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

1. Install X Quartz https://www.xquartz.org/
2. Install MacPorts <https://www.macports.org/install.php>
3. Update MacPorts and Upgrade Packages

sudo port selfupdate

sudo port upgrade outdated

1. Packages to install

gcc5

mpich-gcc5

python27

py27-matplotlib

py27-scipy

py27-numpy

molden +gcc5

grace

gnuplot

bkchem

chemtool

netpbm

pymol

Ex: sudo port install gcc5

You can install more than one at once also, Ex:

sudo port install python27 py27-matplotlib py27-scipy

1. 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

1. 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>