Installing SW4 version 2.0

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Contents

1	Introduction	1		
2	Compilers and third party libraries			
3	Unpacking the source code tar ball			
4	Installing $SW4$ with make4.1Basic compilation and linking of $SW4$ 4.1.1Mac machines4.1.2Linux machines4.1.3Using make4.1.4How do I setup the make.inc file?4.2Building $SW4$ with proj.4 and/or efile support4.3Testing the $SW4$ installation	5 6 7		
5	Installing SW4 with CMake 5.1 CMake Options 5.2 CTest			
6	Installing the proj.4, euclid, and cencalvm packages			
7	Disclaimer 1			

1 Introduction

The sole purpose of this document is to describe the installation process of the seismic wave propagation code SW4. A comprehensive user's guide is provided in the report by Petersson and Sjogreen [1].

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2 Compilers and third party libraries

Before you can build SW4 on your system, you must have

- 1. the lapack and blas libraries. These libraries provide basic linear algebra functionality and are pre-installed on many machines;
- 2. a MPI-2 library. This library provides support for message passing on parallel machines. Examples of open source implementations include Mpich-2 and OpenMPI. Note that the MPI-2 library must be installed even if you are only building SW4 for a single core system.

To avoid incompatibility issues and linking problems, we recommend using the same compiler for the libraries as for SW4.

In order to use geographic projection and material models stored in the rfile format, you need to install the Proj4 before building SW4:

• The Proj.4 library, http://trac.osgeo.org/proj

If you also wish to use material models using the *efile* format, you also need to download and install two additional libraries:

- The Euclid e-tree library, http://www-2.cs.cmu.edu/ euclid
- The cencalvm library, http://earthquake.usgs.gov/data/3dgeologic/cencalvm_doc/index.html

To simplify the build process, all libraries should be installed under the same directory, such that the library files (.so, .a, etc.) are in the lib sub-directory and the include files (.h) end up in the include sub-directory. See Section 6 for details.

Mac computers We recommend using the MacPorts package manager for installing the required compilers and libraries. Simply go to www.macports.org, and install macports on your system. With that in place, you can use the port command as follows

```
shell> sudo port install gcc72
shell> sudo port select --set gcc mp-gcc72
shell> sudo port install mpich-gcc7
shell> sudo port select --set mpi mpich-gcc7
```

Here, gcc72 refers to version 7.2 of the Gnu compiler suite. Compiler versions are bound to change in the future, so the above commands will need to be modified accordingly. Before starting, make sure you install a version of gcc that is compatible with the MPI library package. The above example installs the mpich package using the gcc72 compilers, which includes a compatible Fortran compiler. Alternatively, you can use the openmpi package. Note that the port select commands are used to create shortcuts to the compilers and MPI environment. By using the above setup, the Gnu compilers can be accessed with gcc and gfortran commands, and the MPI compilers and execution environment are called mpicxx, mpif90, and mpirun, respectively.

The lapack and blas libraries are preinstalled on recent Macs and can be accessed using the -framework Accelerate link option. If that is not available or does not work on your machine, you can download lapack and blas from www.netlib.org.

Linux machines We here give detailed instructions for installing the third part libraries under 64 bit, Fedora Core 18 Linux. Other Linux variants use similar commands for installing software packages, but note that the package manager yum is specific to Fedora Core.

You need to have root privileges to install precompiled packages. Start by opening an xterm and set your user identity to root by the command

```
su -
```

Install the compilers by issuing the commands

```
yum install gcc
yum install gcc-c++
yum install gcc-gfortran
```

You install the mpich2 library and include files with the command

```
yum install mpich2-devel
```

The executables and libraries are installed in /usr/lib64/mpich2/bin and /usr/lib64/mpich2/lib respectively. We suggest that you add /usr/lib64/mpich2/bin to your path. This is done with the command

```
export PATH=${PATH}:/usr/lib64/mpich2/bin
```

if your shell is bash. For tcsh users, the command is

```
setenv PATH ${PATH}:/usr/lib64/mpich2/bin
```

It is convenient to put the path setting command in your startup file, .bashrc or .cshrc., for bash or csh/tcsh respectively.

The blas and lapack libraries are installed with

```
yum install blas
yum install lapack
```

On our system, the libraries were installed in /usr/lib64 as libblas.so.3 and liblapack.so.3. For some unknown reason, the install program does not add links to these files with extension .so, which is necessary for the linker to find them. We must therefore add the links explicitly. If the libraries were installed elsewhere on your system, but you don't know where, you can find them with the following command:

```
find / -name "*blas*" -print
```

After locating the directory where the libraries reside (in this case /usr/lib64), we add links to the libraries with the commands:

```
cd /usr/lib64
ln -s libblas.so.3 libblas.so
ln -s liblapack.so.3 liblapack.so
```

Note that you need to have root privileges for this to work.

3 Unpacking the source code tar ball

To unpack the SW4 source code, you place the file sw4-v2.0.tgz in the desired directory and issue the following command:

```
shell> tar xzf sw4-v2.0.tgz
```

As a result a new sub-directory named sw4-v2.0 is created. It contains several files and sub-directories:

- LICENSE.txt License information.
- INSTALL.txt A link to this document.
- README.txt General information about SW4.
- configs Directory containing make configuration files.
- $\operatorname{src} C++$ and Fortran source code of SW4.
- tools Matlab/Octave scripts for post processing and analysis.
- pytest Python script and input files for testing the SW_4 installation.
- examples Sample input files.
- Makefile Main makefile (don't change this file!).
- CMakeLists.txt CMake configuration file (don't change this file either!).
- wave.txt Text for printing the "SW4 Lives" banner at the end of a successful build.

4 Installing SW4 with make

The classical way of building SW4 uses make. We recommend using GNU make, sometimes called gmake. You can check the version of make on you system with the command

```
shell> make -v
```

If you don't have GNU make installed on your system, you can obtain it from www.gnu.org.

We have built SW4 and its supporting libraries on Intel based laptops and desktops running LINUX and OSX. It has also been built on several supercomputers such as the Intel machines cab, quartz (at LLNL) and edison, cori (at LBNL), as well as the IBM BGQ machine vulcan at LLNL. We have successfully used the following versions of Gnu, Intel, and IBM compilers:

```
Gnu: g++/gcc/gfortran versions 4.5 to 7.2

Intel: icpc/icc/ifort versions 16.0 to 18.0

IBM Blue Gene: xlcxx/xlc/xlf versions 12.1 to 14.1
```

SW4 uses the message passing interface (MPI) standard (MPI-2 to be specific) for communication on parallel distributed memory machines. Note that the MPI library often includes wrappers for compiling, linking, and running of MPI programs. For example, the mpich2 package build wrappers for the underlying C++ and Fortran compilers called mpicxx and mpif90, as well as the mpirun script. We highly recommend using these programs for compiling, linking, and running SW4.

4.1 Basic compilation and linking of SW4

The best way of getting started is to first build SW4 without the proj.4 and cencalvm libraries. This process should be very straight forward and the resulting SW4 executable will support all commands except rfile, efile and the proj/ellps options in the grid command. If you need to use these options, you can always recompile SW4 after the proj.4 and cencalvm libraries have been installed. See § 6 for details.

The basic build process is controlled by the environmental variables FC, CXX, EXTRA_FORT_FLAGS, EXTRA_CXX_FLAGS, and EXTRA_LINK_FLAGS. These variables should hold the names of the Fortan and C++ compilers, and any extra options that should be passed to the compilers and linker. The easiest way of assigning these variables is by creating a file in the configs directory called make.inc. The Makefile will look for this file and read it if it is available. There are several examples in the configs directory, e.g. make.osx for Macs and make.linux for Linux machines. You should copy one of these files to your own make.inc and edit it as needed.

4.1.1 Mac machines

If you are on a Mac, you could copy the setup from make.osx,

```
shell> cd configs
shell> cp make.osx make.inc
shell> cat make.inc
etree = no
proj = no
FC = mpif90
CXX = mpicxx
EXTRA_FORT_FLAGS =
EXTRA_LINK_FLAGS = -framework Accelerate -L/opt/local/lib/gcc72 -lgfortran
```

In this case, the blas and lapack libraries are assumed to be provided by the -framework Accelerate option. The libgfortran library is located in the directory /opt/local/lib/gcc72, which is where macports currently installs it.

4.1.2 Linux machines

If you are on a Linux machine, we suggest you copy the configuration options from make.linux,

```
shell> cd configs
shell> cp make.linux make.inc
shell> cat make.inc
FC = gfortran
CXX = mpicxx
EXTRA_LINK_FLAGS = -L/usr/lib64 -llapack -lblas -lgfortran
```

This setup assumes that the blas and lapack libraries are located in the /usr/lib64 directory. In the case of Fedora Core 18, we needed to set the link flag variable to

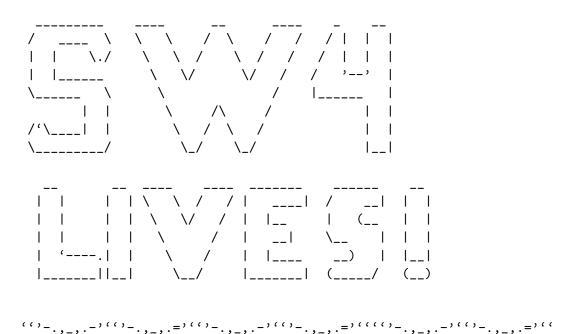
```
EXTRA_LINK_FLAGS = -Wl,-rpath=/usr/lib64/mpich2/lib -llapack -lblas -lgfortran
```

4.1.3 Using make

You build SW4 with the "make" command from the main directory.

```
shell> cd /enter/your/path/sw4-v2.0
shell> make
```

If all goes well, you will see the SW4 Lives banner on your screen after the compilation and linking has completed,



By default, make builds an optimized sw4 executable. It is located in

/enter/your/path/sw4-v2.0/optimize/sw4

You can also build an executable with debugging symbols by adding the debug=yes option to make,

```
shell> cd /enter/your/path/sw4-v2.0
shell> make debug=yes
```

In this case, the executable will be located in

/enter/your/path/sw4-v2.0/debug/sw4

It can be convenient to add the corresponding directory to your PATH environment variable. This can be accomplished by modifying your shell configuration file, e.g. ~/.cshrc if you are using C-shell.

4.1.4 How do I setup the make.inc file?

The input file for make is

```
sw4-v2.0/Makefile
```

Do not change this Makefile. It should only be necessary to edit your configuration file, that is,

```
/my/path/sw4-v2.0/configs/make.inc
```

Note that you must create this file, for example by copying one of the make.xyz files in the same directory. The make.inc file holds all information that is particular for your system, such as the name of the compilers, the location of the third party libraries, and any extra arguments that should be passed to the compiler or linker. This file also tells make whether or not the cencalvm and proj.4 libraries are available and where they are located.

The following make.inc file includes all configurable options:

```
etree = no
proj = no
SW4ROOT = /Users/petersson1

CXX = mpicxx
FC = mpif77

EXTRA_CXX_FLAGS = -DUSING_MPI
EXTRA_FORT_FLAGS = -fno-underscoring
EXTRA_LINK_FLAGS = -framework vecLib
```

The etree variable should be set to yes or no, to indicate whether or not the cencalvm and related libraries are available. The SW4ROOT variable is only used when etree=yes. The CXX and FC variables should be set to the names of the C++ and Fortran compilers, respectively. Finally, the EXTRA_CXX_FLAGS, EXTRA_FORT_FLAGS, and EXTRA_LINK_FLAGS variables should contain any additional arguments that need to be passed to the C++ compiler, Fortran compiler, or linker, on your system.

4.2 Building SW4 with proj.4 and/or effle support

The installation of the proj.4, euclid, and cencalvm libraries is discussed in Section 6. Note that the proj.4 libraray enables the more advanced geographical mapping keywords in the grid command and is also required by the rfile command. To enable the efile command, you have to also install the euclid and cencalvm libraries. Note that the latter two libraries are only needed by the efile command. If you are not planning on using that command, there is no need to install those libraries. This is a change from SW4 version 1.0.

Once you have successfully installed the proj.4, and optionally the euclid and cencalvm libraries, it should be easy to re-configure SW4 to use them. Simply edit your configuration file (make.inc) by adding two lines to the top of the file, setting the etree keyword to yes or no, as appropriate.

```
proj = yes
etree = no
SW4R00T = /thid/party/basedir
```

You then need to re-compile SW4. Go to the SW4 main directory, clean out the previous object files and executable, and re-run make:

```
shell> cd /my/installation/dir/sw4-v2.0
shell> make clean
shell> make
```

If all goes well, the "SW4 lives" banner is shown after the make command is completed. As before, the sw4 executable will be located in the optimize or debug directories.

4.3 Testing the SW4 installation

The SW4 source code distribution includes a python(3) script for running several tests and checking the solutions against previously verified results. Note that the same set of tests can be performed when SW4 is built with CMake, see Section 5.2.

After SW4 has been built with make, go to the pytest directory and run test_sw4.py. If the sw4 executable resides in the optimize directory, you can run the basic tests by doing:

```
shell> cd pytest
shell> ./test_sw4.py
If all goes well, you should see the following output:
>shell test_sw4.py
Running all tests for level 0 ...
Starting test # 1 in directory: meshrefine with input file: refine-el-1.in
Test # 1 Input file: refine-el-1.in PASSED
Starting test # 2 in directory: meshrefine with input file: refine-att-1.in
Test # 2 Input file: refine-att-1.in PASSED
Starting test # 12 in directory: lamb with input file: lamb-1.in
Test # 12 Input file: lamb-1.in PASSED
Out of 12 tests, 12 passed and 0 failed.
Some aspects of the testing can be modified by providing command line arguments to test_sw4.py.
```

For a complete list of options do test_sw4.py --help, which currently give the output: shell> ./test_sw4.py --help

```
usage: test_sw4.py [-h] [-v] [-1 {0,1,2}] [-m MPITASKS] [-d SW4_EXE_DIR]
optional arguments:
 -h, --help
                       show this help message and exit
 -v, --verbose
                       increase output verbosity
 -1 \{0,1,2\}, --level \{0,1,2\}
```

testing level -m MPITASKS, --mpitasks MPITASKS number of mpi tasks

-d SW4_EXE_DIR, --sw4_exe_dir SW4_EXE_DIR

name of directory for sw4 executable

Note that the directory name for the sw4 executable should be given relative to the main sw4 directory.

5 Installing SW4 with CMake

SW4 can also be built with CMake. Compared to using regular make, this build process is easier to use because it is fully automated. However, it gives the user less control of which compilers, linker, and libraries to use. Similar to using regular make, the SW4 CMake configuration allows automated correctness testing of the installation. The test runs the same set of cases as the test_sw4.py script in the pytest directory, see Section 5.2 for details.

To use CMake, navigate to the top sw4 directory and run the following commands:

```
shell> mkdir build
shell> cd build
shell> cmake [options] ..
shell> make
```

The two dots after cmake [options] are essential and instructs it to look in the parent directory for the CMakeLists.txt file.

The cmake command searches for the necessary libraries and other dependencies, then creates makefiles appropriate to your system. Running make compiles SW4 using these makefiles. For details about the exact commands being used in compilation, run make VERBOSE=1. Once SW4 is successfully compiled and linked you will see the "SW4 Lives!" banner on the screen.

NOTE: cmake puts the sw4 executable in the build/bin directory. This is different from regular make, which puts the executable in the optimize directory.

NOTE: If you want to rebuild sw4 with a new set of options, you can force cmake to start from scratch by removing the file CMakeCache.txt in the build directory. Another way is to remove all files in the build directory.

5.1 CMake Options

CMake provides several options to allow customized configuration of SW4. To use any option, add -D<option>=<value> to the options in the cmake command. For example:

```
cmake -DTESTING_LEVEL=1 -DCMAKE_BUILD_TYPE=Debug ..
```

configures SW4 with testing level 1, to be compiled with debugging symbols in the object files. A list of options is shown in the table below.

Option	Default	Details
PROJ4_HOME	(none)	The path to the Proj.4 installation to use when compiling $SW4$.
CENCALVM_HOME	(none)	The path to the cencal m installation to use when compiling $SW4$.
CMAKE_BUILD_TYPE	Release	The type of build to setup. Can be either Debug, Release, or RelWithDebInfo. This affects the type of optimization and debug flags used in compiling $SW4$.
TESTING_LEVEL	0	Specifies the testing level for automated tests. Level 0 corresponds to tests that run in roughly a minute or less (7 total), level 1 to tests that run in roughly 10 minutes or less (13 total) and level 2 to tests that may require up to an hour or more (17 total).
MPI_NUM_TEST_PROCS	4	Number of MPI processes to use in tests. Generally using more processes will result in the tests finishing faster, but there is no point exceeding the number of available cores on your system. We strongly recommend at least 8 processes if TESTING_LEVEL is 1 or higher.
MPIEXEC	mpirun	UNIX command for running an MPI application.
MPIEXEC_NUMPROC_FLAG	-np	MPI command option for specifying the number of processes.
MPIEXEC_PREFLAGS	(none)	Extra MPI command option.

Modifying the MPI execution commands. By default, mpirun is used to start parallel runs when you do make test. However, on Livermore computing (LC) machines the command for running MPI programs is srun, not mpirun. Also, the flag for specifying the number of processors is different, and you must give an additional flag for running interactive jobs on the debug partition. For example, you would say

```
srun -ppdebug -n 128 sw4 inputfile.in
```

to run on the debug partition using 128 cores. To modify the default MPI execution program and other runtime parameters, the variables MPIEXEC, MPIEXEC_NUMPROC_FLAG, and MPIEXEC_PREFLAGS can be set as in the following example:

After the proj.4, euclid and cencalvm libraries have been installed (see next section), you need to tell cmake where to find them. On the LC-machines, all three libraries are currently installed under /usr/apps/wpp, and you can use the following command options to configure sw4:

```
cmake -DTESTING_LEVEL=2 -DMPI_NUM_TEST_PROCS=36 -DMPIEXEC=/usr/bin/srun \
    -DMPIEXEC_NUMPROC_FLAG=-n -DMPIEXEC_PREFLAGS=-ppdebug \
    -DPROJ4_HOME=/usr/apps/wpp -DCENCALVM_HOME=/usr/apps/wpp ..
```

To verify that cmake actually found the libraries, pay attention to the following lines of the output from the cmake command:

```
...
-- Found PROJ4: /usr/apps/wpp/lib/libproj.so
-- Found CENCALVM: /usr/apps/wpp/lib/libcencalvm.so;/usr/apps/wpp/lib/libetree.so
...
```

Sometimes CMake doesn't pick up the correct compiler. Say, for example that the C++ compiler on your system is called mpicxx and the Fortran compiler is mpiifort. You can tell cmake to use those compilers by setting the following envoronment variables *before* running cmake (assuming a csh shell),

- > setenv CXX mpicxx
- > setenv FC mpiifort

5.2 CTest

The SW4 CMake configuration includes several test cases that are used to verify the correctness of the SW4 installation. Each test consists of two parts. First it runs a case using an input file in the pytest directory. Secondly, it checks that the results are within a reasonable error tolerance from previously recorded results.

To run the tests, use either the command make test or ctest as follows:

```
build > ctest
Test project /Users/petersson1/src/sw4-cig/build
     Start 1: Run_twilight/flat-twi-1
 1/24 Test #1: Run_twilight/flat-twi-1 ......
                                                                        0.49 sec
                                                              Passed
     Start 2: Check_Result_twilight/flat-twi-1
 2/24 Test #2: Check_Result_twilight/flat-twi-1 ......
                                                              Passed
                                                                        0.03 sec
     Start 3: Run_twilight/flat-twi-2
     Start 23: Run_pointsource/pointsource-sg-1
23/24 Test #23: Run_pointsource/pointsource-sg-1 .....
                                                              Passed
                                                                       89.56 sec
     Start 24: Check_Result_pointsource/pointsource-sg-1
24/24 Test #24: Check_Result_pointsource/pointsource-sg-1 ...
                                                                        0.03 sec
                                                              Passed
100\% tests passed, 0 tests failed out of 24
Total Test time (real) = 230.91 sec
  You can run tests selectively using ctest -R <regex>, for example:
build > ctest -R meshrefine
Test project /Users/petersson1/src/sw4-cig/build
   Start 15: Run_meshrefine/refine-el-1
1/6 Test #15: Run_meshrefine/refine-el-1 ......
                                                           Passed
                                                                    25.61 sec
```

Passed

0.03 sec

Start 16: Check_Result_meshrefine/refine-el-1 2/6 Test #16: Check_Result_meshrefine/refine-el-1

```
Start 17: Run_meshrefine/refine-att-1
3/6 Test #17: Run_meshrefine/refine-att-1 ......
                                                                     22.00 sec
                                                           Passed
    Start 18: Check_Result_meshrefine/refine-att-1
4/6 Test #18: Check_Result_meshrefine/refine-att-1 ......
                                                                     0.03 sec
                                                            Passed
    Start 19: Run_meshrefine/refine-att-2nd-1
5/6 Test #19: Run_meshrefine/refine-att-2nd-1 .....
                                                            Passed
                                                                     17.63 sec
   Start 20: Check_Result_meshrefine/refine-att-2nd-1
6/6 Test #20: Check_Result_meshrefine/refine-att-2nd-1 ...
                                                           Passed
                                                                      0.03 sec
100% tests passed, 0 tests failed out of 6
Total Test time (real) = 65.35 sec
```

If a test fails you can check the details in the output log at Testing/Temporary/LastTest.log.

6 Installing the proj.4, euclid, and cencalvm packages

If you are only interested in using the advanced geographical mapping options of the grid command, or the rfile command, you only need to install the proj.4 package.

The following instructions describe how to install all three packages. For simplicity all packages are installed under the same top directory. If you are using cmake, you may optionally put the proj.4 package in a separate directory. In the following we shall assume that all packages are installed under the same top directory, and that you assign the name of that directory to the environment variable SW4R00T. When you are finished installing the packages, the corresponding include and library files should be in the sub-directories \${SW4R00T}/include and \${SW4R00T}/lib, respectively.

The cencalvm library was developed by Brad Aagaard at USGS. Instructions for building the cencalvm library as well as downloading the Etree database files for Northern California, can currently be downloaded from

```
http://earthquake.usgs.gov/data/3dgeologic/cencalvm_doc/INSTALL.html
```

The installation process for cencalym, which is outlined below, is described in detail on the above web page. Note that cencalym relies on both the euclid and the proj.4 libraries.

The euclid library must be installed manually by explicitly copying all include files to the include directory and all libraries to the lib directory,

```
shell> cd euclid3-1.2/libsrc
shell> make
shell> cp *.h ${SW4R00T}/include
shell> cp libetree.* ${SW4R00T}/lib

The proj4 library should be configured to be installed in ${SW4R00T}. This is accomplished by
shell> cd proj-4.7.0
shell> configure --prefix=${SW4R00T}
shell> make
shell> make install
```

We remark that the proj.4 library can alternatively be installed using macports (if you are on a Mac OSX machine).

The cencalvm library should also be configured to be installed in \${SW4R00T}. You also have to help the configure script finding the include and library files for the proj.4 and etree libraries,

To verify that the libraries have been installed properly, you should go to the SW4ROOT directory and list the lib sub-directory (cd \${SW4ROOT}; ls lib). You should see the following files (on Mac OSX machines, the .so extension is replaced by .dylib):

```
shell> cd ${SW4ROOT}
shell> ls lib
libetree.so libetree.a
libproj.so libproj.a libproj.la
libcencalvm.a libcencalvm.la libcencalvm.so
Furthermore, if you list the include sub-directory, you should see include files such as
shell> cd ${SW4ROOT} %$
shell> ls include
btree.h etree.h etree_inttypes.h
nad_list.h projects.h proj_api.h
cencalvm
```

Note that the include files for cencalym are in the sub-directory with the same name.

7 Disclaimer

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[1] N. A. Petersson and B. Sjögreen. User's guide to SW4, version 1.1. Technical Report LLNL-SM-662014, Lawrence Livermore National Laboratory, 2014. (Source code available from geodynamics.org/cig/software/sw4/).