3 November 2017

Setting up AMBER on a Mac 10.13 (High Sierra)

1. Install X-Code

Download from App Store, just search "xcode" After installing XCode, you need to agree to the license. So run the following command in a terminal: `sudo xcodebuild -license`

Next you need to install the command-line tools. Running the following command in the terminal installs the command-line tools: `xcode-select --install`

2. Install X Quartz https://www.xquartz.org/

3. Install MacPorts https://www.macports.org/install.php

4. Update MacPorts and Upgrade Packages

```
sudo port selfupdate
sudo port upgrade outdated
```

5. Packages to install

```
gcc5                    py27-numpy              chemtool
mpich-gcc5              molden +gcc5            netpbm
python27                grace                   pymol
py27-matplotlib         gnuplot
py27-scipy              bkchem
```

Ex: `sudo port install gcc5`
You can install more than one at once also, Ex:

```
sudo port install python27 py27-matplotlib py27-scipy
```

6. Prepare for AMBER

```
sudo port install gcc5
sudo port install mpich-gcc5
sudo port select --set gcc mp-gcc5
sudo port select --set mpi mpich-gcc5-fortran
```

7. Other Useful Programs to Download and Install:

UCSF Chimera	https://www.cgl.ucsf.edu/chimera/download.html
iTerm	https://www.iterm2.com/downloads.html
Sublime Text	https://www.sublimetext.com/3
VMD	http://www.ks.uiuc.edu/Development/Download/download.cgi