Installing SW4 version 3.0

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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, Sjogreen, and Tang [1].

2 Installing SW4 with spack

SW4 can be installed with Spack (https://spack.io), which is a package manager for supercomputers, Linux, and macOS. It can automatically install SW4 together with all its dependent libraries, such as MPI, Proj, OpenMP, blas, lapack, HDF5, FFTW, and ZFP.

```
> git clone -c feature.manyFiles=true https://github.com/spack/spack.git
```

- > . spack/share/spack/setup-env.sh
- > spack install sw4

Run the following command to add the installed SW_4 executable to your system PATH:

- > . spack/share/spack/setup-env.sh
- > spack load sw4

3 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. an MPI library. This library provides support for message passing on parallel machines. Examples of open source implementations include Mpich and OpenMPI. Note that the MPI 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 PROJ before building SW4:

• PROJ (version 6+), https://proj.org/download.html

If you also wish to use material models using the *sfile* or *GMG* format, you also need to download and install the HDF5 library:

• HDF5 (version 1.12+), https://www.hdfgroup.org/downloads/hdf5/source-code

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 7 for details.

MacOS 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

```
sudo port install gcc11
sudo port install mpich-gcc11
sudo port install hdf5
```

Here, gcc11 refers to version 11 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 gcc11 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 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. For Ubuntu systems, one can simply change yum to apt-get

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 mpich and hdf5 library and include files with the command

```
yum install mpich-devel
yum install hdf5
```

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

```
export PATH=${PATH}:/usr/lib64/mpich/bin
if your shell is bash. For tcsh users, the command is
setenv PATH ${PATH}:/usr/lib64/mpich/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.

4 Unpacking the source code tar ball

To unpack the SW4 source code, you place the file sw4-v3.0.tar.gz in the desired directory and issue the following command:

```
tar xzf sw4-v3.0.tar.gz
```

As a result a new sub-directory named sw4-v3.0 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.

5 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

```
> 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 quartz (at LLNL), Cori (at LBNL), and Summit (at ORNL). We have successfully used the following versions of Gnu, Intel, and IBM compilers:

```
GNU: g++/gcc/gfortran versions 4.5+
Intel: icpc/icc/ifort versions 16.0+
IBM: xlcxx/xlc/xlf versions 12.1+
```

SW4 uses the message passing interface (MPI) standard 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 mpich 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.

5.1 Basic compilation and linking of SW4

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 Fortran 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.

5.1.1 Mac machines

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

```
cd configs
cp make.osx make.inc
cat make.inc
proj = no
hdf5 = no
FC = mpif90
CXX = mpicxx
EXTRA_FORT_FLAGS =
EXTRA_LINK_FLAGS = -framework Accelerate -L/opt/local/lib/gcc11 -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/gcc11, which is where macports currently installs it.

5.1.2 Linux machines

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

```
cd configs
cp make.linux make.inc
cat make.inc
proj = no
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

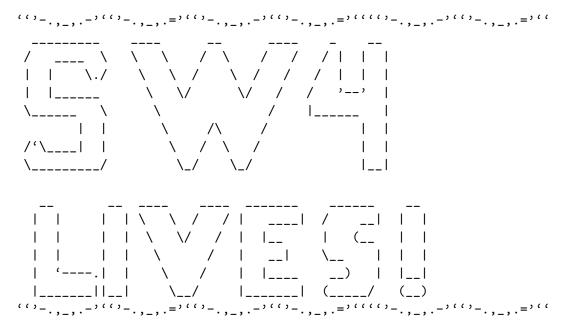
EXTRA_LINK_FLAGS = -W1,-rpath=/usr/lib64/mpich/lib -llapack -lblas -lgfortran

5.1.3 Using make

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

```
cd /enter/your/path/sw4-v3.0
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-v3.0/optimize/sw4

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

```
> cd /enter/your/path/sw4-v3.0
> make debug=yes
```

In this case, the executable will be located in

```
/enter/your/path/sw4-v3.0/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.

5.1.4 How do I setup the make.inc file?

The input file for make is

```
sw4-v3.0/Makefile
```

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

```
/my/path/sw4-v3.0/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.

The following make.inc file includes all configurable options:

```
proj = no
hdf5 = no
SW4R00T = /my/path/to/installed/library
CXX = mpicxx
FC = mpif77
EXTRA_CXX_FLAGS = -DUSING_MPI
EXTRA_FORT_FLAGS = -fno-underscoring
EXTRA_LINK_FLAGS = -framework veclib
```

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.

5.2 Building SW4 with PROJ, HDF5, and ZFP support

The PROJ libraray enables the more advanced geographical mapping keywords in the grid command and is also required by the rfile, sfile and gmg commands. To enable the sfile, ssioutput, and gmg commands, you have to also install the HDF5 library. To use ZFP compression for the ssioutput command, ZFP and H5Z-ZFP are required. See Section 7 for installing these libraries.

Once you have successfully installed the PROJ, and optionally the HDF5 and ZFP libraries, it should be easy to re-configure SW4 to use them. Simply edit your configuration file (make.inc) by adding the following lines to the top of the file, setting the proj, hdf5, and zfp keywords to yes or no, as appropriate.

```
proj = yes
hdf5 = yes
zfp = yes
SW4R00T = /thid/party/basedir
HDF5R00T = /thid/party/basedir
ZFPR00T = /thid/party/basedir
H5ZR00T = /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:

```
> make clean
> 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.

5.3 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 6.2.

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:

```
> cd pytest
> ./test_sw4.py ("./test_sw4.py -u 0" if HDF5 is not installed)
```

If all goes well, you should see the following output:

```
Running all tests for level 0 ...

Test # 1 Input file: energy-nomr-2nd-1.in PASSED

Test # 2 Input file: energy-mr-4th-1.in PASSED

...

Test # 25 Input file: loh1-h100-mr-restart-hdf5-1.in PASSED

Out of 25 tests, 0 failed, 23 passed, and 2 skipped
```

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:

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

6 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 6.2 for details.

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

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

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 that are appropriate for your system. You then run make to compiles and link SW4 using these makefiles. For details about the exact commands being used in compilation, run make VERBOSE=1. Once SW4 has been successfully built, you will see the "SW4 Lives!" banner on the screen.

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.

6.1 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, when building SW4 with the PROJ library:

- > export
- > cmake -DUSE_PROJ=ON -DPROJ_DIR=\${SW4ROOT}/install/lib64/cmake/proj ...

A list of options is shown in the table below.

Option	Default	Details
USE_PROJ	OFF	Enable PROJ library.
PROJ_DIR	(none)	The path to the PROJ installation.
USE_HDF5	OFF	Enable HDF5 library.
HDF5_DIR	(none)	The path to the HDF5 installation.
USE_ZFP	OFF	Enable ZFP compression.
ZFP_DIR	(none)	The path to the ZFP installation.
H5Z_ZFP_DIR	(none)	The path to the H5Z-ZFP installation.
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 and HDF5 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=srun \
    -DMPIEXEC_NUMPROC_FLAG=-n -DMPIEXEC_PREFLAGS=-ppdebug \
    -DUSE_HDF5=ON -DPROJ_DIR=/usr/apps/wpp \
    -DUSE_PROJ=ON -DHDF5_DIR=/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 PROJ: /usr/apps/wpp/lib/libproj.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

6.2 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:

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 ...
                                                               Passed
                                                                         0.03 sec
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 ......
                                                                     25.61 sec
                                                            Passed
    Start 16: Check_Result_meshrefine/refine-el-1
2/6 Test #16: Check_Result_meshrefine/refine-el-1 ......
                                                            Passed
                                                                      0.03 sec
    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 ......
                                                                     17.63 sec
                                                            Passed
    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.

7 Installing the PROJ, HDF5, and ZFP

If you are interested in using the advanced geographical mapping options of the grid command, the sfile, or the gmg command, you need to install the PROJ package. For sfile, ssioutput, and gmg, the HDF5 library is also required. To use the ssioutput command with ZFP compression, both ZFP library and the ZFP HDF5 filter library (H5Z-ZFP) are required.

The following instructions describe how to install the two packages. For simplicity all packages are installed under the same top directory. If you are using cmake, you may optionally put the PROJ and HDF5 packages 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 SW4ROOT. When you are finished installing the packages, the corresponding include and library files should be in the sub-directories \${SW4ROOT}/include and \${SW4ROOT}/lib, respectively.

7.1 PROJ

The PROJ library requires SQLite, if your system does not have it installed already, it can be compiled with the following steps:

Download sqlite from https://www.sqlite.org/download.html (sqlite-autoconf-x)

```
> tar xf sqlite-autoconf-x.tar.gz
  > cd sqlite-autoconf-x/
  > ./configure --prefix=${SW4R00T}
  > make
  > make install
   The PROJ library (version 9 and later is recommended) can be installed by the following steps:
  # Download PROJ from https://proj.org/download.html
  > tar xf proj-x.x.x.tar.gz
  > cd proj-x.x.x
  > mkdir build
  > cd build
  > cmake -DBUILD_APPS=OFF -DCMAKE_INSTALL_PREFIX=${SW4ROOT}
-DSQLITE3_INCLUDE_DIR=${SW4ROOT}/include
-DSQLITE3_LIBRARY=${SW4ROOT}/lib/libsqlite3.so
  # Note that the two -DSQLITE3 flags are needed if you compiled SQLite yourself.
  > make
  > make install
```

7.2 HDF5

Installing HDF5 (version 1.12 and later is recommended) can be done with the following steps:

```
# Download HDF5 from https://www.hdfgroup.org/downloads/hdf5/source-code
> tar xf hdf5-1.xx.x.tar.gz
> cd hdf5-1.xx.x
> mkdir build
> cd build
> cmake -DHDF5_ENABLE_PARALLEL=ON -DCMAKE_INSTALL_PREFIX=${SW4ROOT}}
> make
> make install
```

7.3 ZFP and H5Z-ZFP

We recommend to use use ZFP and H5Z-ZFP's latest stable release version. Installing ZFP can be done with the following steps:

```
# Download ZFP from https://github.com/LLNL/zfp/releases
> tar xf zfp-x.x.x.tar.gz
> cd zfp-x.x.x
> mkdir build
```

```
> cd build
> cmake -DZFP_BIT_STREAM_WORD_SIZE=8 -DCMAKE_INSTALL_PREFIX=${SW4R00T} ...
> make
> make install

Installing H5Z-ZFP can be done with the following steps:
# Download H5Z-ZFP from https://github.com/LLNL/H5Z-ZFP/releases
> tar xf vx.x.x.tar.gz
> cd H5Z-ZFP-x.x.x
> mkdir build
> cd build
> export HDF_DIR=/path/to/hdf5/install
> export ZFP_DIR=/path/to/zfp/install
> cmake -DCMAKE_INSTALL_PREFIX=${SW4R00T} ...
> make
> make install
```

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 lib64). You should see the following files (on Mac OSX machines, the .so extension is replaced by .dylib):

```
> cd ${SW4R00T}
> ls lib lib64
> lib
> libhdf5.so ...
> lib64
> libproj.so ...
```

Furthermore, if you list the include sub-directory, you should see include files such as

```
> cd ${SW4R00T}
> ls include
> proj.h hdf5.h ...
```

7.4 SW4 with PROJ, HDF5, and ZFP

To build SW4 with all the libraries can be done using CMake with the following commands:

```
> export PROJ_ROOT=/path/to/proj/install
> export HDF5_ROOT=/path/to/hdf5/install
> export ZFP_ROOT=/path/to/zfp/install
> export H5Z_ZFP_ROOT=/path/to/h5z_zfp/install
> cmake -DUSE_HDF5=ON -DUSE_PROJ=ON -DUSE_ZFP=ON ...
> make
```

8 Disclaimer

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References

[1] N. A. Petersson, B. Sjögreen, and H. Tang. User's guide to SW4, version 3.0. Technical Report LLNL-SM-741439, Lawrence Livermore National Laboratory, 2022. (Source code available from https://github.com/geodynamics/sw4).