Lab 0: Preparing your laptop for the course – Linux

Four pieces of software are needed to complete this course:

1. VMD – Views and analyses molecular models.
2. NAMD – Performs molecular dynamics simulations.
3. Gnuplot – Plots data
4. 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 are using 64 bit Linux (if not then select the 32 bit versions of VMD and NAMD and correct all paths accordingly)
4. You understand the difference between a text editor and word processor.
5. 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 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

In either case you need to select the 'LINUX_64 OpenGL, CUDA' link 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

- In the terminal, migrate to the download directory.
- Run the command:

```
tar xvfz vmd-1.9.2.bin.LINUXAMD64.opengl.tar.gz
```

- Change into the vmd-1.9.2 directory.
- Open the 'configure' file in a text editor; change the values for $install_library_dir and $install_bin_dir to the directories in which VMD data files and executables should be installed.
    - Note: the $install_bin_dir value should be in your PATH

- With admin access good choices might be:

```
$install_bin_dir="/usr/local/bin"
```

and

```
$install_library_dir="/usr/local/lib/$install_name"
```

- Run the command:

```
./configure
```

This will generate a Makefile based on these configuration variables

- Change into the src directory,
- Type:

```
sudo make install
```

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 Binaries' link
- Select the Linux-x86_64-multicore 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 run the command

```
sudo tar xvfz NAMD_2.9_Linux-x86_64-multicore.tar.gz -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_Linux-x86_64-multicore
```

  3. Save the file

Gnuplot

Download & Installation

You should be able to obtain Gnuplot via your standard package manager, for example:

Ubuntu/Debian:

```
sudo apt-get install gnuplot
```

CentOS:

```
sudo yum install gnuplot
```

Testing NAMD and Gnuplot Installations

To ensue that the various packages are available in your path you will need to start a new terminal. This will ensure that the .bashrc file is read. You can manually do this in an existing terminal using the command:

```
source ~/.bashrc
```

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.