PFLOTRAN installation instructions on MacOS (arm64)

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REQUIREMENTS: xcode command-line utils

Step 0: If not already done, install Xcode command line tools and gcc, and make gcc aliases

At a new terminal window, type the following:

```
xcode-select --install
```

This will prompt a window from MacOS asking if you want to install Xcode, and whether you agree to the terms. Click Yes/Agree, and proceed with installation.

Once installation completes, restart computer.

After restart, open a new terminal window and install gcc with homebrew:

```
brew install gcc
```

Determine version of gcc installed:

```
brew info gcc
```

This will display somehting like:

```
==> gcc: stable 12.2.0 (bottled), HEAD
GNU compiler collection
https://gcc.gnu.org/
/opt/homebrew/Cellar/gcc/12.2.0 (1,470 files, 358.8MB) *
Poured from bottle on 2023-02-07 at 17:42:04
From: https://github.com/Homebrew/homebrew-
core/blob/HEAD/Formula/gcc.rb
License: GPL-3.0-or-later with GCC-exception-3.1
==> Dependencies
Required: gmp ✔, isl ✔, libmpc ✔, mpfr ✔, zstd ✔
==> Options
--HEAD
    Install HEAD version
==> Analytics
install: 78,057 (30 days), 227,784 (90 days), 1,395,629 (365 days)
install-on-request: 38,183 (30 days), 112,782 (90 days), 666,694 (365
```

```
  days)
      build-error: 252 (30 days)
```

gcc version in shown in line 0; the location of the install is shown in line 3

Now create aliases for gcc. MacOS defaults to clang. The aliases force gcc to be used.

Open ~/.zshrc:

```
    vi ~/.zshrc
```

Add the following lines to the file, where [VERSION] corresponds to the first number (e.g., '12') of the gcc version:

```
    alias gcc=gcc-[VERSION]
    alias g++=g++-[VERSION]
```

Write and save the changes in the ~/.zshrc, and then resource the file, or quit the terminal and reopen it.

Step 1: Install required packages with hombrew

```
    brew install open-mpi
    brew install hdf5-mpi
    brew install lapack
    brew install cmake
```

Determine installed versions and locations of install, as above with gcc:

```
    brew info open-mpi
    brew info hdf5-mpi
```

Step 2: Clone PETSc

Move to the location where you wish to save PETSc. Then clone with:

```
    git clone https://gitlab.com/petsc/petsc.git petsc
    cd petsc
    git checkout v3.17.1
```

Step 3: Configure and make PETSc

Enter the topmost PETSc dir and run configure:

```
    cd petsc

    ./configure --with-debugging=no --with-shared-libraries=0 --known-mpi-
shared-libraries=1 --with-mpi-dir=/opt/homebrew/Cellar/open-mpi/4.1.4_2/ -
-known-64-bit-blas-indices --with-hdf5-dir=/opt/homebrew/Cellar/hdf5-
mpi/1.12.2_1 / --download-hdf5-fortran-bindings=yes
```

Note that if the versions of hdf5-mpi and/or open-mpi differ from hdf5-mpi/1.12.2_1 and open-mpi/4.1.4_2, replace --with-mpi-dir= and --with-hdf5-dir= paths with correct values

After the configuration is complete, it will prompt you to make PETSc and provide a command for doing so. If PETSc compiles, it will prompt you test the compilation, and provide a command to do so. Note that the test may partially fail -- this is not necessarily a problem.

Check that PETSC_DIR and PETSC_ARCH are defined:

```
    echo $PETSC_DIR
    echo $PETSC_ARCH
```

Step 4: Clone PFLOTRAN

From $HOME, make a new directory for PFLOTRAN. Enter the directory and clone PFLOTRAN

```
    git clone https://gitlab.com/pflotran/pflotran.git
```

Step 5: Make PFLOTRAN

```
    cd pflotran/src/pflotran
    git checkout maint/v4.0
    make pflotran
```

This will take ~10 min.