Lab 0: Preparing your laptop for the course – OS X

Five pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. Textmate 2.0
4. Gnuplot – Plots data
5. A modern web browser – Internet Explorer 10 or newer, recent versions of Chrome or Firefox.

Several assumptions in this document:

1. You have admin access (i.e. permission to install new packages to you system)
2. You know what a terminal is.
3. You understand the difference between a text editor and word processor.
4. You will have a web browser already installed, if you need a more modern version then one is only a web search and standard installation away.

We will also add NAMD and Gnuplot to your PATH for ease of use.

VMD

Download

Click on this link http://www.ks.uiuc.edu/Research/vmd/ or use your web browser to navigate to the web page.

- Locate the 'Downloads' section that is highlighted (below the 'Overview' section) on the left side of the page
- Click on the 'Download (all versions)' link

Then you need to select the 'MacOS X OpenGL' link appropriate for your version of OS X for the most recent version of VMD (Version 1.9.2 at the time of writing).

- Click the appropriate link
- You now need to register an account
    - Enter a username and password
    - Click "Continue with registration or download'
    - Fill in the form (including confirming your password)
    - Click 'Register'
- Confirm that you are you and agree to the license
- The download should begin automatically

Installation

- Once the file has downloaded double click on it to run it
- Drag the icon that resembles a water molecule into your Applications folder

To open VMD from a terminal window (optional)

- Add the following to your ~/.bashrc file:
    - alias vmd='Applications/VMD\ 1.9.2.app/Contents/vmd/vmd_MACOSXX86'
    - VMDFILECHOOSER=FLTK
    - Export VMDFILECHOOSER

- Then type “source ~/.bashrc”

NAMD

Download

Click on this link http://www.ks.uiuc.edu/Research/namd/ or use your web browser to navigate to the web page.

- Follow the 'Download NAMD' link on the left side of the page
- Select the MacOSX-x86_64 link from the “Version 2.9 (2012-04-30) Platforms” section
    - We use version 2.9 to ensure that all input and output formats are compatible with other software used in the tutorial
- Enter the username and password you created before when installing VMD.
- Agree to the license and the download should start automatically

Installation

- In the terminal navigate to the directory where the file was downloaded and run the command:

```
sudo tar xvf NAMD_2.9_MacOSX-x86_64-multicore.tar -C /usr/local/bin
```

- You will need to enter your password to gain admin rights
- Now we need to make the program easily accessible from the command prompt, this involves setting an Environment Variable:

1. Open the file ~/.bashrc in your text editor
2. Add the following line:

```
export PATH=$PATH:/usr/local/bin/NAMD_2.9_MacOSX-x86_64-multicore
```

3. Save the file
4. Type `source ~/.bashrc`
5. Open the file ~/.bash_profile in your text editor
6. Add the following line:

```
if [-f ~/.bashrc];then . ~/.bashrc;fi
```

Textmate (optional – the TextEdit app that comes with OS X can be used)

Download

Navigate to http://macromates.com/

- Click on the download icon

Installation

- Once the file has downloaded double click on it to run it
- Drag the icon that resembles a water molecule into your Applications folder

Gnuplot

Download

There are a variety of ways of installing Gnuplot. All of which have different dependencies. Ask one of the course administrators which option is best for you.

Perhaps the nicest is via homebrew (http://brew.sh/)but even this requires a working installation of Xcode.

Testing NAMD and Gnuplot Installations

If the installation has worked then NAMD and Gnuplot should be available from the command line.

- To test NAMD type:

  ```
  namd2
  ```

  - If NAMD is installed and setup correctly then a message stating:

```
FATAL ERROR: No simulation config file specified on command line.
```

- To test Gnuplot type:

```
gnuplot
```

  - If Gnuplot is installed correctly a message giving the version of the code should appear and the terminal prompt should look like:

```
gunplot>
```

  - Try making a plot by typing:

```
plot sin(x)
```

  - Exit by typing:

```
exit
```

Getting the Course Files

All course content is available from:

https://sassie-web.chem.utk.edu/training/aps_2016/main.html

Download each days zip file onto your desktop as you progress.