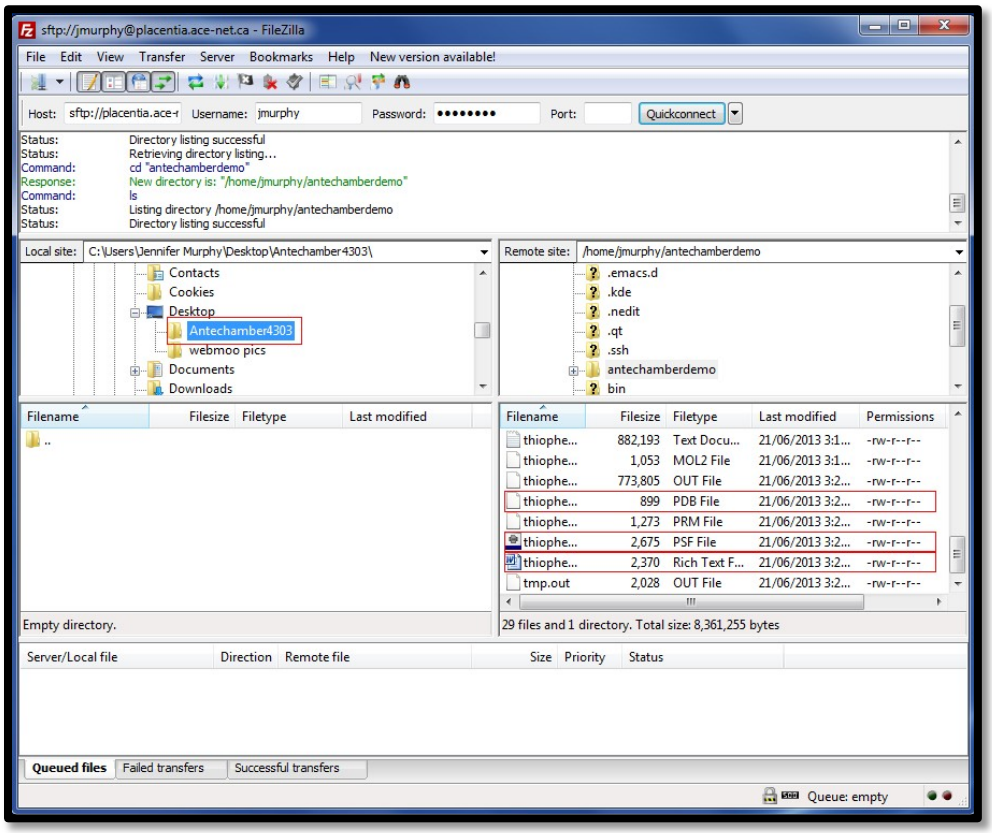
CHEM 4305 Term Project:

Simulating Molecular Liquids

Part 2: Building a Molecular Liquid and Equilibrating the System

18. Get your .psf, .pdb and .rtf back onto the desktop using Filezilla.

This is similar to Step 9. Open Filezilla and make a folder on your desktop to transfer the files to.



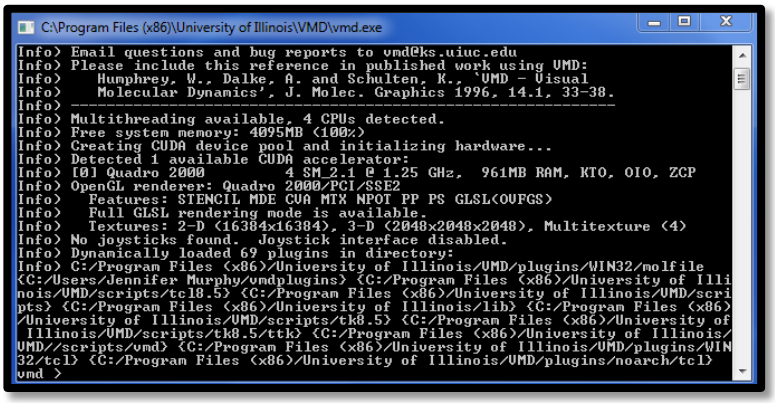
19. Download the liquefy.tcl plugin

Enter the URL: http://www.chem.mun.ca/homes/cnrhome/liquefy.tcl into your web browser. Save the file to your computer.

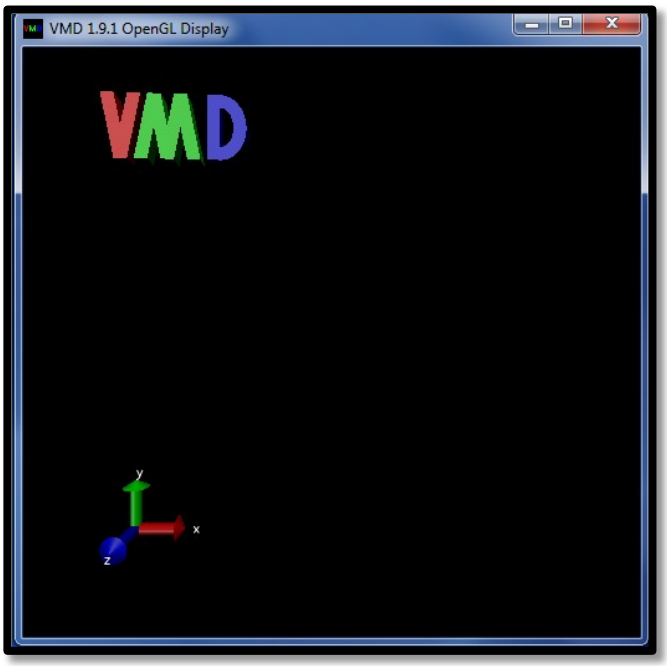
19. Open VMD from the desktop

Find the program "VMD" in your Program Files directory under "University of Illinois." There should be three windows that come up, shown below.

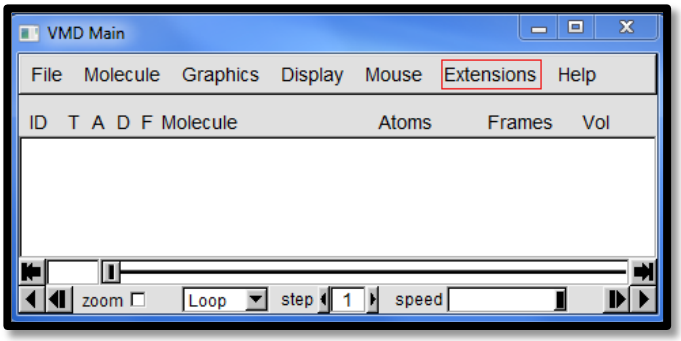
Command Window



Graphics Window



Program Window

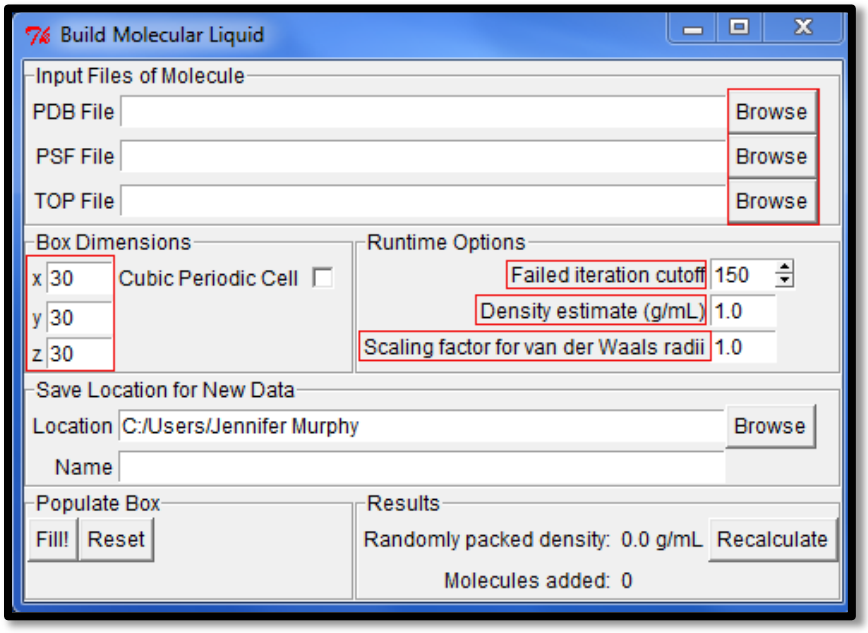


20. Execute the Liquefy Script

In the command window, type the following commands:

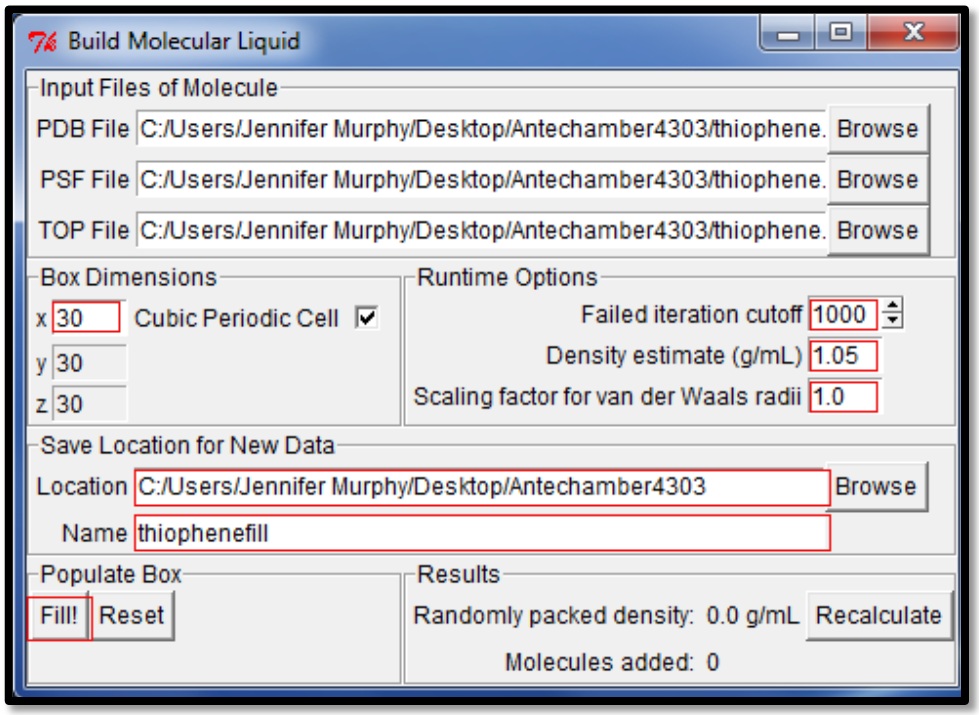
```
vmd > source Downloads/liquefy.tcl
vmd > Liquefy::liquefy_gui
```

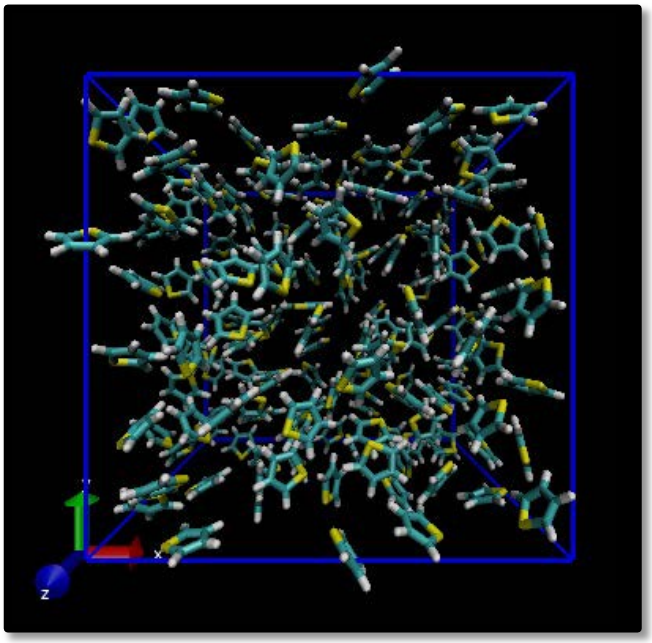
A new window will appear. You will use this extension to build a unit cell of your liquid.



Browse to put in the .pdb, .psf and .rtf files that you have transferred over from placentia in the "Input Files of Molecule" section. For your project, change x, y, and z lengths under "Box Dimensions" to $40\ \text{Å} \times 40\ \text{Å} \times 40\ \text{Å}$. Enter the density of your liquid in the "Density estimate" box. Give your liquid an appropriate name and be sure you save it to the same folder as your other files. When you are sure everything is put in the plugin correctly, click 'fill' to construct the unit cell of randomly oriented molecules. Click the "Fill!" button to generate a unit cell for your simulation.

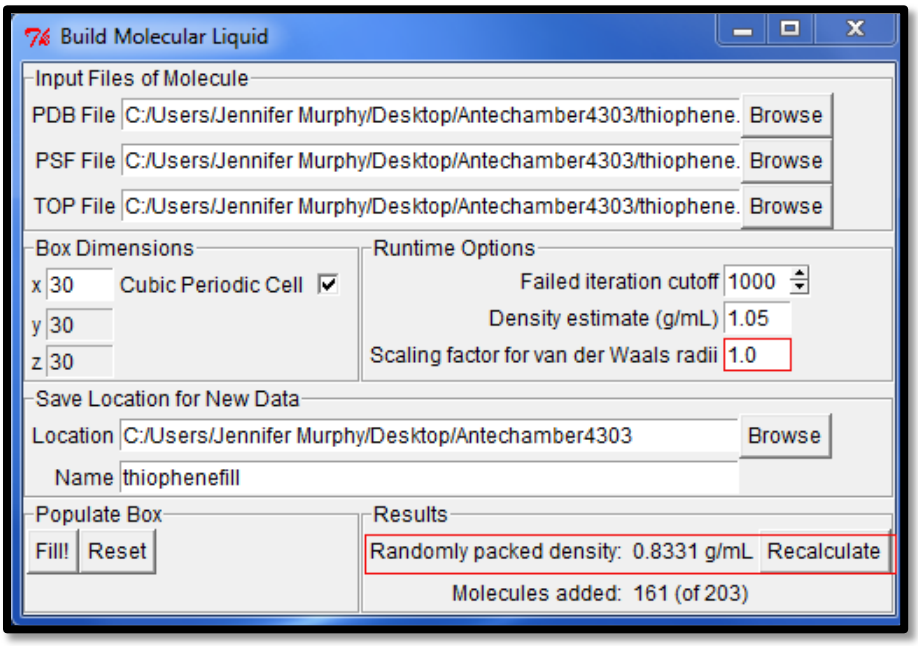
You may need to make several attempts to generate a unit cell with the correct density. You can increase the number of iterations up to a maximum of 1000 and the scaling for the van der Waals radii can be decreased to a minimum of 0.75 if your density is too low. It is OK if your density is too low – the box size will decrease during the simulation to achieve the optimal density.


Build Molecular Liquid
Input Files of Molecule
PDB File C:/Users/Jennifer Murphy/Desktop/Antechamber4303/thiophene. Browse
PSF File C:/Users/Jennifer Murphy/Desktop/Antechamber4303/thiophene. Browse
TOP File C:/Users/Jennifer Murphy/Desktop/Antechamber4303/thiophene. Browse
Box Dimensions
x 30
Cubic Periodic Cell
y 30
z 30
Runtime Options
Failed iteration cutoff 1000
Density estimate (g/mL) 1.05
Scaling factor for van der Waals radii 1.0
Save Location for New Data
Location C:/Users/Jennifer Murphy/Desktop/Antechamber4303 Browse
Name thiophenefill
Populate Box
Fill!
Reset
Results
Randomly packed density: 0.0 g/mL
Recalculate
Molecules added: 0



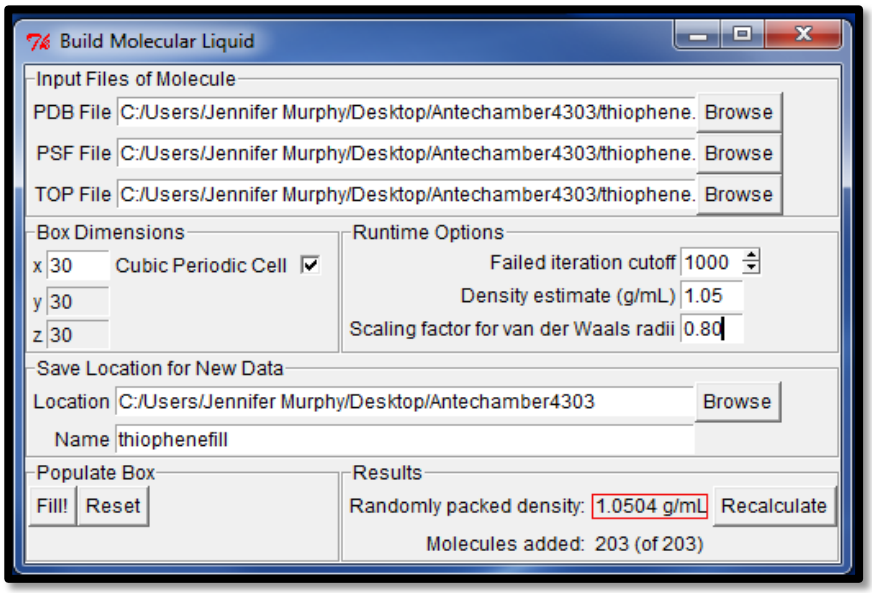
21. Check your density value

Your box should be filled with the molecule like the picture shown above. Look at the main VMD window to see what the density of the liquid is. It's OK if your density differs somewhat from the experimental density; the equilibration simulation will correct this.



As you can see, the density is only 0.8331 g/mL. Now we can play around with the scaling factor for van der Waals radii to get the density approximation closer to the experimental value. Also, only 161 molecules out of a possible 203 based on the dimensions of the box were used, this should be higher. You can start by changing the scaling factor to 0.80 and filling the box again.

In this case, the density after altering the scaling factor works out to 1.0504 g/mL and all 203 molecules are used. This may not be true for your liquid and you may have to play around with the scaling factor before you get a density that is close to the experimental value.



22. Copy the sample NAMD configuration file to your directory on placentia

Edit the NAMD file so that is matches your molecule.

```
$ cp /home/crowley/chm4305/moleculefill.namd .
$ nano moleculefill.namd
```

Your input file will look like the following. You should edit the lines like “moleculefile.pdb” to reflect the names of the PSF and PDB files generated using `Liquefy` and the prm file generated using `antechamber.`

```
# input
coordinates             moleculefill.pdb
extendedSystem          moleculefill.xsc
structure               moleculefill.psf
parameters              molecule.prm
paratypecharmm          on

# output
set output              moleculefill
outputname              $output
dcdfile                 ${output}.dcd
xstFile                 ${output}.xst
dcdfreq                 10000
xstFreq                 10000
binaryoutput            no

binaryrestart           no
outputEnergies          100
restartfreq             1000

fixedAtoms              off

# Basic dynamics
exclude                 scaled1-4
1-4scaling              1
COMmotion               no
dielectric              1.0

# Simulation space partitioning
switching               on
switchdist              9
cutoff                  10
pairlistdist            12

# Multiple timestepping
firsttimestep           0
timestep                1
```

```
stepspercycle           20
nonbondedFreq           2
fullElectFrequency      4

# Temperature control

set temperature         298
temperature             $temperature;  # initial temperature

# Langevin Dynamics
langevin            on;  # do langevin dynamics
langevinDamping     1;   # damping coefficient (gamma) of 1/ps
langevinTemp        $temperature;   # bath temperature
langevinHydrogen    no; # don't couple langevin bath to hydrogens
seed                    12345

# Pressure control
langevinPiston          on
langevinPistonTarget    1.01325; # in bar -> 1.01325 bar = 1 atm
langevinPistonPeriod    2000
langevinPistonDecay     100
langevinPistonTemp      $temperature
useFlexibleCell         no
useGroupPressure        no
fixedAtomsForces        off

# PBC
wrapAll                 on
PME                     yes
PMEGridSpacing          1.0

# Scripting
minimize            1000
reinitvels          $temperature
run                 1000000
```

23. Submit the NAMD simulation to the queue on placentia

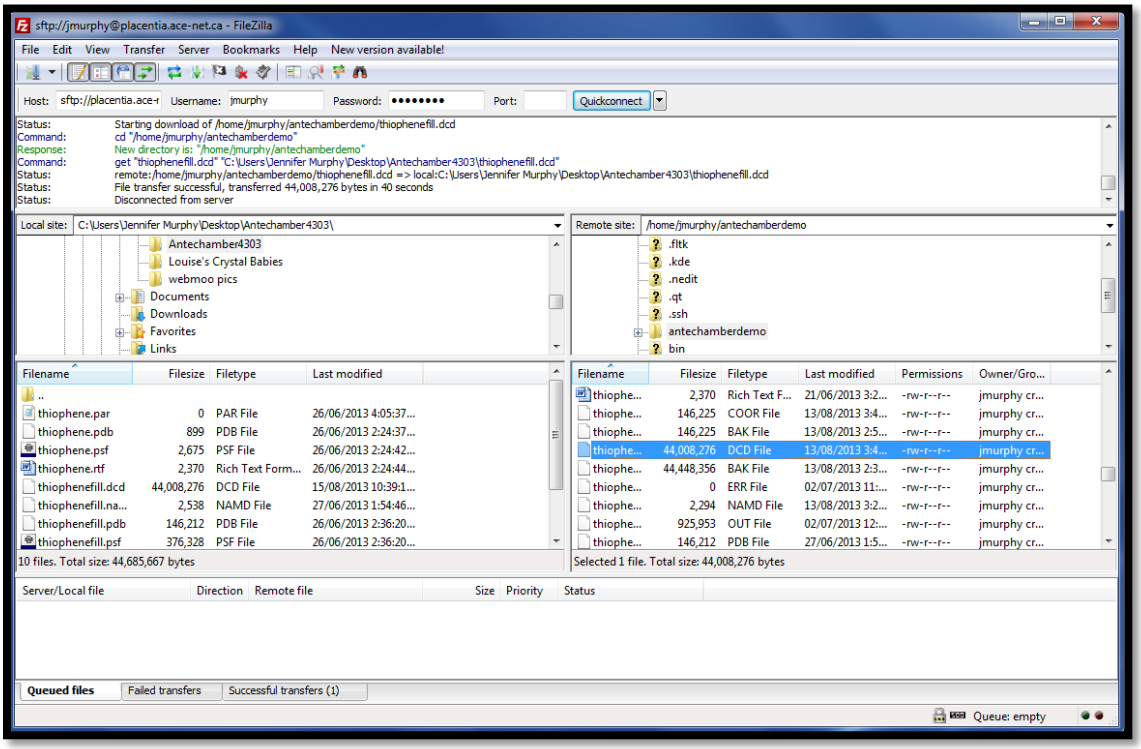
```
$ nano script-2.sh
```

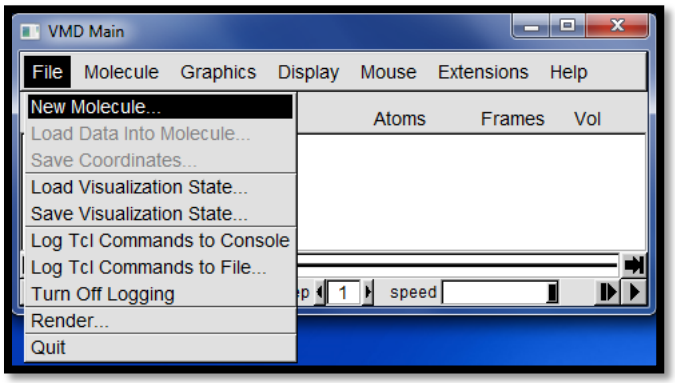
```
#!/bin/bash
#$ -l h_rt=24:00:00
#$ -cwd

module load namd
namd2 moleculefill.namd 1> moleculefill.out 2> moleculefill.err
```

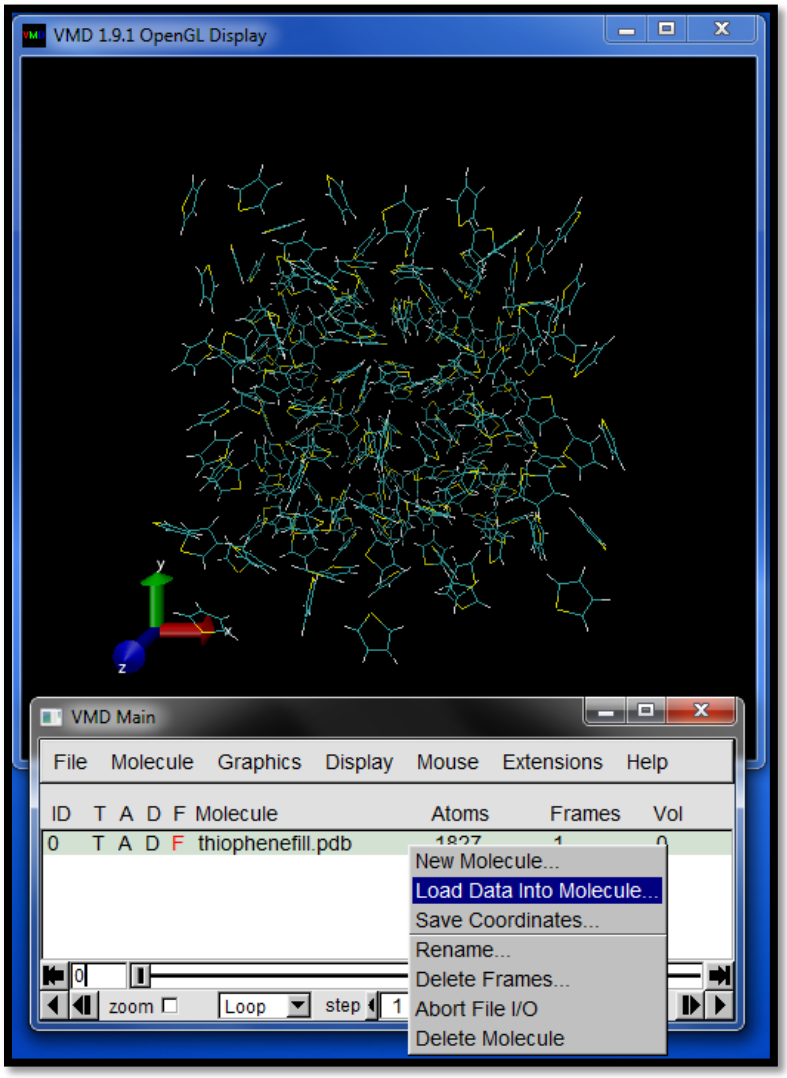
```
$ qsub script-2.sh
```

24. Lights, camera, action!

It is time to check out you movie! The trajectory of your MD simulation will be saved to a DCD file in this directory. To view the trajectory, use filezilla to transfer your .dcd file to your desktop. Open vmd and load your moleculefill.psf. Then, right click on the moleculefill.psf file so that the whole line turns green and a drop down menu comes down. Select 'load data onto molecule' and browse for the thiophenefill.dcd file, click 'load'.




VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
New Molecule...
Load Data Into Molecule...
Save Coordinates...
Load Visualization State...
Save Visualization State...
Log Tcl Commands to Console
Log Tcl Commands to File...
Turn Off Logging
Render...
Quit
Atoms
Frames
Vol
1
speed


VMD 1.9.1 OpenGL Display
y
x
z
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
0 T A D F thiophenefill.pdb
New Molecule...
Load Data Into Molecule...
Save Coordinates...
Rename...
Delete Frames...
Abort File I/O
Delete Molecule
0
zoom
Loop
step
1

25. Extracting energies/volumes and making graphs in gnuplot.

Use the following commands to extract the potential and total energy from your .namd output file.

```
$ grep "^ENERGY": moleculefill.out > energy_eq.txt
```

You need to look at your .namd output files to see what columns the potential and total energy are in. The potential energy is in 14 and total energy is in 12. An example, from the end of an output file is shown below. The timestep is in column 2.

```
ETITLE:      TS           BOND          ANGLE          DIHED          IMPRP
ELECT            VDW
 BOUNDARY           MISC        KINETIC               TOTAL           TEMP
POTENTIAL         TOTAL3        TEMP
AVG             PRESSURE      GPRESSURE          VOLUME       PRESSAVG      GPRESSAVG

ENERGY:  100000      2418.5540       435.0343       304.9260        35.2647          -
1108.3803      -330.4578
   0.0000         0.0000      1580.1563           3335.0973       290.1554
1754.9410      3354.8077       291.0
053           1278.5353       751.4656      27477.3849        15.7136         3.1915
```

Write a script for your graphs, copy and paste the one below.

```
$ nano liquidenergygraphs_eq
```

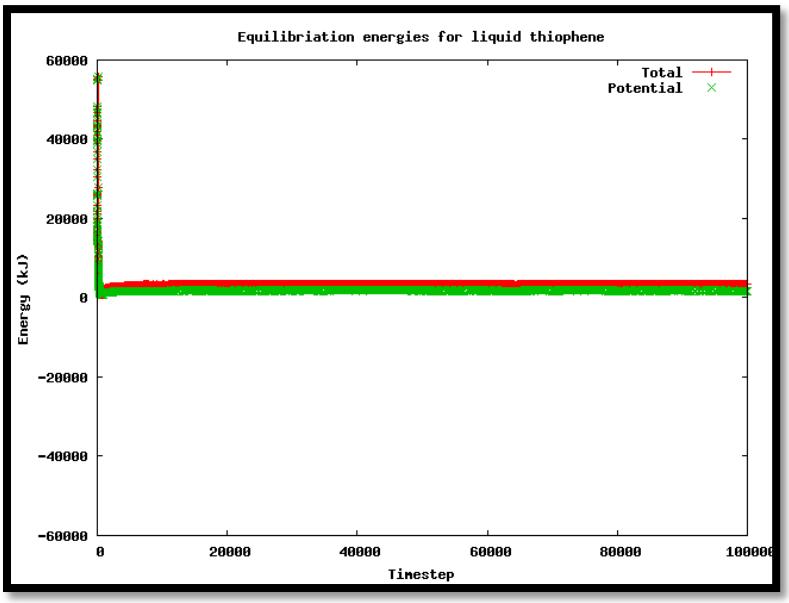
```
# Gnuplot script file for plotting data in file "energy_eq.txt"
      # This file is called   liquidenergygraphs_eq
      set terminal png
      set output "liquidenergygraphs_eq.png"
      set   autoscale                        # scale axes automatically
      unset log                              # remove any log-scaling
      unset label                            # remove any previous labels
      set xtic auto                          # set xtics automatically
      set ytic auto                          # set ytics automatically
      set title   "Equilibriation   energies for liquid thiophene"
      set xlabel "Timestep"
      set ylabel "Energy (kJ)"
      set key auto
      set xr [0.0:100000]
      set yr [-60000:60000]
      plot    "energy_eq.txt" using 2:12 title 'Total' with linespoints , \
                "energy_eq.txt" using 2:14 title 'Potential' with points
```

We are using GNUPLOT to make our graphs. For more information about GNUPLOT, check out this website: http://people.duke.edu/~hpgavin/gnuplot.html

```
$ module load gnuplot
$ gnuplot

      G N U P L O T
      Version 4.6 patchlevel 0    last modified 2012-03-04
      Build System: Linux x86_64

      Copyright (C) 1986-1993, 1998, 2004, 2007-2012
      Thomas Williams, Colin Kelley and many others

      gnuplot home:     http://www.gnuplot.info
      faq, bugs, etc:   type "help FAQ"
      immediate help:   type "help"  (plot window: hit 'h')

gnuplot> load 'liquidenergygraphs_eq'
```

To get your graph, you must transfer your liquidenergygraphs_eq.png file back to your PC using Filezilla.

You may need to adjust the scale of the plot to a value that's appropriate for your data. You can adjust the scale by changing the "`set yr [-60000:60000]`" line in the gnuplot input file.

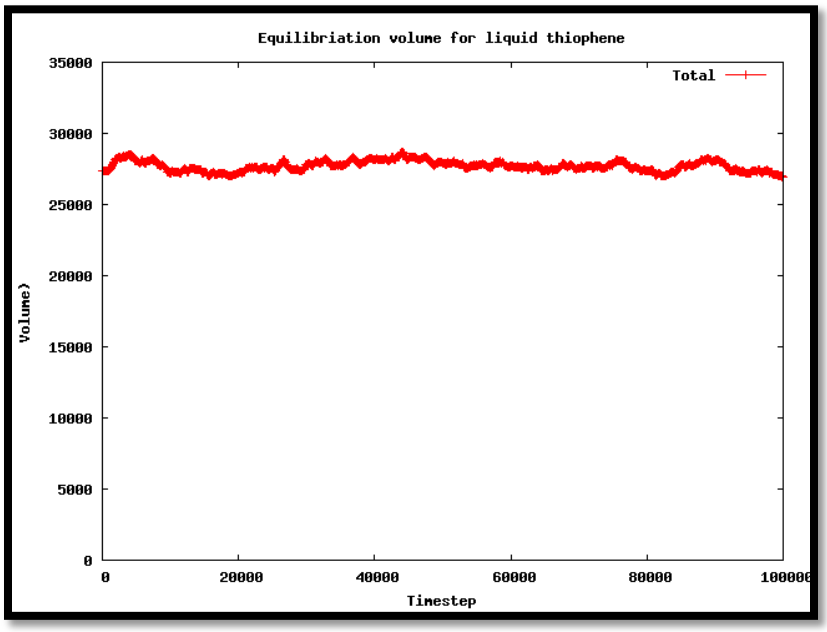


You should also plot of volume to make sure density of the simulation has reached equilibrium. Note: Volume is in column 19.

```
$ nano liquidvol_eq
```

```
# Gnuplot script file for plotting data in file "energy_eq.txt"
      #     This file is called   thiophenevol_eq
      set terminal png
      set output "liquidvol_eq.png"
      set   autoscale                                # scale axes automatically
      unset log                                      # remove any log-scaling
      unset label                                    # remove any previous labels
      set xtic auto                                  # set xtics automatically
      set ytic auto                                  # set ytics automatically
      set title   "Equilibriation   volume for liquid thiophene"
      set xlabel "Timestep"
      set ylabel "Volume)"
      set key auto
      set xr [0.0:100000]
      set yr [0:35000]
      plot    "energy_eq.txt" using 2:19 title 'Volume' with linespoints
```

```
$ gnuplot

      G N U P L O T
      Version 4.6 patchlevel 0    last modified 2012-03-04
      Build System: Linux x86_64

      Copyright (C) 1986-1993, 1998, 2004, 2007-2012
      Thomas Williams, Colin Kelley and many others

      gnuplot home:     http://www.gnuplot.info
      faq, bugs, etc:   type "help FAQ"
      immediate help:   type "help"  (plot window: hit 'h')

gnuplot> load 'liquidvol_eq'
```



Stage 2 Complete

Download the initial PDB generated by Liquefy and the final coordinates from the NAMD simulation (moleculefill.coor), and the PNG files of the plots of the cell volume and potential energy to show convergence of this simulation.