

# HPRC Short Course: Classical Molecular Dynamics with NAMD

This tutorial is designed specifically for TAMU HPRC's terra cluster.

## I. Set up environment and prepare protein with VMD

1. Connect to the HPRC Terra Portal: <https://portal-terra.hprc.tamu.edu/>
2. Launch a VNC Session. Under Interactive Apps, choose VNC, request a session with:

Number of hours: 3  
Number of cores: 28  
Total Memory (GB): 54  
Node type: GPU

and then click Launch. When the desktop is ready, click the launch noVNC in a new Tab button. You should now see a simple desktop with a terminal.

3. Prepare your environment for this tutorial. In the terminal, type:

```
source /scratch/training/namd/pre.bash
```

Note that the script executes the following module commands needed for vmd.

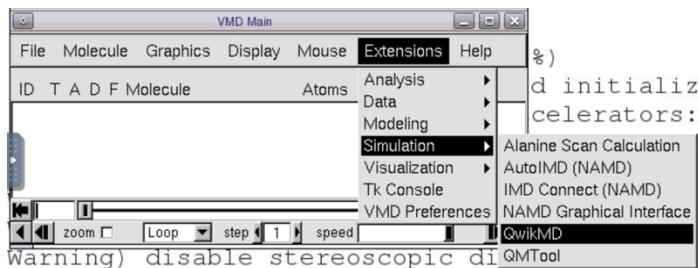
```
ml purge
```

```
ml VMD/1.9.3-LINUXAMD64-opengl
```

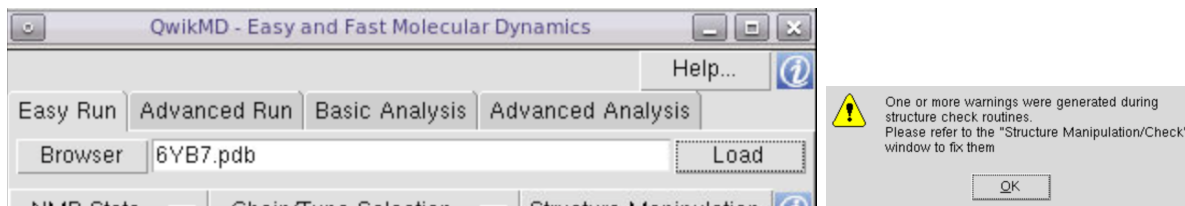
4. Run the VMD software. Type in the terminal:

```
vglrun vmd
```

5. In the VMD main panel, select Extensions > Simulation > QwikMD

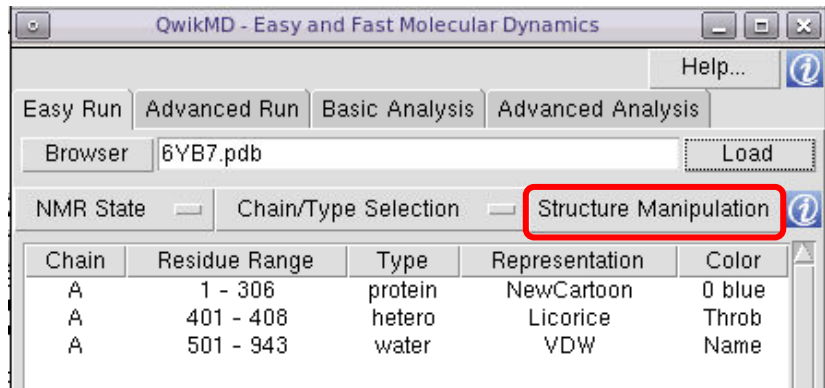


6. In the QwikMD panel, type in the file name: **6YB7.pdb**, and click Load. Alternatively, you can click the Browser button and load the file. Click OK to accept warnings with the structure.

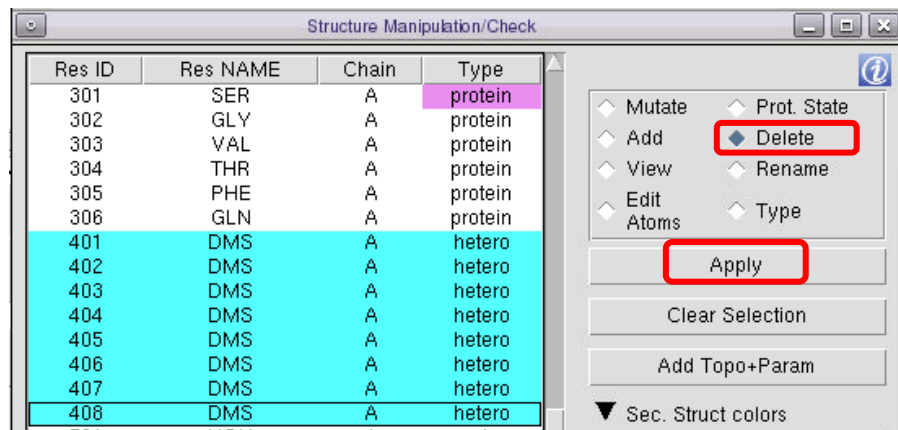


# HPRC Short Course: Classical Molecular Dynamics with NAMD

7. In the QwikMD panel, click Structure Manipulation. In the new window, under the “Structure Check” box, click “Topologies and Parameters” to check the issues found in the structure.



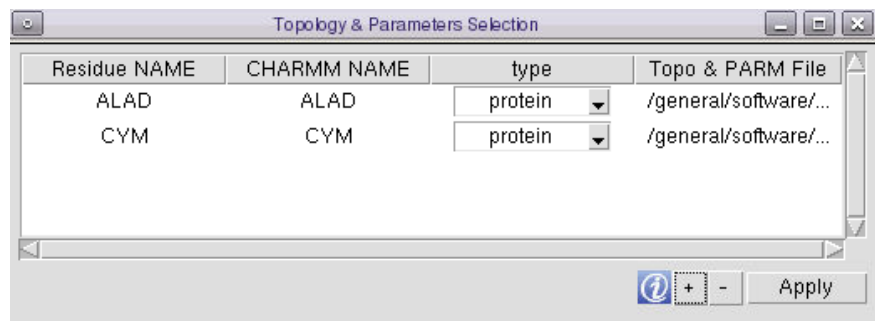
8. Scroll down and select/highlight residue 401 to 408. On the right side of the window, choose delete and click Apply. The residue 401-408 should display in grey color.



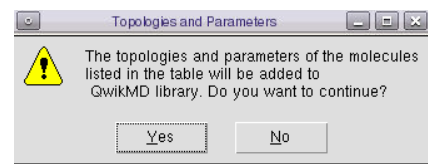
9. Check the structure again by clicking “Check” at the bottom right of the window to make sure the

problems have been fixed (red icons disappear in the Structure Check section).

10. Click “Add Topo+Param”. In the new window, click the “+” button and select “top\_all36\_prot.rtf”, then click “Open”. Then click Apply.



11. The warning window shows that “The topologies and parameters of the molecules listed in the table will be added to QwikMD library”, click yes to continue.



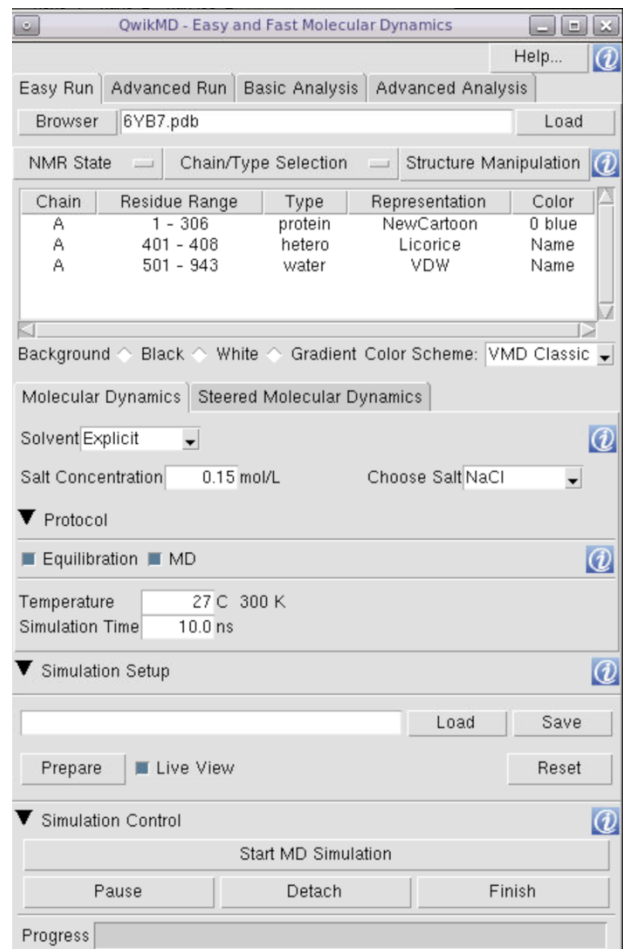
# HPRC Short Course: Classical Molecular Dynamics with NAMD

12. Return to the QwikMD window. In the “Molecular Dynamics” tab, change Solvent to “Explicit”. We are going to run both “Equilibration” and “MD” calculations, so check both options under the “Protocol” section. Keep the temperature at 27C and change the simulation time to **1.0 ns**.

13. In the “Simulation Setup” menu, check “Live View” and click “Prepare”. In the pop-up window, save the input file as 6yb7 in the /scratch/user/username/hprc\_sc\_namd/ directory.

When the Prepare button is pressed, a series of operations is performed to prepare the system and the simulation configuration files with the settings selected by user. Two folders will be created in the working directory: files created during the preparation step are stored in the “setup” folder, while files needed to run the MD simulations are stored in the “run” folder.

When finished, a yellow box should appear around the protein. You can close vmd now. In the VMD Main menu, navigate to File > Quit.



## II. Edit configuration files and run simulations with NAMD

1. Go to the “run” folder by typing in the terminal:

```
cd $SCRATCH/hprc_sc_namd/6yb7/run/↵  
ls↵
```

2. Now that you have the pdb and psf files for solvated 6yb7, along with the parameter file for proteins in general. You will edit the QuickMD generated NAMD configuration files to equilibrate your protein-water system.

3. Modify the configuration file by typing into the terminal:

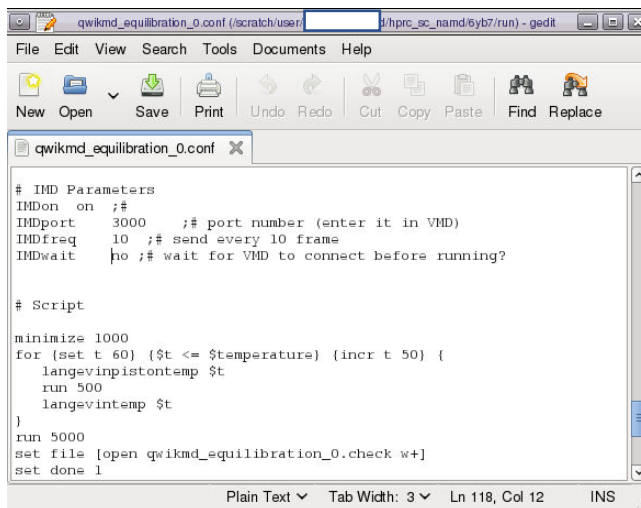
```
gedit qwickmd_equilibration_0.conf↵
```

# HPRC Short Course: Classical Molecular Dynamics with NAMD

(Line number is displayed on the status bar on the bottom of the window)

- Change line 118, IMD wait to **no**
  - Change line 124, {incr t 50}
  - Change line 129, run **5000**
- Save and exit.

4. Modify the production configuration file by typing into the terminal:  
**gedit qwikmd\_production\_1.conf**↵  
Change line 106, IMD wait to **no**  
Change line 111, run **5000**  
Save and exit.



```
# IMD Parameters
IMDon on ;#
IMDport 3000 ;# port number (enter it in VMD)
IMDfreq 10 ;# send every 10 frame
IMDwait no ;# wait for VMD to connect before running?

# Script
minimize 1000
for {set t 60} { $t <= $temperature } {incr t 50} {
  langevinpiston temp $t
  run 500
  langevin temp $t
}
run 5000
set file [open qwikmd_equilibration_0.check w+]
set done 1
```

5. Copy the job file to your working directory:  
**cp /scratch/training/namd/md.job md.job**↵  
and submit the job by typing:  
**sbatch md.job**↵

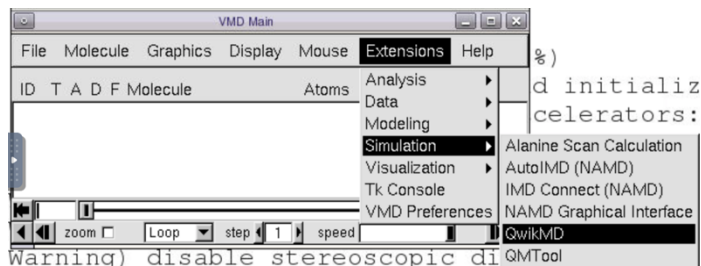
6. Check the status of all jobs for a user: **squeue -u username**↵  
The job takes about 20 minutes to complete.

## III. Visualization and Analysis with VMD & the QuickMD plugin

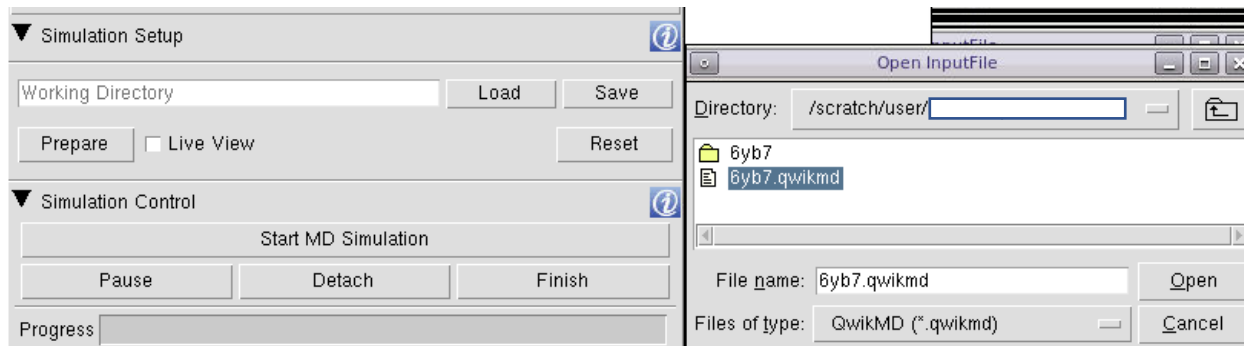
1. When the calculation is finished, open VMD by typing in the terminal:

**vglrun vmd**↵

2. In the VMD main panel, select  
Extensions > Simulation > QwikMD



3. Under Simulation Setup, click on Load. In the new Open InputFile window, Navigate to the directory with the 6yb7.qwikmd file, select 6yb7.qwikmd, and click Open:



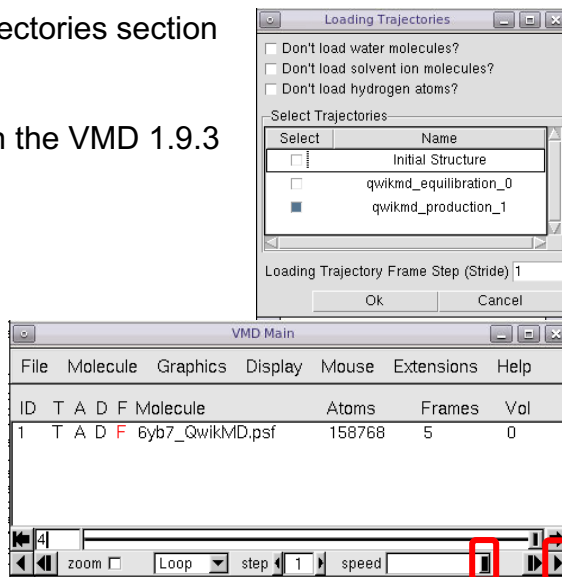
# HPRC Short Course: Classical Molecular Dynamics with NAMD

Select `qwikmd_production_1` in the Select Trajectories section and click Ok:

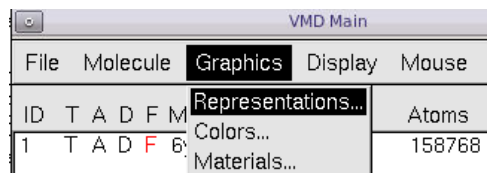
You should now see your protein with waters in the VMD 1.9.3 OpenGL Display window.

## 5. View the trajectory.

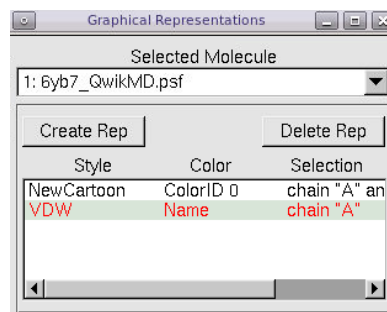
- In the VMD Main window, click on the Play button in the lower right hand corner:
- Change the speed of the playback using the slider



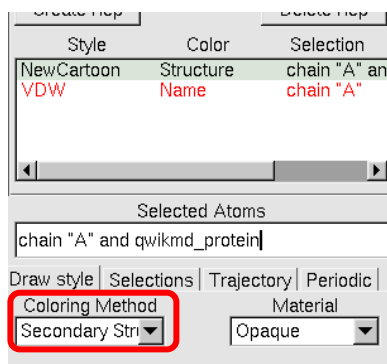
- open the Graphics > Representations... menu



- Turn off the waters by double clicking on the line that starts with VDW. It should turn red and the waters should no longer be displayed. You can turn them back on by double clicking the VDW line again.



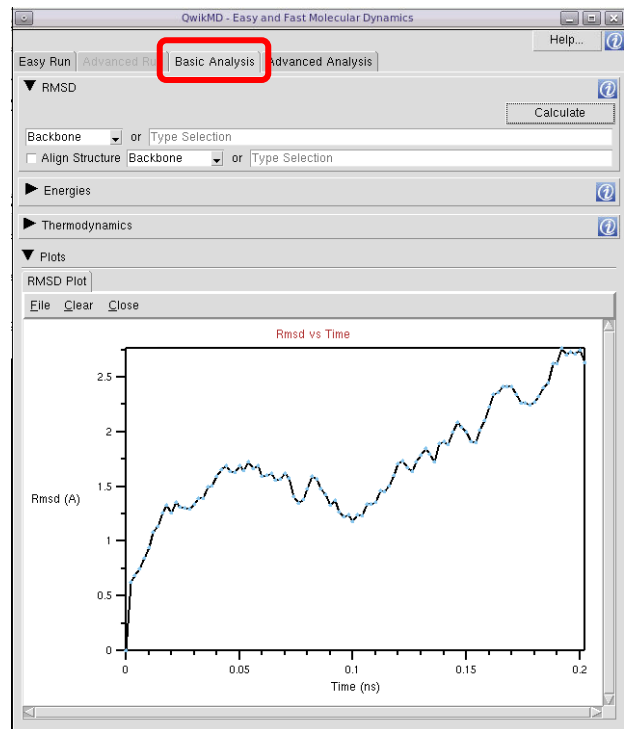
- Color the NewCartoon by secondary structure. Click once on the line that starts with NewCartoon and select Secondary Structure in the dropdown menu under Coloring Method. Your protein should now display with a Cartoon representation that is colored by secondary structure (ie. Beta strand = yellow, Alpha Helix = Magenta, etc)



# HPRC Short Course: Classical Molecular Dynamics with NAMD

## 4. Basic Analysis.

- Click on the Basic Analysis Tab in the QwikMD – Easy and Fast Molecular Dynamics window.
- Expand the RMSD section by clicking on the black triangle next to RMSD
- Click Calculate
- Expand Energies and Plot the different components: Total, Kinetic, Potential, Bond, Angle Dihedral, VDW
- Expand Thermodynamics and plot the different components: Temperature, Pressure, Volume



## 5. Advanced Analysis

- Click on the Advanced Analysis Tab in the QwikMD – Easy and Fast Molecular Dynamics window.
- Using the Analysis drop down menu, investigate the different analysis options: H Bonds, SMD Forces, RMSF, SASA, etc

