Setup Guide for a Linux Development Environment

Nick Macey

 $March\ 16,\ 2021$

1. Assumptions

- 1.1 Libraries, and executables built manually, should be placed in a /prod directory. Access to this should be controlled, but can (and should) be a group distinct to the sudoers.
- 1.2 The instructions are for a Debian-like disto (Ubuntu, Mint). Broadly, they'll work for any distro, but note that anything using apt will be different.

2. **LLVM**

- 2.1 LLVM version 11.0 onwards includes the flang (Fortran) compiler.
- **2.2** Unfortunately, LLVM 11.0 does not exist in any useful pre-built binary or package file.
- 2.3 Easiest way to build and install LLVM 11.0 is to use the following script:
 - https://www.dropbox.com/s/87115qvebssjack/build_llvm.sh?dl=0
 - Will install into /prod/bin, /prod/lib and /prod/include
 - Note: Building LLVM requires a recent copy of both gcc and gfortran

3. **HDF5**

 $\bf 3.1 \quad \mbox{Pre-built binaries are only available for CentOS – not terribly helpful given that CentOS is dead. . .$

- **3.2** Download source code from here:
 - https://www.hdfgroup.org/downloads/hdf5/source-code/
 - Ideally, you want the Cmake version (bottom of the page)
- ${\bf 3.3}$ $\,$ Modify the HDF5 options.cmake configuration file (NOT the HDF5 config.cmake file)
 - Switch between MPI and serial builds
 - Switch on Fortran build
 - Modify install prefix
- **3.4** Export compiler executables. E.g. for GCC:
 - export CC=gcc CXX=g++ FC=gfortran
- **3.5** Build via cmake and make (or cmake –build)
- 3.6 Note that HDF5 v1.12 does not seem to work with Clang
- 3.7 Export HDF5_DIR as described here: https://portal.hdfgroup.org/display/support/CMake+Scripts+for+Building+Application

4. **SILO**

- **4.1** SILO is probably the most reliable mesh output format for a general Linux install, although it does suffer from a really bad Fortran API (so we'll install NetCDF too).
- **4.2** If you want to use HDF5 with SILO, you'll need an older HDF5 library (1.10). But SILO works perfectly well with its own file format.

4.3 Download from here: https://wci.llnl.gov/simulation/computer-codes/silo and follow the build instructions in the INSTALL file.

5. NetCDF

- **5.1** Download from here:
 - https://www.unidata.ucar.edu/downloads/netcdf/
 - You want both the C and Fortran libraries, and possibly the C++ one
- **5.2** Build using Cmake, following these guides:
 - https://www.unidata.ucar.edu/software/netcdf/docs/getting_and_ building_netcdf.html#netCDF-CMake
 - https://www.unidata.ucar.edu/software/netcdf/docs/building_netcdf_fortran.html
 - Remember to set the installation directory to /prod, not the default of /usr/local

6. Module Environment

- $6.1~{\rm Download~from~https://sourceforge.net/projects/modules/files/Modules/$
- **6.2** Build instructions are here: https://modules.readthedocs.io/en/stable/INSTALL.html
 - You'll need telsh installed (sudo apt install tel tel-dev)
 - Probably does make sense to install this into /usr/share (see example at bottom of installation guide
 - Make sure to follow the instructions in the Configuration section in order to have the module environment load

7. AMReX

- $\textbf{7.1} \quad \textbf{Clone AMReX repository: https://github.com/AMReX-Codes/amrex}$
- 7.2 Create BUILD directory
- 7.3 Run cmake
 - cmake -DAMReX_OMP=YES -DAMReX_FORTRAN_INTERFACES=YES DAMReX_HDF5=YES -DAMReX_SPACEDIM=2 -DCMAKE_INSTALL_PREFIX=/
 prod/AMReX2D_CMAKE ..
 - (Requires that HDF5_ROOT be set to the root of a parallel HDF5 build)
- 7.4 Make and install
 - make; make install