Installation Guide for SUNDIALS v5.6.1

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CONTRIBUTORS

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Chapter 1

SUNDIALS Package Installation Procedure

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

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

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

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

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

• The remainder of this chapter will follow these conventions:

solverdir is the directory solver-x.y.z created above; i.e., the directory containing the SUNDI-ALS sources.

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

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

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



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

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

1.1 CMake-based installation

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

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

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

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

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

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

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

Building with the GUI

Using CMake with the GUI follows this general process:

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

- For file and directories, the <tab> key can be used to complete
- Repeat until all values are set as desired and the generate option is available (g key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (t key)
- To search for a variable press / key, and to repeat the search, press the n key

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

% ccmake ../solverdir

The default configuration screen is shown in Figure 1.1.

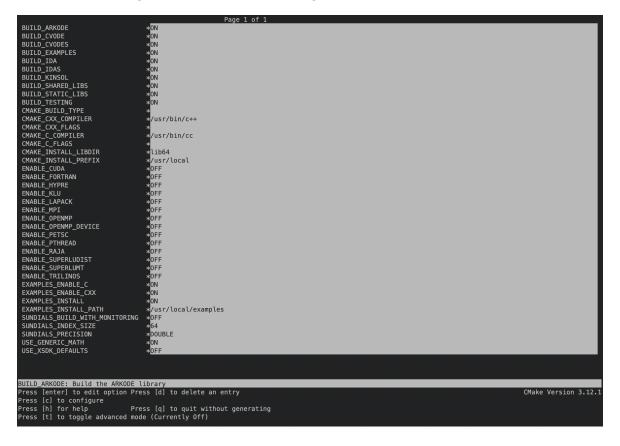


Figure 1.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the CMAKE_INSTALL_PREFIX and the EXAMPLES_INSTALL_PATH as shown in figure 1.2.

Pressing the (g key) will generate makefiles including all dependencies and all rules to build 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

```
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BUILD_CVODE
BUILD_CVODES
 BUILD EXAMPLES
 BUILD_IDA
BUILD_IDAS
 BUILD_KINSOL
BUILD_SHARED_LIBS
BUILD_STATIC_LIBS
 CMAKE_CXX_COMPILER
CMAKE_CXX_FLAGS
CMAKE_C_COMPILER
                                                                 */usr/bin/c++
                                                                   /usr/bin/cc
 CMAKE_C_FLAGS
CMAKE_INSTALL_LIBDIR
CMAKE_INSTALL_PREFIX
                                                                  /usr/casc/sundials/instdir
OFF
 ENABLE CUDA
 ENABLE_FORTRAN
ENABLE_HYPRE
 ENABLE_KLU
ENABLE_LAPACK
ENABLE_MPI
 ENABLE_OPENMP
ENABLE_OPENMP_DEVICE
ENABLE_PETSC
 ENABLE_PTHREAD
ENABLE_RAJA
ENABLE_SUPERLUDIST
ENABLE_SUPERLUDIST
ENABLE_SUPERLUMT
ENABLE_TRILINOS
EXAMPLES_ENABLE_C
EXAMPLES_ENABLE_CXX
EXAMPLES_INSTALL
EXAMPLES_INSTALL
                                                               */usr/casc/sundials/instdir/examples
*OFF
*64
 SUNDIALS_BUILD_WITH_MONITORING
SUNDIALS_INDEX_SIZE
 SUNDIALS PRECISION
                                                                   DOUBL F
 USE_XSDK_DEFAULTS
EXAMPLES_INSTALL_PATH: Output directory for installing example files
Press [enter] to edit option Press [d] to delete an entry
 ress [c] to configure
ress [h] for help Press [q] to quit without generating
ress [t] to toggle advanced mode (Currently Off)
```

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

Building from the command line

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

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

```
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.

 ${\tt CMAKE_CXX_FLAGS}$ - 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 LAPACK support is enabled (ENABLE_LAPACK 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

ENABLE_CUDA - Build the SUNDIALS CUDA modules.

Default: OFF

CUDA_ARCH - Specifies the CUDA architecture to compile for.

Default: sm_30

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 unless ENABLE TRILINGS is ON.

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples

Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90 examples

Default: ON (if F77_INTERFACE_ENABLE is ON)

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.

F77_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 77 interfaces

Default: OFF

BUILD_FORTRAN_MODULE_INTERFACE - Enable Fortran-C support via the Fortran 2003 interfaces

Default: OFF

ENABLE_HYPRE - 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

ENABLE_KLU - 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

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 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.

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:

 ${\tt MPI_CXX_COMPILER\ -\ mpicxx\ program}$

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 - mpif77 or mpif90 program

Default:

Note: This option is triggered only if MPI is enabled (ENABLE_MPI is ON) and Fortran-C support is enabled (F77_INTERFACE_ENABLE or BUILD_FORTRAN_MODULE_INTERFACE 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).

ENABLE_OPENMP - 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

OPENMP_DEVICE_WORKS - advanced option - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.

Default: OFF

ENABLE_PETSC - Enable PETSc support

Default: OFF

Note: See additional information on building with PETSc enabled in ??.

PETSC_DIR - Path to PETSc installation

Default:

PETSC_LIBRARIES - advanced option - 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:

PETSC_INCLUDES - advanced option - 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:

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 and HIP.

Default: CUDA

ENABLE_SUPERLUDIST - Enable SuperLU_DIST support

Default: OFF

Note: See additional information on building with SuperLU_DIST enabled in 1.1.4.

SUPERLUDIST_INCLUDE_DIR - Path to SuperLU_DIST header files (typically SRC directory)

SUPERLUDIST_LIBRARY_DIR - Path to SuperLU_DIST installed library files

SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST

SUPERLUDIST_OpenMP - Enable SUNDIALS support for SuperLU_DIST built with OpenMP

Default: OFF

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

ENABLE_SUPERLUMT - Enable SUPERLUMT support

Default: OFF

Note: See additional information on building with SUPERLUMT 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_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_MT

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP

Default: Pthread

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

Default: OFF

Trilinos_DIR - Path to the Trilinos install directory.

Default:

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

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

CMAKE_C_COMPILER or MPI_C_COMPILER if USE_XSDK_DEFAULTS=ON.

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

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

Default: The C compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=0FF.

CMAKE_C_FLAGS if USE_XSDK_DEFAULTS=ON.

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

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

 $Default: \ The \ C^{++} \ compiler \ exported \ from \ the \ found \ Trilinos \ installation \ if \ USE_XSDK_DEFAULTS=OFF.$

CMAKE_CXX_COMPILER or MPI_CXX_COMPILER if USE_XSDK_DEFAULTS=ON.

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

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

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

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

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

Default: OFF

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

SUNDIALS_BUILD_PACKAGE_FUSED_KERNELS - Build specialized fused kernels inside CVODE.

Default: OFF

Note: This option is currently only available when building with CUDA_ENABLE = ON. Building with fused kernels requires linking to either libsundials_cvode_fused_cuda. lib or libsundials_cvode_fused_stud where the latter provides CPU-only placeholders for the fused routines, in addition to libsundials_cvode. lib.

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

Default: 11

Note: Options are 99, 11, 14, 17. This option only used when a C++ compiler is required.

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.

 ${\tt SUNDIALS_INDEX_TYPE-advanced\ option-Integer\ type\ used\ for\ SUNDIALS\ indices.}\ The\ size\ must}$ 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

SUNDIALS_INSTALL_CMAKEDIR - Installation directory for the SUNDIALS cmake files (relative to CMAKE_INSTALL_PREFIX).

Default: CMAKE_INSTALL_PREFIX/cmake/sundials

 $\begin{tabular}{ll} {\tt USE_GENERIC_MATH~-Use~generic~(stdc)~math~libraries} \\ {\tt Default:~ON} \end{tabular}$

USE_XSDK_DEFAULTS - Enable xSDK (see 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

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 mpic and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DENABLE_MPI=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 \
> -DENABLE_MPI=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 any external libraries used with SUNDIALS must also be build as a shared library or as a static library compiled with the -fPIC flag.



Building with LAPACK

To enable LAPACK, set the ENABLE_LAPACK 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 rquired for LAPACK.

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

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 5.7.2. 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. The CMake configure will result in populating the following variables: AMD_LIBRARY, AMD_LIBRARY_DIR, BTF_LIBRARY_DIR, COLAMD_LIBRARY, COLAMD_LIBRARY_DIR, and KLU_LIBRARY.

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt. SUNDIALS has been

tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set 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 ws 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.

Building with SuperLU_DIST

The SuperLU_DIST libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_dist. SUNDIALS has been tested with SuperLU_DIST 6.1.1. To enable SuperLU_DIST, set ENABLE_SUPERLUDIST to ON, set SUPERLUDIST_INCLUDE_DIR to the include directory of the SuperLU_DIST installation (typically SRC), and set the variable

SUPERLUDIST_LIBRARY_DIR to the path to library directory of the SuperLU_DIST installation (typically lib). At the same time, the variable SUPERLUDIST_LIBRARIES must be set to a semi-colon separated list of other libraries SuperLU_DIST depends on. For example, if SuperLU_DIST was built with LAPACK, then include the LAPACK library in this list. If SuperLU_DIST was built with OpenMP support, then you may set SUPERLUDIST_OPENMP to ON to utilize the OpenMP functionality of SuperLU_DIST.



Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having ENABLE_PTHREAD set to ON then SuperLU_DIST should not be set to use OpenMP.

Building with PETSc

The PETSC libraries are available for download from the Argonne National Laboratory website: http://www.mcs.anl.gov/SUNDIALS has been tested with PETSC version 3.10.0-3.14.0. To enable PETSC, set ENABLE_PETSC to ON and then 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 libraries needed in PETSC_LIBRARIES.

Building with hypre

The hypre libraries are available for download from the Lawrence Livermore National Laboratory website: http://computing.llnl.gov/projects/hypre. SUNDIALS has been tested with hypre version 2.14.0-2.19.0. 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 (or equivalently, XSDK_INDEX_SIZE) equals the precision of HYPRE_BigInt in the corresponding hypre installation.

Building with CUDA

SUNDIALS CUDA modules and examples have been tested with versions 9 through 11.0.2 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 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.

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 up to version 0.12.1. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set ENABLE_CUDA and ENABLE_RAJA to ON. If RAJA is installed in a nonstandard location you will be prompted to set the variable RAJA_DIR with the path to the RAJA CMake configuration file. To enable building the RAJA examples set EXAMPLES_ENABLE_CUDA to ON.

Building with Trilinos

Trilinos is a suite of numerical libraries developed by Sandia National Laboratories. It can be obtained at https://github.com/trilinos/Trilinos. SUNDIALS Trilinos modules and examples have been tested with Trilinos version 12.14.1 – 12.18.1. To enable Trilinos, set ENABLE_TRILINOS to ON. If Trilinos is installed in a nonstandard location you will be prompted to set the variable Trilinos_DIR with the path to the Trilinos CMake configuration file. It is desireable to build the Trilinos vector interface with same compiler and options that were used to build Trilinos. CMake will try to find the correct compiler settings automatically from the Trilinos configuration file. If that is not successful, the compilers and options can be manually set with the following CMake variables:

- Trilinos_INTERFACE_C_COMPILER
- Trilinos_INTERFACE_C_COMPILER_FLAGS
- Trilinos_INTERFACE_CXX_COMPILER
- Trilinos_INTERFACE_CXX_COMPILER_FLAGS

1.1.5 Testing the build and installation

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

% make test

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

% make test_install

1.2 Building and Running Examples

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

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

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



1.3 Configuring, building, and installing on Windows

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

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

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

1.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

% make install

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

The installed libraries and exported header files are listed for reference in Table 1.1. The file extension .lib is typically .so for shared libraries and .a for static libraries. Note that, in the Tables, names are relative to 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 <code>includedir/include/sundials</code> directory since they are explicitly included by the appropriate solver header files (e.g., <code>cvode_dense.h</code> includes <code>sundials_dense.h</code>). However, it is both legal and safe to do so, and would be useful, for example, if the functions declared in <code>sundials_dense.h</code> are to be used in building a preconditioner.

1.4.1 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.

```
# 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

find_project(SUNDIALS 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)
```

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
		sundials/sundials_cuda_policies.hpp
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.lib
		libsundials_fnvecserial_mod. lib
		libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module	fnvector_serial_mod.mod
	files	
NVECTOR_PARALLEL	Libraries	$libsundials_nvecparallel. lib$
		libsundials_fnvecparallel.a

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NVECTOR_MPIPLUSX	Libraries	libsundials_nvecmpiplusx.lib	
	TT 1 C1	libsundials_nvecmpiplusx_mod.lib	
	Header files	nvector/nvector_mpiplusx.h	
	Module	fnvector_mpiplusx_mod.mod	
	files	101 10 1 17	
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.lib	
		libsundials_fnvecopenmp_mod.lib	
	II 1 C1	libsundials_fnvecopenmp.a	
	Header files	nvector/nvector_openmp.h	
	Module files	fnvector_openmp_mod.mod	
NIVECTOR OPENADDEN	Libraries	libaun diala museen en man dess lib	
NVECTOR_OPENMPDEV	Header files	libsundials_nvecopenmpdev.lib	
NULCEON DELINEADS	Libraries	nvector/nvector_openmpdev.h	
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.lib	
		libsundials_fnvecpthreads_mod.lib	
	Header files	libsundials_fnvecpthreads.a nvector/nvector_pthreads.h	
	Module	fnvector_pthreads_mod.mod	
	files	mvector_ptnreads_mod.mod	
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp.lib	
	Header files	nvector/nvector_parhyp.h	
NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.lib	
	Header files	nvector/nvector_petsc.h	
NVECTOR_CUDA	Libraries	libsundials_nveccuda.lib	
	Header files	nvector/nvector_cuda.h	
NVECTOR_RAJA	Libraries	libsundials_nveccudaraja.lib	
		libsundials_nvechipraja.lib	
	Header files	nvector/nvector_raja.h	
NVECTOR_TRILINOS	Libraries	libsundials_nvectrilinos.lib	
	Header files	nvector/nvector_trilinos.h	
		nvector/trilinos/SundialsTpetraVectorInterface.hpp	
		nvector/trilinos/SundialsTpetraVectorKernels.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	
S STANTITUMED DINGE	11.51.00100	libsundials_fsunmatrixdense_mod.lib	
		libsundials_fsunmatrixdense.a	
	Header files	sunmatrix/sunmatrix_dense.h	
	11Cadel IIIes	continued on next page	

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	Module	fsunmatrix_dense_mod.mod
	files	
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse.lib
		libsundials_fsunmatrixsparse_mod.lib
		libsundials_fsunmatrixsparse.a
	Header files	sunmatrix/sunmatrix_sparse.h
	Module	fsunmatrix_sparse_mod.mod
	files	•
SUNMATRIX_SLUNRLOC	Libraries	libsundials_sunmatrixslunrloc.lib
	Header files	sunmatrix/sunmatrix_slunrloc.h
SUNLINSOL_CUSPARSE	Libraries	libsundials_sunmatrixcusparse.lib
	Header files	sunmatrix/sunmatrix_cusparse.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.lib
		libsundials_fsunlinsolband_mod.lib
		libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module	fsunlinsol_band_mod.mod
	files	
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.lib
		$libsundials_fsunlinsoldense_mod. \it lib$
		libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	Module	fsunlinsol_dense_mod.mod
	files	
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.lib
		libsundials_fsunlinsolklu_mod. lib
		libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module	fsunlinsol_klu_mod.mod
	files	
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.lib
		libsundials_fsunlinsollapackband.a
	Header files	sunlinsol/sunlinsol_lapackband.h
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.lib
		libsundials_fsunlinsollapackdense.a
	Header files	sunlinsol/sunlinsol_lapackdense.h
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.lib
		libsundials_fsunlinsolpcg_mod. lib
		libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module	fsunlinsol_pcg_mod.mod
	files	
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SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.lib
		libsundials_fsunlinsolspbcgs_mod.lib
		libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module	fsunlinsol_spbcgs_mod.mod
	files	
SUNLINSOL_SPFGMR	Libraries	$libsundials_sunlinsolspfgmr. \\ lib$
		$libsundials_fsunlinsolspfgmr_mod.lib$
		libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module	fsunlinsol_spfgmr_mod.mod
	files	
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.lib
		libsundials_fsunlinsolspgmr_mod.lib
		libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module	fsunlinsol_spgmr_mod.mod
	files	
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.lib
		$lib sundials_f sunlins olsptf qmr_mod. \\ lib$
		libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
	Module	fsunlinsol_sptfqmr_mod.mod
	files	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.lib
		libsundials_fsunlinsolsuperlumt.a
	Header files	sunlinsol/sunlinsol_superlumt.h
SUNLINSOL_SUPERLUDIST	Libraries	$libsundials_sunlinsolsuperludist.lib$
	Header files	sunlinsol/sunlinsol_superludist.h
SUNLINSOL_CUSOLVERSP_BAT		$libsundials_sunlinsolcusolversp.lib$
	Header files	sunlinsol/sunlinsol_cusolverp_batchqr.h
SUNNONLINSOL_NEWTON	Libraries	$lib sundials_sunnon linsol newton. \it lib$
		$lib sundials_f sunnon lins olnewton_mod. \\ lib$
		libsundials_fsunnonlinsolnewton.a
	Header files	sunnonlinsol/sunnonlinsol_newton.h
	Module	fsunnonlinsol_newton_mod.mod
	files	
SUNNONLINSOL_FIXEDPOINT	Libraries	$lib sundials_sunnon lins of fixed point. \it lib$
		$lib sundials_f sunnon lins of fixed point. a$
		$libsundials_fsunnonlinsolfixed point_mod. lib$
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h
	Module	fsunnonlinsol_fixedpoint_mod.mod
	files	
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	Header files	sunnonlinsol/sunnonlinsol_petscsnes.h		
CVODE	Libraries	libsundials_cvode.lib		
		libsundials_fcvode.a		
		libsundials_fcvode_mod.lib		
	Header files	cvode/cvode.h cvode/cvode_impl.h		
		cvode/cvode_direct.h	cvode/cvode_ls.h	
		cvode/cvode_spils.h	cvode/cvode_bandpre.h	
		cvode/cvode_bbdpre.h	· · · · · · · · · · · · · · · · · · ·	
	Module	fcvode_mod.mod		
	files	10 10 40 1110 411110 4		
CVODES	Libraries	libsundials_cvodes.lib		
CVODES	Listaires	libsundials_fcvodes_mod.lib		
	Header files	cvodes/cvodes.h	cvodes/cvodes_impl.h	
	Treader mes	cvodes/cvodes_direct.h	cvodes/cvodes_ls.h	
		cvodes/cvodes_spils.h	cvodes/cvodes_bandpre.h	
		cvodes/cvodes_bbdpre.h	evodes/evodes_bandpre.n	
	Module	fcvodes_mod.mod		
	files	ic vodes_mod.mod		
ARKODE	Libraries	libsundials_arkode.lib		
ARRODE	Libraries	libsundials_farkode.a		
		libsundials_farkode_mod.lib		
	Header files	arkode/arkode.h	arkode/arkode_impl.h	
	licadei mes	arkode/arkode_ls.h	arkode/arkode_bandpre.h	
		arkode/arkode_bbdpre.h	arkode/arkode_bandpre.n	
	Module	farkode_mod.mod	farkode_arkstep_mod.mod	
	files	larkode_mod.mod	rarkode_arkstep_mod.mod	
	IIICS	farkode_erkstep_mod.mod	farkode_mristep_mod.mod	
IDA	Libraries	libsundials_ida.lib	iaino do imiliotop imo di imo	
15.1	Libraries	libsundials_fida.a		
		libsundials_fida_mod.lib		
	Header files	ida/ida.h	ida/ida_impl.h	
	1100000111100	ida/ida_direct.h	ida/ida_ls.h	
		ida/ida_spils.h	ida/ida_bbdpre.h	
	Module	fida_mod.mod	ida/ida_ssapiem	
	files			
IDAS	Libraries	libsundials_idas.lib		
	210101100	libsundials_fidas_mod.lib		
	Header files	idas/idas.h	idas/idas_impl.h	
		idas/idas_direct.h	idas/idas_ls.h	
		idas/idas_spils.h	idas/idas_bbdpre.h	
	Module	fidas_mod.mod	1440/14402004pittiii	
	files			
	11100		continued on next pag	

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KINSOL	Libraries	libsundials_kinsol.lib	
		libsundials_fkinsol.a	
		libsundials_fkinsol_mod. lib	
	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
	Module	fkinsol_mod.mod	
	files		