SUNDIALS Installation Guide v7.2.1

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CONTRIBUTORS

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Chapter 1

Acquiring SUNDIALS

There are two supported ways for building and installing SUNDIALS from source. One option is to use the Spack HPC package manager:

```
spack install sundials
```

The second supported option for building and installing SUNDIALS is with CMake. Before proceeding with CMake, the source code must be downloaded. This can be done by cloning the SUNDIALS GitHub repository (run `git clone https://github.com/LLNL/sundials`), or by downloading the SUNDIALS release compressed archives (`.tar.gz`) from the SUNDIALS website.

The compressed archives allow for downloading of individual SUNDIALS packages. The name of the distribution archive is of the form `SOLVER-7.1.0.tar.gz`, where `SOLVER` is one of: `sundials`, `cvode`, `cvodes`, `arkode`, `ida`, `idas`, or `kinsol`, and `7.1.0` represents the version number (of the SUNDIALS suite or of the individual solver). After downloading the relevant archives, uncompress and expand the sources, by running

```
% tar -zxf SOLVER-7.1.0.tar.gz
```

This will extract source files under a directory `SOLVER-7.1.0`.

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

1. The remainder of this chapter will follow these conventions:

   `SOLVERDIR` is the directory `SOLVER-7.1.0` 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.

2. 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.

3. The installation directory `INSTDIR` can not be the same as the source directory `SOLVERDIR`.

4. 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.)

Further details on the CMake-based installation procedures, instructions for manual compilation, and a roadmap of the resulting installed libraries and exported header files, are provided in §2 and §2.8.

Chapter 2

Building and Installing with CMake

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 3.18.0 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` or `cmake-gui`), while on Windows it requires Visual Studio. While many Linux distributions offer CMake, the version included may be out of date. CMake adds new features regularly, 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` or `cmake-gui` (depending on the version of CMake), 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.

2.1 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, or from a wxWidgets or QT based GUI by using the `cmake-gui` command. Examples for using both text and graphical 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 (...)/INSTDIR
$ mkdir (...)/BUILDDIR
$ cd (...)/BUILDDIR
```

2.1.1 Building with the GUI

Using CMake with the `ccmake` GUI follows the general process:

1. Select and modify values, run configure (`c` key)
2. New values are denoted with an asterisk
3. 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
4. Repeat until all values are set as desired and the generate option is available (`g` key)
5. Some variables (advanced variables) are not visible right away; to see advanced variables, toggle to advanced mode (`t` key)
6. To search for a variable press the `/` key, and to repeat the search, press the `n` key

Using CMake with the `cmake-gui` GUI follows a similar process:

1. Select and modify values, click `Configure`
2. The first time you click `Configure`, make sure to pick the appropriate generator (the following will assume generation of Unix Makefiles).
3. New values are highlighted in red
4. To set a variable, click on or move the cursor to the variable and press enter
    - If it is a boolean (`ON/OFF`) it will check/uncheck the box
    - If it is string or file, it will allow editing of the string. Additionally, an ellipsis button will appear `...` on the far right of the entry. Clicking this button will bring up the file or directory selection dialog.
    - For files and directories, the `<tab>` key can be used to complete
5. Repeat until all values are set as desired and click the `Generate` button
6. Some variables (advanced variables) are not visible right away; to see advanced variables, click the `advanced` button

To build the default configuration using the curses GUI, from the `BUILDDIR` enter the `ccmake` command and point to the `SOLVERDIR`:

```
$ ccmake (...)/SOLVERDIR
```

Similarly, to build the default configuration using the wxWidgets GUI, from the `BUILDDIR` enter the `cmake-gui` command and point to the `SOLVERDIR`:

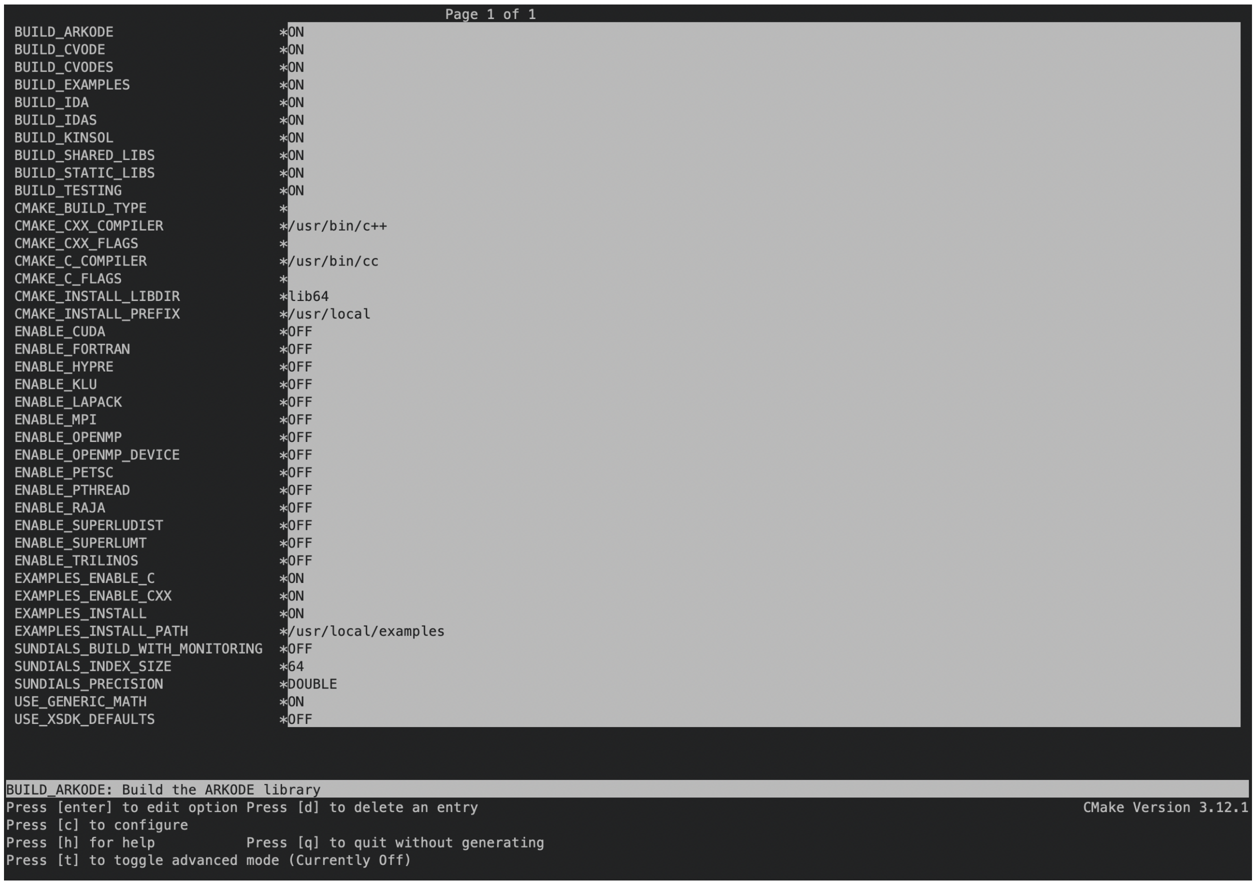
```
$ cmake-gui (...)/SOLVERDIR
```

The default curses configuration screen is shown in the following figure.

The default INSTDIR for both SUNDIALS and the corresponding examples can be changed by setting the `CMAKE_INSTALL_PREFIX` and the `EXAMPLES_INSTALL_PATH` as shown in the following figure.

Pressing the `g` key or clicking `generate` will generate Makefiles including all dependencies and all rules to build SUNDIALS on this system. Back at the command prompt, you can now run:

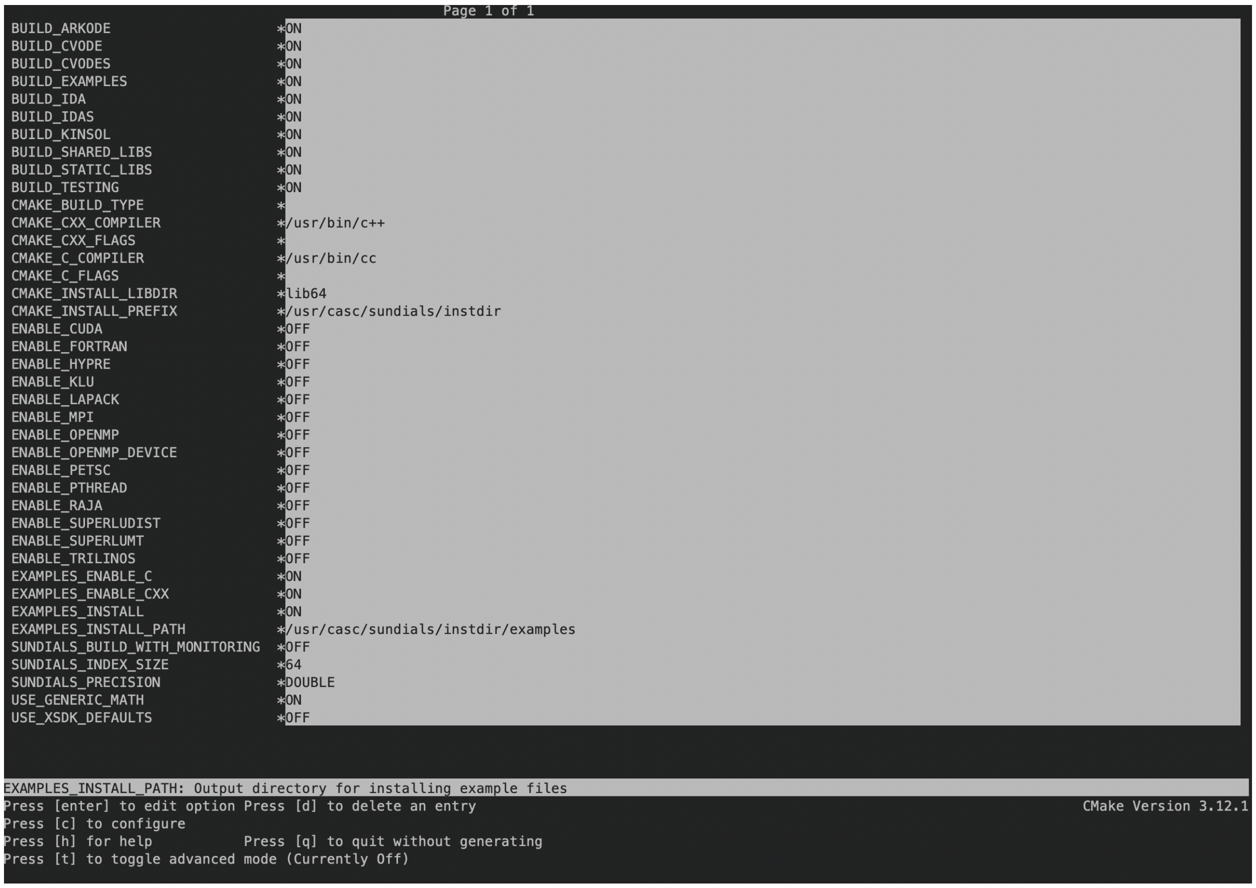
```
$ make
```



```
                                                    Page 1 of 1
 BUILD_ARKODE                    *ON
 BUILD_CVODE                     *ON
 BUILD_CVODES                    *ON
 BUILD_EXAMPLES                  *ON
 BUILD_IDA                       *ON
 BUILD_IDAS                      *ON
 BUILD_KINSOL                    *ON
 BUILD_SHARED_LIBS               *ON
 BUILD_STATIC_LIBS               *ON
 BUILD_TESTING                   *ON
 CMAKE_BUILD_TYPE                *
 CMAKE_CXX_COMPILER              */usr/bin/c++
 CMAKE_CXX_FLAGS                 *
 CMAKE_C_COMPILER                */usr/bin/cc
 CMAKE_C_FLAGS                   *
 CMAKE_INSTALL_LIBDIR            *lib64
 CMAKE_INSTALL_PREFIX            */usr/local
 ENABLE_CUDA                     *OFF
 ENABLE_FORTRAN                  *OFF
 ENABLE_HYPRE                    *OFF
 ENABLE_KLU                      *OFF
 ENABLE_LAPACK                   *OFF
 ENABLE_MPI                      *OFF
 ENABLE_OPENMP                   *OFF
 ENABLE_OPENMP_DEVICE            *OFF
 ENABLE_PETSC                    *OFF
 ENABLE_PTHREAD                  *OFF
 ENABLE_RAJA                     *OFF
 ENABLE_SUPERLUDIST              *OFF
 ENABLE_SUPERLUMT                *OFF
 ENABLE_TRILINOS                 *OFF
 EXAMPLES_ENABLE_C               *ON
 EXAMPLES_ENABLE_CXX             *ON
 EXAMPLES_INSTALL                *ON
 EXAMPLES_INSTALL_PATH           */usr/local/examples
 SUNDIALS_BUILD_WITH_MONITORING  *OFF
 SUNDIALS_INDEX_SIZE             *64
 SUNDIALS_PRECISION              *DOUBLE
 USE_GENERIC_MATH                *ON
 USE_XSDK_DEFAULTS               *OFF


BUILD_ARKODE: Build the ARKODE library
Press [enter] to edit option Press [d] to delete an entry                                         CMake Version 3.12.1
Press [c] to configure
Press [h] for help           Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Fig. 2.1: 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.



```
                                                   Page 1 of 1
 BUILD_ARKODE                     *ON
 BUILD_CVODE                      *ON
 BUILD_CVODES                     *ON
 BUILD_EXAMPLES                   *ON
 BUILD_IDA                        *ON
 BUILD_IDAS                       *ON
 BUILD_KINSOL                     *ON
 BUILD_SHARED_LIBS                *ON
 BUILD_STATIC_LIBS                *ON
 BUILD_TESTING                    *ON
 CMAKE_BUILD_TYPE                 *
 CMAKE_CXX_COMPILER               */usr/bin/c++
 CMAKE_CXX_FLAGS                  *
 CMAKE_C_COMPILER                 */usr/bin/cc
 CMAKE_C_FLAGS                    *
 CMAKE_INSTALL_LIBDIR             *lib64
 CMAKE_INSTALL_PREFIX             */usr/casc/sundials/instdir
 ENABLE_CUDA                      *OFF
 ENABLE_FORTRAN                   *OFF
 ENABLE_HYPRE                     *OFF
 ENABLE_KLU                       *OFF
 ENABLE_LAPACK                    *OFF
 ENABLE_MPI                       *OFF
 ENABLE_OPENMP                    *OFF
 ENABLE_OPENMP_DEVICE             *OFF
 ENABLE_PETSC                     *OFF
 ENABLE_PTHREAD                   *OFF
 ENABLE_RAJA                      *OFF
 ENABLE_SUPERLUDIST               *OFF
 ENABLE_SUPERLUMT                 *OFF
 ENABLE_TRILINOS                  *OFF
 EXAMPLES_ENABLE_C                *ON
 EXAMPLES_ENABLE_CXX              *ON
 EXAMPLES_INSTALL                 *ON
 EXAMPLES_INSTALL_PATH            */usr/casc/sundials/instdir/examples
 SUNDIALS_BUILD_WITH_MONITORING   *OFF
 SUNDIALS_INDEX_SIZE              *64
 SUNDIALS_PRECISION               *DOUBLE
 USE_GENERIC_MATH                 *ON
 USE_XSDK_DEFAULTS                *OFF


EXAMPLES_INSTALL_PATH: Output directory for installing example files
Press [enter] to edit option Press [d] to delete an entry                                        CMake Version 3.12.1
Press [c] to configure
Press [h] for help           Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Fig. 2.2: Changing the INSTDIR for SUNDIALS and corresponding EXAMPLES.

or for a faster parallel build (e.g. using 4 threads), you can run

```
$ make -j 4
```

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

```
$ make install
```

2.1.2 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
```

2.2 Configuration options

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.

`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: `Debug`, `Release`, `RelWithDebInfo`, and `MinSizeRel`

Default: `RelWithDebInfo`

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_C_STANDARD`

The C standard to build C parts of SUNDIALS with.

Default: 99

Options: 99, 11, 17.

`CMAKE_C_EXTENSIONS`

Enable compiler specific C extensions.

Default: `OFF`

`CMAKE_CXX_COMPILER`

C++ compiler

Default: `/usr/bin/c++`

Note

A C++ compiler is only required when a feature requiring C++ is enabled (e.g., CUDA, HIP, SYCL, RAJA, etc.) or the C++ examples are enabled.

All SUNDIALS solvers can be used from C++ applications 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_CXX_STANDARD`

The C++ standard to build C++ parts of SUNDIALS with.

Default: 11

Options: 98, 11, 14, 17, 20.

`CMAKE_CXX_EXTENSIONS`

Enable compiler specific C++ extensions.

Default: `OFF`

`CMAKE_Fortran_COMPILER`

Fortran compiler

Default: `/usr/bin/gfortran`

Note

Fortran support (and all related options) are triggered only if either Fortran-C support (`BUILD_FORTRAN_MODULE_INTERFACE`) or LAPACK (`ENABLE_LAPACK`) support is enabled.

`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_LIBDIR`

The directory under which libraries will be installed.

Default: Set based on the system: `lib`, `lib64`, or `lib/<multiarch-tuple>`

`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.

`ENABLE_CUDA`

Build the SUNDIALS CUDA modules.

Default: `OFF`

`CMAKE_CUDA_ARCHITECTURES`

Specifies the CUDA architecture to compile for i.e., `60` for Pascal, `70` Volta, `80` for Ampere, `90` for Hopper, etc. See the GPU compute capability tables on the NVIDIA webpage and the GPU Compilation section of the CUDA documentation for more information.

Default: Determined automatically by CMake. Users are encouraged to override this value with the architecture for their system as the default varies across compilers and compiler versions.

Changed in version 7.2.0: In prior versions `CMAKE_CUDA_ARCHITECTURES` defaulted to `70`.

`EXAMPLES_ENABLE_C`

Build the SUNDIALS C examples

Default: `ON`

`EXAMPLES_ENABLE_CXX`

Build the SUNDIALS C++ examples

Default: `OFF`

`EXAMPLES_ENABLE_CUDA`

Build the SUNDIALS CUDA examples

Default: `OFF`

Note

You need to enable CUDA support to build these examples.

`EXAMPLES_ENABLE_F2003`

Build the SUNDIALS Fortran2003 examples

Default: `ON` (if `BUILD_FORTRAN_MODULE_INTERFACE` 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`.

`BUILD_FORTRAN_MODULE_INTERFACE`

Enable Fortran 2003 interface

Default: `OFF`

Warning

There is a known issue with MSYS/gfortran and SUNDIALS shared libraries that causes linking the Fortran interfaces to fail when building SUNDIALS. For now the work around is to only build with static libraries when using MSYS with gfortran on Windows.

`SUNDIALS_LOGGING_LEVEL`

Set the maximum logging level for the SUNLogger runtime API. The higher this is set, the more output that may be logged, and the more performance may degrade. The options are:

- `0` – no logging
- `1` – log errors

- `2` – log errors + warnings
- `3` – log errors + warnings + informational output
- `4` – log errors + warnings + informational output + debug output
- `5` – log all of the above and even more (e.g. vector valued variables may be logged)

Default: 2

`SUNDIALS_BUILD_WITH_MONITORING`

Build SUNDIALS with capabilities for fine-grained monitoring of solver progress and statistics. This is primarily useful for debugging.

Default: OFF

Warning

Building with monitoring may result in minor performance degradation even if monitoring is not utilized.

`SUNDIALS_BUILD_WITH_PROFILING`

Build SUNDIALS with capabilities for fine-grained profiling. This requires POSIX timers or the Windows `profileapi.h` timers.

Default: OFF

Warning

Profiling will impact performance, and should be enabled judiciously.

`SUNDIALS_ENABLE_ERROR_CHECKS`

Build SUNDIALS with more extensive checks for unrecoverable errors.

Default: `OFF` when `CMAKE_BUILD_TYPE=Release|RelWithDebInfo `` and ``ON` otherwise.

Warning

Error checks will impact performance, but can be helpful for debugging.

`SUNDIALS_ENABLE_EXTERNAL_ADDONS`

Build SUNDIALS with any external addons that you have put in `sundials/external`.

Default: `OFF`

Warning

Addons are not maintained by the SUNDIALS team. Use at your own risk.

`ENABLE_GINKGO`

Enable interfaces to the Ginkgo linear algebra library.

Default: `OFF`

`Ginkgo_DIR`

Path to the Ginkgo installation.

Default: None

`SUNDIALS_GINKGO_BACKENDS`

Semi-colon separated list of Ginkgo target architectures/executors to build for. Options currently supported are REF (the Ginkgo reference executor), OMP, CUDA, HIP, and SYCL.

Default: “REF;OMP”

`ENABLE_KOKKOS`

Enable the Kokkos based vector.

Default: `OFF`

`Kokkos_DIR`

Path to the Kokkos installation.

Default: None

`ENABLE_KOKKOS_KERNELS`

Enable the Kokkos based dense matrix and linear solver.

Default: `OFF`

`KokkosKernels_DIR`

Path to the Kokkos-Kernels installation.

Default: None

`ENABLE_HIP`

Enable HIP Support

Default: `OFF`

`AMDGPU_TARGETS`

Specify which AMDGPU processor(s) to target.

Default: None

`ENABLE_HYPRE`

Flag to enable *hypre* support

Default: `OFF`

Note

See additional information on building with *hypre* enabled in §2.4.

`HYPRE_INCLUDE_DIR`

Path to *hypre* header files

Default: none

`HYPRE_LIBRARY`

Path to *hypre* installed library files

Default: none

ENABLE_KLU

Enable KLU support

Default: `OFF`

> **Note**
>
> See additional information on building with KLU enabled in §2.4.

KLU_INCLUDE_DIR

Path to SuiteSparse header files

Default: none

KLU_LIBRARY_DIR

Path to SuiteSparse installed library files

Default: none

ENABLE_LAPACK

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 §2.4.

BLAS_LIBRARIES

BLAS libraries

Default: none (CMake will try to find a BLAS installation)

BLAS_LINKER_FLAGS

BLAS required linker flags

Default: none (CMake will try to determine the necessary flags)

LAPACK_LIBRARIES

LAPACK libraries

Default: none (CMake will try to find a LAPACK installation)

LAPACK_LINKER_FLAGS

LAPACK required linker flags

Default: none (CMake will try to determine the necessary flags)

ENABLE_MAGMA

Enable MAGMA support.

Default: `OFF`

> **Note**
>
> Setting this option to `ON` will trigger additional options related to MAGMA.

`MAGMA_DIR`

Path to the root of a MAGMA installation.

Default: none

`SUNDIALS_MAGMA_BACKENDS`

Which MAGMA backend to use under the SUNDIALS MAGMA interface.

Default: `CUDA`

`ENABLE_MPI`

Enable MPI support. This will build the parallel nvector and the MPI-aware version of the ManyVector library.

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 (`ENABLE_MPI` 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 `ENABLE_MPI`.

`MPI_Fortran_COMPILER`

`mpif90` program

Default:

Note

This option is triggered only if MPI is enabled (`ENABLE_MPI` is `ON`) and Fortran-C support is enabled (`EXAMPLES_ENABLE_F2003` is `ON`).

`MPIEXEC_EXECUTABLE`

Specify the executable for running MPI programs

Default: `mpirun`

Note

This option is triggered only if MPI is enabled (`ENABLE_MPI` is `ON`).

`MPIEXEC_PREFLAGS`

Specifies flags that come directly after `MPIEXEC_EXECUTABLE` and before `MPIEXEC_NUMPROC_FLAG` and `MPIEXEC_MAX_NUMPROCS`.

Default: none

Note

This option is triggered only if MPI is enabled (`ENABLE_MPI` is `ON`).

`MPIEXEC_POSTFLAGS`

Specifies flags that come after the executable to run but before any other program arguments.

Default: none

Note

This option is triggered only if MPI is enabled (`ENABLE_MPI` is `ON`).

`ENABLE_ONEMKL`

Enable oneMKL support.

Default: `OFF`

`ONEMKL_DIR`

Path to oneMKL installation.

Default: none

`SUNDIALS_ONEMKL_USE_GETRF_LOOP`

This advanced debugging option replaces the batched LU factorization with a loop over each system in the batch and a non-batched LU factorization.

Default: OFF

`SUNDIALS_ONEMKL_USE_GETRS_LOOP`

This advanced debugging option replaces the batched LU solve with a loop over each system in the batch and a non-batched solve.

Default: OFF

`ENABLE_OPENMP`

Enable OpenMP support (build the OpenMP NVector)

Default: `OFF`

`ENABLE_PETSC`

Enable PETSc support

Default: `OFF`

Note

See additional information on building with PETSc enabled in §2.4.

`PETSC_DIR`

Path to PETSc installation

Default: none

`PETSC_LIBRARIES`

Semi-colon separated list of PETSc link libraries. Unless provided by the user, this is autopopulated based on the PETSc installation found in `PETSC_DIR`.

Default: none

`PETSC_INCLUDES`

Semi-colon separated list of PETSc include directories. Unless provided by the user, this is autopopulated based on the PETSc installation found in `PETSC_DIR`.

Default: none

`ENABLE_PTHREAD`

Enable Pthreads support (build the Pthreads NVector)

Default: `OFF`

`ENABLE_RAJA`

Enable RAJA support.

Default: OFF

Note

You need to enable CUDA or HIP in order to build the RAJA vector module.

`SUNDIALS_RAJA_BACKENDS`

If building SUNDIALS with RAJA support, this sets the RAJA backend to target. Values supported are CUDA, HIP, or SYCL.

Default: CUDA

`ENABLE_SUPERLUDIST`

Enable SuperLU_DIST support

Default: `OFF`

Note

See additional information on building with SuperLU_DIST enabled in §2.4.

`SUPERLUDIST_DIR`

Path to SuperLU_DIST installation.

Default: none

`SUPERLUDIST_OpenMP`

Enable SUNDIALS support for SuperLU_DIST built with OpenMP

Default: none

Note: SuperLU_DIST must be built with OpenMP support for this option to function. Additionally the environment variable `OMP_NUM_THREADS` must be set to the desired number of threads.

SUPERLUDIST_INCLUDE_DIRS

List of include paths for SuperLU_DIST (under a typical SuperLU_DIST install, this is typically the SuperLU_-DIST SRC directory)

Default: none

Note

This is an advanced option. Prefer to use *SUPERLUDIST_DIR*.

SUPERLUDIST_LIBRARIES

Semi-colon separated list of libraries needed for SuperLU_DIST

Default: none

Note

This is an advanced option. Prefer to use *SUPERLUDIST_DIR*.

SUPERLUDIST_INCLUDE_DIR

Path to SuperLU_DIST header files (under a typical SuperLU_DIST install, this is typically the SuperLU_DIST SRC directory)

Default: none

Note

This is an advanced option. This option is deprecated. Use *SUPERLUDIST_INCLUDE_DIRS*.

SUPERLUDIST_LIBRARY_DIR

Path to SuperLU_DIST installed library files

Default: none

Note

This option is deprecated. Use *SUPERLUDIST_DIR*.

ENABLE_SUPERLUMT

Enable SuperLU_MT support

Default: `OFF`

Note

See additional information on building with SuperLU_MT enabled in §2.4.

SUPERLUMT_INCLUDE_DIR

Path to SuperLU_MT header files (under a typical SuperLU_MT install, this is typically the SuperLU_MT SRC directory)

Default: none

`SUPERLUMT_LIBRARY_DIR`

Path to SuperLU_MT installed library files

Default: none

`SUPERLUMT_THREAD_TYPE`

Must be set to Pthread or OpenMP, depending on how SuperLU_MT was compiled.

Default: Pthread

`ENABLE_SYCL`

Enable SYCL support.

Default: OFF

Note

Building with SYCL enabled requires a compiler that supports a subset of the of SYCL 2020 specification (specifically `sycl/sycl.hpp` must be available).

CMake does not currently support autodetection of SYCL compilers and `CMAKE_CXX_COMPILER` must be set to a valid SYCL compiler. At present the only supported SYCL compilers are the Intel oneAPI compilers i.e., `dpcpp` and `icpx`. When using `icpx` the `-fsycl` flag and any ahead of time compilation flags must be added to `CMAKE_CXX_FLAGS`.

`SUNDIALS_SYCL_2020_UNSUPPORTED`

This advanced option disables the use of *some* features from the SYCL 2020 standard in SUNDIALS libraries and examples. This can be used to work around some cases of incomplete compiler support for SYCL 2020.

Default: OFF

`ENABLE_TRILINOS`

Enable Trilinos (Tpetra) support

Default: OFF

`Trilinos_DIR`

Path to the Trilinos installation.

Default: None

`ENABLE_CALIPER`

Enable CALIPER support

Default: OFF

Note

Using Caliper requires setting *`SUNDIALS_BUILD_WITH_PROFILING`* to `ON`.

`CALIPER_DIR`

Path to the root of a Caliper installation

Default: None

`ENABLE_ADIAK`

Enable Adiak support

Default: OFF

`adiak_DIR`

Path to the root of an Adiak installation

Default: None

`SUNDIALS_LAPACK_CASE`

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_LAPACK_UNDERSCORES` must also be set.

`SUNDIALS_LAPACK_UNDERSCORES`

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_LAPACK_CASE` must also be set.

`SUNDIALS_INDEX_TYPE`

Integer type used for SUNDIALS indices. The size must match the size provided for the `SUNDIALS_INDEX_SIZE` option.

Default: Automatically determined based on *`SUNDIALS_INDEX_SIZE`*

> **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`

The floating-point precision used in SUNDIALS packages and class implementations, options are: `double`, `single`, or `extended`

Default: `double`

`SUNDIALS_MATH_LIBRARY`

The standard C math library (e.g., `libm`) to link with.

Default: `-lm` on Unix systems, none otherwise

`SUNDIALS_INSTALL_CMAKEDIR`

Installation directory for the SUNDIALS cmake files (relative to *`CMAKE_INSTALL_PREFIX`*).

Default: `CMAKE_INSTALL_PREFIX/cmake/sundials`

`ENABLE_XBRAID`

Enable or disable the ARKStep + XBraid interface.

Default: `OFF`

Note

See additional information on building with *XBraid* enabled in §2.4.

`XBRAID_DIR`

The root directory of the XBraid installation.

Default: `OFF`

`XBRAID_INCLUDES`

Semi-colon separated list of XBraid include directories. Unless provided by the user, this is autopopulated based on the XBraid installation found in `XBRAID_DIR`.

Default: none

`XBRAID_LIBRARIES`

Semi-colon separated list of XBraid link libraries. Unless provided by the user, this is autopopulated based on the XBraid installation found in `XBRAID_DIR`.

Default: none

`USE_XSDK_DEFAULTS`

Enable xSDK (see https://xsdk.info for more information) default configuration settings. This sets `CMAKE_BUILD_TYPE` to `Debug`, `SUNDIALS_INDEX_SIZE` to 32 and `SUNDIALS_PRECISION` to double.

Default: `OFF`

2.3 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 `mpif90` 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 \
> -DENABLE_MPI=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 \
> -DENABLE_MPI=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/srcdir

% make install
```

2.4 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.

2.4.1 Building with Ginkgo

Ginkgo is a high-performance linear algebra library for manycore systems, with a focus on solving sparse linear systems. It is implemented using modern C++ (you will need at least a C++14 compliant compiler to build it), with GPU kernels implemented in CUDA (for NVIDIA devices), HIP (for AMD devices) and SYCL/DPC++ (for Intel devices and other supported hardware). To enable Ginkgo in SUNDIALS, set the *`ENABLE_GINKGO`* to `ON` and provide the path to the root of the Ginkgo installation in *`Ginkgo_DIR`*. Additionally, *`SUNDIALS_GINKGO_BACKENDS`* must be set to a list of Ginkgo target architectures/executors. E.g.,

```
% cmake \
> -DENABLE_GINKGO=ON \
> -DGinkgo_DIR=/path/to/ginkgo/installation \
> -DSUNDIALS_GINKGO_BACKENDS="REF;OMP;CUDA" \
> /home/myname/sundials/srcdir
```

The SUNDIALS interfaces to Ginkgo are not compatible with *`SUNDIALS_PRECISION`* set to `extended`.

2.4.2 Building with Kokkos

Kokkos is a modern C++ (requires at least C++14) programming model for witting performance portable code for multi-core CPU and GPU-based systems including NVIDIA, AMD, and Intel accelerators. To enable Kokkos in SUNDIALS, set the *ENABLE_KOKKOS* to ON and provide the path to the root of the Kokkos installation in *Kokkos_DIR*. Additionally, the Kokkos-Kernels library provides common computational kernels for linear algebra. To enable Kokkos-Kernels in SUNDIALS, set the *ENABLE_KOKKOS_KERNELS* to ON and provide the path to the root of the Kokkos-Kernels installation in *KokkosKernels_DIR* e.g.,

```
% cmake \
> -DENABLE_KOKKOS=ON \
> -DKokkos_DIR=/path/to/kokkos/installation \
> -DENABLE_KOKKOS_KERNELS=ON \
> -DKokkosKernels_DIR=/path/to/kokkoskernels/installation \
> /home/myname/sundials/srcdir
```

Note

The minimum supported version of Kokkos-Kernels 3.7.00.

2.4.3 Building with LAPACK

To enable LAPACK, set the *ENABLE_LAPACK* option to ON. CMake will attempt to find BLAS and LAPACK installations on the system and set the variables *BLAS_LIBRARIES*, *BLAS_LINKER_FLAGS*, *LAPACK_LIBRARIES*, and *LAPACK_-LINKER_FLAGS*. To explicitly specify the LAPACK library to build with, manually set the aforementioned variables to the desired values when configuring the build.

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DENABLE_LAPACK=ON \
> -DBLAS_LIBRARIES=/mylapackpath/lib/libblas.so \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/srcdir

% make install
```

Note

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.

SUNDIALS has been tested with OpenBLAS 0.3.27.

2.4.4 Building with KLU

KLU is a software package for the direct solution of sparse nonsymmetric linear systems of equations that arise in circuit simulation and is part of SuiteSparse, a suite of sparse matrix software. The library is developed by Texas A&M University and is available from the SuiteSparse GitHub repository.

To enable KLU, set `ENABLE_KLU` 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. In that case, 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`.

For SuiteSparse 7.4.0 and newer, the necessary information can also be gathered from a CMake import target. If SuiteSparse is installed in a non-default prefix, the path to the CMake Config file can be set using `CMAKE_PREFIX_-PATH`. In that case, the CMake configure step won't populate the previously mentioned variables. It is still possible to set `KLU_INCLUDE_DIR` and `KLU_LIBRARY_DIR` which take precedence over a potentially installed CMake import target file.

In either case, a CMake target `SUNDIALS::KLU` will be created if the KLU library could be found. Dependent targets should link to that target.

SUNDIALS has been tested with SuiteSparse version 5.10.1.

2.4.5 Building with SuperLU_DIST

SuperLU_DIST is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations in a distributed memory setting. The library is developed by Lawrence Berkeley National Laboratory and is available from the SuperLU_DIST GitHub repository.

To enable SuperLU_DIST, set *`ENABLE_SUPERLUDIST`* to `ON`, set *`SUPERLUDIST_DIR`* to the path where SuperLU_DIST is installed. If SuperLU_DIST was built with OpenMP then the option *`SUPERLUDIST_OpenMP`* and *`ENABLE_OPENMP`* should be set to `ON`.

SUNDIALS supports SuperLU_DIST v7.0.0 – v8.x.x and has been tested with v7.2.0 and v8.1.0.

2.4.6 Building with SuperLU_MT

SuperLU_MT is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations on shared memory parallel machines. The library is developed by Lawrence Berkeley National Laboratory and is available from the SuperLU_MT GitHub repository.

To enable SuperLU_MT, set `ENABLE_SUPERLUMT` 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_LIBRARIES` must be set to a semi-colon separated list of other libraries SuperLU_MT depends on. For example, if SuperLU_MT was build with an external blas library, then include the full path to the blas library in this list. Additionally, 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 `ENABLE_OPENMP` or `ENABLE_PTHREAD` set to `ON` then SuperLU_MT should be set to use the same threading type.

SUNDIALS has been tested with SuperLU_MT version 3.1.

2.4.7 Building with PETSc

The Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of data structures and routines for simulating applications modeled by partial differential equations. The library is developed by Argonne National Laboratory and is available from the PETSc GitLab repository.

To enable PETSc, set `ENABLE_PETSC` to `ON`, and set `PETSC_DIR` to the path of the PETSc installation. Alternatively, a user can provide a list of include paths in `PETSC_INCLUDES` and a list of complete paths to the PETSc libraries in `PETSC_LIBRARIES`.

SUNDIALS is regularly tested with the latest PETSc versions, specifically up to version 3.18.1 as of SUNDIALS version v7.2.1. SUNDIALS requires PETSc 3.5.0 or newer.

2.4.8 Building with *hypre*

hypre is a library of high performance preconditioners and solvers featuring multigrid methods for the solution of large, sparse linear systems of equations on massively parallel computers. The library is developed by Lawrence Livermore National Laboratory and is available from the hypre GitHub repository.

To enable *hypre*, set `ENABLE_HYPRE` 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.

Note

SUNDIALS must be configured so that `SUNDIALS_INDEX_SIZE` is compatible with `HYPRE_BigInt` in the *hypre* installation.

SUNDIALS is regularly tested with the latest versions of *hypre*, specifically up to version 2.26.0 as of SUNDIALS version v7.2.1.

2.4.9 Building with MAGMA

The Matrix Algebra on GPU and Multicore Architectures (MAGMA) project provides a dense linear algebra library similar to LAPACK but targeting heterogeneous architectures. The library is developed by the University of Tennessee and is available from the UTK webpage.

To enable the SUNDIALS MAGMA interface set `ENABLE_MAGMA` to `ON`, `MAGMA_DIR` to the MAGMA installation path, and `SUNDIALS_MAGMA_BACKENDS` to the desired MAGMA backend to use with SUNDIALS e.g., `CUDA` or `HIP`.

SUNDIALS has been tested with MAGMA version v2.6.1 and v2.6.2.

2.4.10 Building with oneMKL for SYCL

The Intel oneAPI Math Kernel Library (oneMKL) includes CPU and SYCL/DPC++ interfaces for LAPACK dense linear algebra routines. The SUNDIALS oneMKL interface targets the SYCL/DPC++ routines, to utilize the CPU routine see §2.4.3.

To enable the SUNDIALS oneMKL interface set `ENABLE_ONEMKL` to `ON` and `ONEMKL_DIR` to the oneMKL installation path.

SUNDIALS has been tested with oneMKL version 2021.4.

2.4.11 Building with CUDA

The NVIDIA CUDA Toolkit provides a development environment for GPU-accelerated computing with NVIDIA GPUs. The CUDA Toolkit and compatible NVIDIA drivers are available from the NVIDIA developer website.

To enable CUDA, set `ENABLE_CUDA` 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`.

SUNDIALS has been tested with the CUDA toolkit versions 10 and 11.

2.4.12 Building with HIP

HIP(heterogeneous-compute interface for portability) allows developers to create portable applications for AMD and NVIDIA GPUs. HIP can be obtained from HIP GitHub repository.

To enable HIP, set `ENABLE_HIP` to `ON` and set `AMDGPU_TARGETS` to the desired target(ex. gfx705). In addition, set `CMAKE_C_COMPILER` and `CMAKE_CXX_COMPILER` to point to an installation of `hipcc`.

SUNDIALS has been tested with HIP versions between 5.0.0 to 5.4.3.

2.4.13 Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from the RAJA GitHub repository.

Building SUNDIALS RAJA modules requires a CUDA, HIP, or SYCL enabled RAJA installation. To enable RAJA, set `ENABLE_RAJA` to `ON`, set `SUNDIALS_RAJA_BACKENDS` to the desired backend (`CUDA`, `HIP`, or `SYCL`), and set `ENABLE_CUDA`, `ENABLE_HIP`, or `ENABLE_SYCL` to `ON` depending on the selected backend. 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_CXX` to `ON`.

SUNDIALS has been tested with RAJA version 0.14.0.

2.4.14 Building with XBraid

XBraid is parallel-in-time library implementing an optimal-scaling multigrid reduction in time (MGRIT) solver. The library is developed by Lawrence Livermore National Laboratory and is available from the XBraid GitHub repository.

To enable XBraid support, set `ENABLE_XBRAID` to `ON`, set `XBRAID_DIR` to the root install location of XBraid or the location of the clone of the XBraid repository.

Note

At this time the XBraid types `braid_Int` and `braid_Real` are hard-coded to `int` and `double` respectively. As such SUNDIALS must be configured with `SUNDIALS_INDEX_SIZE` set to `32` and `SUNDIALS_PRECISION` set to `double`. Additionally, SUNDIALS must be configured with `ENABLE_MPI` set to `ON`.

SUNDIALS has been tested with XBraid version 3.0.0.

2.4.15 Building with Trilinos

Trilinos is a collection of C++ libraries of linear solvers, non-linear solvers, optimization solvers, etc. To enable the SUNDIALS interface to the Trilinos Tpetra vector, set the *ENABLE_TRILINOS* to `ON` and provide the path to the root of the Trilinos installation in *Trilinos_DIR*.

```
% cmake \
> -DENABLE_TRILONOS=ON \
> -DTRILINOS_DIR=/path/to/ginkgo/installation \
> /home/myname/sundials/srcdir
```

2.5 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
```

2.6 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` or `cmake-gui` 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.

2.7 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.

2.8 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 the table below. The file extension `.LIB` is typically `.so` for shared libraries and `.a` for static libraries. Note that, in this table names are relative to `LIBDIR` for libraries and to `INCLUDEDIR` for header files.

Warning

SUNDIALS installs some header files to `INSTDIR/include/sundials/priv`. All of the header files in this directory are private and **should not be included in user code**. The private headers are subject to change without any notice and relying on them may break your code.

2.9 Using SUNDIALS in your project

After building and installing SUNDIALS, using SUNDIALS in your application involves two steps: including the right header files and linking to the right libraries.

Depending on what features of SUNDIALS that your application uses, the header files needed will vary. For example, if you want to use CVODE for serial computations you need the following includes:

```
#include <cvode/cvode.h>
#include <nvector/nvector_serial.h>
```

If you wanted to use CVODE with the GMRES linear solver and our CUDA enabled vector:

```
#include <cvode/cvode.h>
#include <nvector/nvector_cuda.h>
#include <sunlinsol/sunlinsol_spgmr.h>
```

The story is similar for linking to SUNDIALS. Starting in v7.0.0, all applications will need to link to `libsundials_core`. Furthermore, depending on the packages and modules of SUNDIALS of interest an application will need to link to a few more libraries. Using the same examples as for the includes, we would need to also link to `libsundials_cvode`, `libsundials_nvecserial` for the first example and `libsundials_cvode`, `libsundials_nveccuda`, `libsundials_sunlinsolspgmr` for the second.

Refer to the documentations sections for the individual packages and modules of SUNDIALS that interest you for the proper includes and libraries to link to.

Furthermore, each of the sundials solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set both `EXAMPLES_ENABLE_<lang>` and *`EXAMPLES_INSTALL`* to `ON` and specify the example installation directory *`EXAMPLES_INSTALL_PATH`*. CMake will generate a `CMakeLists.txt` configuration file (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`.

2.10 Using SUNDIALS as a Third Party Library in other CMake Projects

The `make install` command will also install a CMake package configuration file that other CMake projects can load to get all the information needed to build against SUNDIALS. In the consuming project's CMake code, the `find_package` command may be used to search for the configuration file, which will be installed to `instdir/SUNDIALS_INSTALL_CMAKEDIR/SUNDIALSConfig.cmake` alongside a package version file `instdir/SUNDIALS_INSTALL_CMAKEDIR/SUNDIALSConfigVersion.cmake`. Together these files contain all the information the consuming project needs to use SUNDIALS, including exported CMake targets. The SUNDIALS exported CMake targets follow the same naming convention as the generated library binaries, e.g. the exported target for CVODE is `SUNDIALS::cvode`. The CMake code snipped below shows how a consuming project might leverage the SUNDIALS package configuration file to build against SUNDIALS in their own CMake project.

```
project(MyProject)

# Set the variable SUNDIALS_DIR to the SUNDIALS instdir.
# When using the cmake CLI command, this can be done like so:
#   cmake -D SUNDIALS_DIR=/path/to/sundials/installation
```

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```
# Find any SUNDIALS version...
find_package(SUNDIALS REQUIRED)

# ... or find any version newer than some minimum...
find_package(SUNDIALS 7.1.0 REQUIRED)

# ... or find a version in a range
find_package(SUNDIALS 7.0.0...7.1.0 REQUIRED)

add_executable(myexec main.c)

# Link to SUNDIALS libraries through the exported targets.
# This is just an example, users should link to the targets appropriate
# for their use case.
target_link_libraries(myexec PUBLIC SUNDIALS::cvode SUNDIALS::nvecpetsc)
```

Note

Changed in version 7.1.0: A single version provided to `find_package` denotes the minimum version of SUNDIALS to look for, and any version equal or newer than what is specified will match. In prior versions `SUNDIALSConfig.cmake` required the version found to have the same major version number as the single version provided to `find_package`.

2.11 Table of SUNDIALS libraries and header files

Table 2.1: SUNDIALS shared libraries and header files

Core	Libraries	`libsundials_core.LIB`
	Headers	`sundials/sundials_band.h`
		`sundials/sundials_config.h`
		`sundials/sundials_context.h`
		`sundials/sundials_cuda_policies.hpp`
		`sundials/sundials_dense.h`
		`sundials/sundials_direct.h`
		`sundials/sundials_hip_policies.hpp`
		`sundials/sundials_iterative.h`
		`sundials/sundials_linearsolver.h`
		`sundials/sundials_math.h`
		`sundials/sundials_matrix.h`
		`sundials/sundials_memory.h`
		`sundials/sundials_mpi_types.h`
		`sundials/sundials_nonlinearsolver.h`
		`sundials/sundials_nvector.h`
		`sundials/sundials_types.h`
		`sundials/sundials_version.h`
		`sundials/sundials_xbraid.h`
NVECTOR Modules		

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SERIAL	Libraries	`libsundials_nvecserial.LIB`
	Headers	`nvector/nvector_serial.h`
PARALLEL	Libraries	`libsundials_nvecparallel.LIB`
	Headers	`nvector/nvector_parallel.h`
OPENMP	Libraries	`libsundials_nvecopenmp.LIB`
	Headers	`nvector/nvector_openmp.h`
PTHREADS	Libraries	`libsundials_nvecpthreads.LIB`
	Headers	`nvector/nvector_pthreads.h`
PARHYP	Libraries	`libsundials_nvecparhyp.LIB`
	Headers	`nvector/nvector_parhyp.h`
PETSC	Libraries	`libsundials_nvecpetsc.LIB`
	Headers	`nvector/nvector_petsc.h`
CUDA	Libraries	`libsundials_nveccuda.LIB`
	Headers	`nvector/nvector_cuda.h`
HIP	Libraries	`libsundials_nvechip.LIB`
	Headers	`nvector/nvector_hip.h`
RAJA	Libraries	`libsundials_nveccudaraja.LIB`
		`libsundials_nvechipraja.LIB`
	Headers	`nvector/nvector_raja.h`
SYCL	Libraries	`libsundials_nvecsycl.LIB`
	Headers	`nvector/nvector_sycl.h`
MANYVECTOR	Libraries	`libsundials_nvecmanyvector.LIB`
	Headers	`nvector/nvector_manyvector.h`
MPIMANYVECTOR	Libraries	`libsundials_nvecmpimanyvector.LIB`
	Headers	`nvector/nvector_mpimanyvector.h`
MPIPLUSX	Libraries	`libsundials_nvecmpiplusx.LIB`
	Headers	`nvector/nvector_mpiplusx.h`
SUNMATRIX Modules		
BAND	Libraries	`libsundials_sunmatrixband.LIB`
	Headers	`sunmatrix/sunmatrix_band.h`
CUSPARSE	Libraries	`libsundials_sunmatrixcusparse.LIB`
	Headers	`sunmatrix/sunmatrix_cusparse.h`
DENSE	Libraries	`libsundials_sunmatrixdense.LIB`
	Headers	`sunmatrix/sunmatrix_dense.h`
Ginkgo	Headers	`sunmatrix/sunmatrix_ginkgo.hpp`
MAGMADENSE	Libraries	`libsundials_sunmatrixmagmadense.LIB`
	Headers	`sunmatrix/sunmatrix_magmadense.h`
ONEMKLDENSE	Libraries	`libsundials_sunmatrixonemkldense.LIB`
	Headers	`sunmatrix/sunmatrix_onemkldense.h`
SPARSE	Libraries	`libsundials_sunmatrixsparse.LIB`
	Headers	`sunmatrix/sunmatrix_sparse.h`
SLUNRLOC	Libraries	`libsundials_sunmatrixslunrloc.LIB`
	Headers	`sunmatrix/sunmatrix_slunrloc.h`
SUNLINSOL Modules		
BAND	Libraries	`libsundials_sunlinsolband.LIB`
	Headers	`sunlinsol/sunlinsol_band.h`
CUSOLVERSP_BATCHQR	Libraries	`libsundials_sunlinsolcusolversp.LIB`
	Headers	`sunlinsol/sunlinsol_cusolversp_batchqr.h`
DENSE	Libraries	`libsundials_sunlinsoldense.LIB`
	Headers	`sunlinsol/sunlinsol_dense.h`
Ginkgo	Headers	`sunlinsol/sunlinsol_ginkgo.hpp`

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KLU	Libraries	`libsundials_sunlinsolklu.LIB`
	Headers	`sunlinsol/sunlinsol_klu.h`
LAPACKBAND	Libraries	`libsundials_sunlinsollapackband.LIB`
	Headers	`sunlinsol/sunlinsol_lapackband.h`
LAPACKDENSE	Libraries	`libsundials_sunlinsollapackdense.LIB`
	Headers	`sunlinsol/sunlinsol_lapackdense.h`
MAGMADENSE	Libraries	`libsundials_sunlinsolmagmadense.LIB`
	Headers	`sunlinsol/sunlinsol_magmadense.h`
ONEMKLDENSE	Libraries	`libsundials_sunlinsolonemkldense.LIB`
	Headers	`sunlinsol/sunlinsol_onemkldense.h`
PCG	Libraries	`libsundials_sunlinsolpcg.LIB`
	Headers	`sunlinsol/sunlinsol_pcg.h`
SPBCGS	Libraries	`libsundials_sunlinsolspbcgs.LIB`
	Headers	`sunlinsol/sunlinsol_spbcgs.h`
SPFGMR	Libraries	`libsundials_sunlinsolspfgmr.LIB`
	Headers	`sunlinsol/sunlinsol_spfgmr.h`
SPGMR	Libraries	`libsundials_sunlinsolspgmr.LIB`
	Headers	`sunlinsol/sunlinsol_spgmr.h`
SPTFQMR	Libraries	`libsundials_sunlinsolsptfqmr.LIB`
	Headers	`sunlinsol/sunlinsol_sptfqmr.h`
SUPERLUDIST	Libraries	`libsundials_sunlinsolsuperludist.LIB`
	Headers	`sunlinsol/sunlinsol_superludist.h`
SUPERLUMT	Libraries	`libsundials_sunlinsolsuperlumt.LIB`
	Headers	`sunlinsol/sunlinsol_superlumt.h`
SUNNONLINSOL Modules		
NEWTON	Libraries	`libsundials_sunnonlinsolnewton.LIB`
	Headers	`sunnonlinsol/sunnonlinsol_newton.h`
FIXEDPOINT	Libraries	`libsundials_sunnonlinsolfixedpoint.LIB`
	Headers	`sunnonlinsol/sunnonlinsol_fixedpoint.h`
PETSCSNES	Libraries	`libsundials_sunnonlinsolpetscsnes.LIB`
	Headers	`sunnonlinsol/sunnonlinsol_petscsnes.h`
SUNMEMORY Modules		
SYSTEM	Libraries	`libsundials_sunmemsys.LIB`
	Headers	`sunmemory/sunmemory_system.h`
CUDA	Libraries	`libsundials_sunmemcuda.LIB`
	Headers	`sunmemory/sunmemory_cuda.h`
HIP	Libraries	`libsundials_sunmemhip.LIB`
	Headers	`sunmemory/sunmemory_hip.h`
SYCL	Libraries	`libsundials_sunmemsycl.LIB`
	Headers	`sunmemory/sunmemory_sycl.h`
SUNDIALS Packages		
CVODE	Libraries	`libsundials_cvode.LIB`
	Headers	`cvode/cvode.h`
		`cvode/cvode_bandpre.h`
		`cvode/cvode_bbdpre.h`
		`cvode/cvode_diag.h`
		`cvode/cvode_impl.h`
		`cvode/cvode_ls.h`
		`cvode/cvode_proj.h`
CVODES	Libraries	`libsundials_cvodes.LIB`
	Headers	`cvodes/cvodes.h`

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		cvodes/cvodes_bandpre.h
		cvodes/cvodes_bbdpre.h
		cvodes/cvodes_diag.h
		cvodes/cvodes_impl.h
		cvodes/cvodes_ls.h
ARKODE	Libraries	libsundials_arkode.LIB
		libsundials_xbraid.LIB
	Headers	arkode/arkode.h
		arkode/arkode_arkstep.h
		arkode/arkode_bandpre.h
		arkode/arkode_bbdpre.h
		arkode/arkode_butcher.h
		arkode/arkode_butcher_dirk.h
		arkode/arkode_butcher_erk.h
		arkode/arkode_erkstep.h
		arkode/arkode_impl.h
		arkode/arkode_ls.h
		arkode/arkode_mristep.h
		arkode/arkode_xbraid.h
IDA	Libraries	libsundials_ida.LIB
	Headers	ida/ida.h
		ida/ida_bbdpre.h
		ida/ida_impl.h
		ida/ida_ls.h
IDAS	Libraries	libsundials_idas.LIB
	Headers	idas/idas.h
		idas/idas_bbdpre.h
		idas/idas_impl.h
KINSOL	Libraries	libsundials_kinsol.LIB
	Headers	kinsol/kinsol.h
		kinsol/kinsol_bbdpre.h
		kinsol/kinsol_impl.h
		kinsol/kinsol_ls.h

2.12 Installing SUNDIALS on HPC Clusters

This section is a guide for installing SUNDIALS on specific HPC clusters. In general, the procedure is the same as described previously for Linux machines. The main differences are in the modules and environment variables that are specific to different HPC clusters. We aim to keep this section as up to date as possible, but it may lag the latest software updates to each cluster.

2.12.1 Frontier

Frontier is an Exascale supercomputer at the Oak Ridge Leadership Computing Facility. If you are new to this system, then we recommend that you review the Frontier user guide.

A Standard Installation

Clone SUNDIALS:

```
git clone https://github.com/LLNL/sundials.git && cd sundials
```

Next we load the modules and set the environment variables needed to build SUNDIALS. This configuration enables both MPI and HIP support for distributed and GPU parallelism. It uses the HIP compiler for C and C++ and the Cray Fortran compiler. Other configurations are possible.

```
# required dependencies
module load PrgEnv-cray-amd/8.5.0
module load craype-accel-amd-gfx90a
module load rocm/5.3.0
module load cmake/3.23.2

# GPU-aware MPI
export MPICH_GPU_SUPPORT_ENABLED=1

# compiler environment hints
export CC=$(which hipcc)
export CXX=$(which hipcc)
export FC=$(which ftn)
export CFLAGS="-I${ROCM_PATH}/include"
export CXXFLAGS="-I${ROCM_PATH}/include -Wno-pass-failed"
export LDFLAGS="-L${ROCM_PATH}/lib -lamdhip64 ${PE_MPICH_GTL_DIR_amd_gfx90a} -lmpi_gtl_hsa"
```

Now we can build SUNDIALS. In general, this is the same procedure described in the previous sections. The following command builds and installs SUNDIALS with MPI, HIP, and the Fortran interface enabled, where <*install path*> is your desired installation location, and <*account*> is your allocation account on Frontier:

```
cmake -S . -B builddir -DCMAKE_INSTALL_PREFIX=<install path> -DAMDGPU_TARGETS=gfx90a \
-DENABLE_HIP=ON -DENABLE_MPI=ON -DBUILD_FORTRAN_MODULE_INTERFACE=ON
cd builddir
make -j8 install
# Need an allocation to run the tests:
salloc -A <account> -t 10 -N 1 -p batch
make test
make test_install_all
```

2.13 Building with SUNDIALS Addons

SUNDIALS "addons" are community developed code additions for SUNDIALS that can be subsumed by the SUNDIALS build system so that they have full access to all internal SUNDIALS symbols. The intent is for SUNDIALS addons to function as if they are part of the SUNDIALS library, while allowing them to potentially have different licenses (although we encourage BSD-3-Clause still), code style (although we encourage them to follow the SUNDIALS style outlined here).

Warning

SUNDIALS addons are not maintained by the SUNDIALS team and may come with different licenses. Use them at your own risk.

To build with SUNDIALS addons,

1. Clone/copy the addon(s) into `<sundials root>/external/`
2. Copy the `sundials-addon-example` block in the `<sundials root>/external/CMakeLists.txt`, paste it below the example block, and modify the path listed for your own external addon(s).
3. When building SUNDIALS, set the CMake option *`SUNDIALS_ENABLE_EXTERNAL_ADDONS`* to *ON*
4. Build SUNDIALS as usual.

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