGS_RELEASE - Flags used by the C++ compiler during release builds
Default: -O3 -DNDEBUG

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

CMAKE_Fortran_FLAGS - Flags for Fortran compiler
Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the Fortran compiler during debug builds
Default: -g

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

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the Fortran compiler during release builds
Default: -O3

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

CMAKE_INSTALL_LIBDIR - Library installation directory
Default:
Note: This is the directory within CMAKE_INSTALL_PREFIX that the SUNDIALS libraries will be installed under. The default is automatically set based on the operating system using the GNUInstallDirs CMake module.

Fortran_INSTALL_MODDIR - Fortran module installation directory
Default: fortran

CUDA_ENABLE - Build the SUNDIALS CUDA vector module.
Default: OFF

EXAMPLES_ENABLE_C - Build the SUNDIALS C examples
Default: ON

EXAMPLES_ENABLE_CUDA - Build the SUNDIALS CUDA examples
Default: OFF
Note: You need to enable CUDA support to build these examples.

EXAMPLES_ENABLE_CXX - Build the SUNDIALS C++ examples
Default: OFF

EXAMPLES_ENABLE_RAJA - Build the SUNDIALS RAJA examples
Default: OFF
Note: You need to enable CUDA and RAJA support to build these examples.

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples
Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90/Fortran2003 examples
Default: ON (if F77_INTERFACE_ENABLE or F2003_INTERFACE_ENABLE is ON)

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

EXAMPLES_INSTALL_PATH - Output directory for installing example files
Default: /usr/local/examples
Note: The actual default value for this option will be an examples subdirectory created under CMAKE_INSTALL_PREFIX.

F77_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 77 interfaces
Default: OFF

F2003_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 2003 interfaces
Default: OFF

HYPRE_ENABLE - Enable *hypre* support
Default: OFF
Note: See additional information on building with *hypre* enabled in 1.1.4.

HYPRE_INCLUDE_DIR - Path to *hypre* header files

HYPRE_LIBRARY_DIR - Path to *hypre* installed library files

KLU_ENABLE - Enable KLU support
Default: OFF
Note: See additional information on building with KLU enabled in 1.1.4.

KLU_INCLUDE_DIR - Path to SuiteSparse header files

KLU_LIBRARY_DIR - Path to SuiteSparse installed library files

LAPACK_ENABLE - Enable LAPACK support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in 1.1.4.

LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

MPI_ENABLE - Enable MPI support (build the parallel nvector).
Default: OFF
Note: Setting this option to ON will trigger several additional options related to MPI.

MPI_C_COMPILER - mpicc program
Default:

MPI_CXX_COMPILER - mpicxx program
Default:
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON) and C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than MPI_ENABLE.

MPI_Fortran_COMPILER - mpif77 or mpif90 program
Default:
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON) and Fortran-C support is enabled (F77_INTERFACE_ENABLE or F2003_INTERFACE_ENABLE is ON).

MPIEXEC_EXECUTABLE - Specify the executable for running MPI programs
Default: mpirun
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON).

OPENMP_ENABLE - Enable OpenMP support (build the OpenMP nvector).
Default: OFF

OPENMP_DEVICE_ENABLE - Enable OpenMP device offloading (build the OpenMPDEV nvector) if supported by the provided compiler.
Default: OFF

SKIP_OPENMP_DEVICE_CHECK - **advanced option** - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.
Default: OFF

PETSC_ENABLE - Enable PETSc support
Default: OFF
Note: See additional information on building with PETSc enabled in 1.1.4.

PETSC_INCLUDE_DIR - Path to PETSc header files

PETSC_LIBRARY_DIR - Path to PETSc installed library files

PTHREAD_ENABLE - Enable Pthreads support (build the Pthreads nvector).
Default: OFF

RAJA_ENABLE - Enable RAJA support (build the RAJA nvector).
Default: OFF
Note: You need to enable CUDA in order to build the RAJA vector module.

SUNDIALS_F77_FUNC_CASE - **advanced option** - Specify the case to use in the Fortran name-mangling scheme, options are: lower or upper
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (lower) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_UNDERSCORES must also be set.

SUNDIALS_F77_FUNC_UNDERSCORES - **advanced option** - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: none, one, or two
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (one) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_CASE must also be set.

SUNDIALS_INDEX_TYPE - **advanced option** - Integer type used for SUNDIALS indices. The size must match the size provided for the
SUNDIALS_INDEX_SIZE option.
Default:
Note: In past SUNDIALS versions, a user could set this option to INT64_T to use 64-bit integers, or INT32_T to use 32-bit integers. Starting in SUNDIALS 3.2.0, these special values are deprecated. For SUNDIALS 3.2.0 and up, a user will only need to use the SUNDIALS_INDEX_SIZE option in most cases.

SUNDIALS_INDEX_SIZE - Integer size (in bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 64
Note: The build system tries to find an integer type of appropriate size. Candidate 64-bit integer types are (in order of preference): int64_t, __int64, long long, and long. Candidate 32-bit integers are (in order of preference): int32_t, int, and long. The advanced option, SUNDIALS_INDEX_TYPE can be used to provide a type not listed here.

SUNDIALS_PRECISION - Precision used in SUNDIALS, options are: double, single, or extended
Default: double

SUPERLUMT_ENABLE - Enable SuperLU_MT support
Default: OFF
Note: See additional information on building with SuperLU_MT enabled in 1.1.4.

SUPERLUMT_INCLUDE_DIR - Path to SuperLU_MT header files (typically SRC directory)

SUPERLUMT_LIBRARY_DIR - Path to SuperLU_MT installed library files

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP
Default: Pthread

USE_GENERIC_MATH - Use generic (stdc) math libraries
Default: ON

xSDK Configuration Options

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

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

TPL_BLAS_LIBRARIES - BLAS library
Default: /usr/lib/libblas.so
SUNDIALS equivalent: BLAS_LIBRARIES
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

TPL_ENABLE_BLAS - Enable BLAS support
Default: OFF
SUNDIALS equivalent: BLAS_ENABLE

TPL_ENABLE_HYPRE - Enable *hypre* support
Default: OFF
SUNDIALS equivalent: HYPRE_ENABLE

TPL_ENABLE_KLU - Enable KLU support
Default: OFF
SUNDIALS equivalent: KLU_ENABLE

TPL_ENABLE_PETSC - Enable PETSc support
Default: OFF
SUNDIALS equivalent: PETSC_ENABLE

TPL_ENABLE_LAPACK - Enable LAPACK support
Default: OFF
SUNDIALS equivalent: LAPACK_ENABLE

TPL_ENABLE_SUPERLUMT - Enable SuperLU_MT support
Default: OFF
SUNDIALS equivalent: SUPERLUMT_ENABLE

TPL_HYPRE_INCLUDE_DIRS - Path to *hypre* header files
SUNDIALS equivalent: HYPRE_INCLUDE_DIR

TPL_HYPRE_LIBRARIES - *hypre* library
SUNDIALS equivalent: N/A

TPL_KLU_INCLUDE_DIRS - Path to KLU header files
SUNDIALS equivalent: KLU_INCLUDE_DIR

TPL_KLU_LIBRARIES - KLU library
SUNDIALS equivalent: N/A

TPL_LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
SUNDIALS equivalent: LAPACK_LIBRARIES
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

TPL_PETSC_INCLUDE_DIRS - Path to PETSc header files
SUNDIALS equivalent: PETSC_INCLUDE_DIR

TPL_PETSC_LIBRARIES - PETSc library
SUNDIALS equivalent: N/A

TPL_SUPERLUMT_INCLUDE_DIRS - Path to SuperLU_MT header files
SUNDIALS equivalent: SUPERLUMT_INCLUDE_DIR

TPL_SUPERLUMT_LIBRARIES - SuperLU_MT library
SUNDIALS equivalent: N/A

TPL_SUPERLUMT_THREAD_TYPE - SuperLU_MT library thread type
SUNDIALS equivalent: SUPERLUMT_THREAD_TYPE

USE_XSDK_DEFAULTS - Enable xSDK default configuration settings
Default: OFF
SUNDIALS equivalent: N/A
Note: Enabling xSDK defaults also sets CMAKE_BUILD_TYPE to Debug

XSDK_ENABLE_FORTRAN - Enable SUNDIALS Fortran interfaces
Default: OFF
SUNDIALS equivalent: F77_INTERFACE_ENABLE/F2003_INTERFACE_ENABLE

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

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

1.1.3 Configuration examples

The following examples will help demonstrate usage of the CMake configure options.
To configure SUNDIALS using the default C and Fortran compilers, and default mpicc and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

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

To disable installation of the examples, use:

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

1.1.4 Working with external Libraries

The SUNDIALS suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries. When building SUNDIALS as a shared library external libraries any used with SUNDIALS must also be build as a shared library or as a static library compiled with the -fPIC flag.

Building with BLAS

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

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

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

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

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

Building with LAPACK

To enable LAPACK, set the LAPACK_ENABLE option to ON. If the directory containing the LAPACK library is in the LD_LIBRARY_PATH environment variable, CMake will set the LAPACK_LIBRARIES variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations.

To explicitly tell CMake what library to use, the LAPACK_LIBRARIES variable can be set to the desired libraries. When setting the LAPACK location explicitly the location of the corresponding BLAS library will also need to be set. Example:

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

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

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

Building with KLU

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

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: `http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt`. SUNDIALS has been tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set `SUPERLUMT_ENABLE` to `ON`, set `SUPERLUMT_INCLUDE_DIR` to the `SRC` path of the SuperLU_MT installation, and set the variable `SUPERLUMT_LIBRARY_DIR` to the `lib` path of the SuperLU_MT installation. At the same time, the variable `SUPERLUMT_THREAD_TYPE` must be set to either `Pthread` or `OpenMP`.
Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either `OPENMP_ENABLE` or `PTHREAD_ENABLE` set to `ON` then SuperLU_MT should be set to use the same threading type.

Building with PETSc

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

Building with *hypre*

The *hypre* libraries are available for download from the Lawrence Livermore National Laboratory website: `http://computation.llnl.gov/projects/hypre`. SUNDIALS has been tested with *hypre* version 2.11.1. To enable *hypre*, set `HYPRE_ENABLE` to `ON`, set `HYPRE_INCLUDE_DIR` to the `include` path of the *hypre* installation, and set the variable `HYPRE_LIBRARY_DIR` to the `lib` path of the *hypre* installation.

Building with CUDA

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

Building with RAJA

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

1.1.5 Testing the build and installation

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

```
% make test
```

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

```
% make test_install
```

1.2 Building and Running Examples

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

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

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

1.3 Configuring, building, and installing on Windows

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

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

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

1.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

```
% make install
```

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

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

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

Table 1.1: SUNDIALS libraries and header files

SHARED	Libraries	n/a
	Header files	sundials/sundials_config.h sundials/sundials_fconfig.h sundials/sundials_types.h sundials/sundials_math.h sundials/sundials_nvector.h sundials/sundials_fnvector.h sundials/sundials_matrix.h sundials/sundials_linearsolver.h sundials/sundials_iterative.h sundials/sundials_direct.h sundials/sundials_dense.h sundials/sundials_band.h sundials/sundials_nonlinearsolver.h sundials/sundials_version.h sundials/sundials_mpi_types.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib* libsundials_fnvecserial_mod.*lib* libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module files	fnvector_serial_mod.mod
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib* libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.*lib* libsundials_fnvecopenmp_mod.*lib* libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h
	Module files	fnvector_openmp_mod.mod
NVECTOR_OPENMPDEV	Libraries	libsundials_nvecopenmpdev.*lib*
	Header files	nvector/nvector_openmpdev.h
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.*lib* libsundials_fnvecpthreads_mod.*lib* libsundials_fnvecpthreads.a
	Header files	nvector/nvector_pthreads.h
	Module files	fnvector_pthreads_mod.mod
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp.*lib*
	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 Libraries	libsundials_nveccuda.*lib* 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 Libraries	libsundials_nveccudaraja.*lib* libsundials_nveccudampiraja.*lib*
	Header files	nvector/nvector_raja.h nvector/nvector_mpiraja.h nvector/raja/Vector.hpp
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.*lib* libsundials_fsunmatrixband_mod.*lib* libsundials_fsunmatrixband.a
	Header files	sunmatrix/sunmatrix_band.h
	Module files	fsunmatrix_band_mod.mod
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.*lib* libsundials_fsunmatrixdense_mod.*lib* libsundials_fsunmatrixdense.a
	Header files	sunmatrix/sunmatrix_dense.h
	Module files	fsunmatrix_dense_mod.mod
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse.*lib* libsundials_fsunmatrixsparse_mod.*lib* libsundials_fsunmatrixsparse.a
	Header files	sunmatrix/sunmatrix_sparse.h
	Module files	fsunmatrix_sparse_mod.mod
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.*lib* libsundials_fsunlinsolband_mod.*lib* libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module files	fsunlinsol_band_mod.mod
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.*lib* libsundials_fsunlinsoldense_mod.*lib* libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h

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	Module files	fsunlinsol_dense_mod.mod
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.*lib* libsundials_fsunlinsolklu_mod.*lib* libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module files	fsunlinsol_klu_mod.mod
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 files	fsunlinsol_pcg_mod.mod
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.*lib* libsundials_fsunlinsolspbcgs_mod.*lib* libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module files	fsunlinsol_spbcgs_mod.mod
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.*lib* libsundials_fsunlinsolspfgmr_mod.*lib* libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module files	fsunlinsol_spfgmr_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.*lib* libsundials_fsunlinsolspgmr_mod.*lib* libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.*lib* libsundials_fsunlinsolsptfqmr_mod.*lib* libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h

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	Module files	fsunlinsol_sptfqmr_mod.mod	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.*lib* libsundials_fsunlinsolsuperlumt.a	
	Header files	sunlinsol/sunlinsol_superlumt.h	
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnewton.*lib* libsundials_fsunnonlinsolnewton_mod.*lib* libsundials_fsunnonlinsolnewton.a	
	Header files	sunnonlinsol/sunnonlinsol_newton.h	
	Module files	fsunnonlinsol_newton_mod.mod	
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint.*lib* libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod.*lib*	
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h	
	Module files	fsunnonlinsol_fixedpoint_mod.mod	
CVODE	Libraries	libsundials_cvode.*lib*	libsundials_fcvode.a
	Header files	cvode/cvode.h cvode/cvode_direct.h cvode/cvode_spils.h cvode/cvode_bbdpre.h	cvode/cvode_impl.h cvode/cvode_ls.h cvode/cvode_bandpre.h
	Module files	fcvode_mod.mod	
CVODES	Libraries	libsundials_cvodes.*lib*	
	Header files	cvodes/cvodes.h cvodes/cvodes_direct.h cvodes/cvodes_spils.h cvodes/cvodes_bbdpre.h	cvodes/cvodes_impl.h cvodes/cvodes_ls.h cvodes/cvodes_bandpre.h
ARKODE	Libraries	libsundials_arkode.*lib*	libsundials_farkode.a
	Header files	arkode/arkode.h arkode/arkode_ls.h arkode/arkode_bbdpre.h	arkode/arkode_impl.h arkode/arkode_bandpre.h
IDA	Libraries	libsundials_ida.*lib*	libsundials_fida.a
	Header files	ida/ida.h ida/ida_direct.h ida/ida_spils.h	ida/ida_impl.h ida/ida_ls.h ida/ida_bbdpre.h
IDAS	Libraries	libsundials_idas.*lib*	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_spils.h	idas/idas_impl.h idas/idas_ls.h idas/idas_bbdpre.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a

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