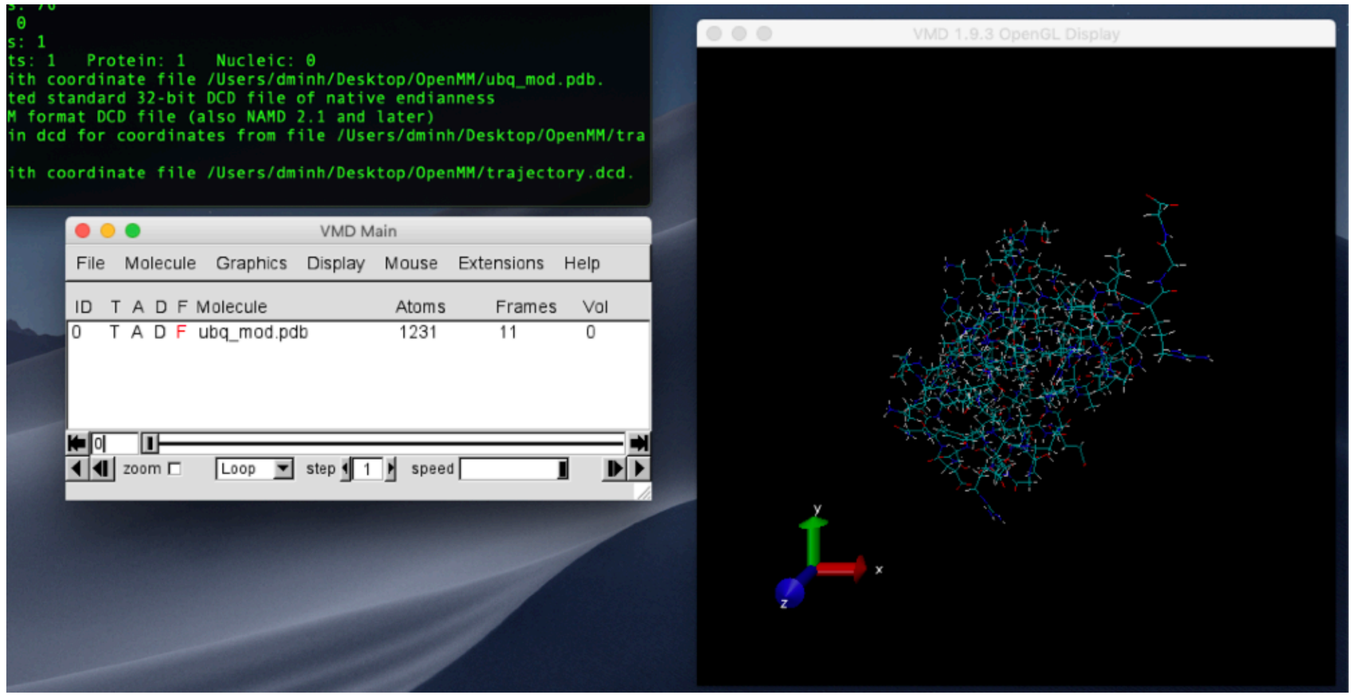
- Now look at the “VMD Main” window
  - “Frames” reads 11 instead of 1
  - You can use the bottom of the window to start a movie and control where we are
- There probably won’t be much going on in your movie, but all of molecular dynamics is just like this, just rinse and repeat



Some complications

- Most simulations are not going to be this easy to set up
  - Crystal structures may have missing atoms, which often can be added by homology modeling
  - The added hydrogens should depend on the pH you're trying to model
  - You need to do extra work for non-standard residues, cofactors, and ligands
  - Most of the time it is better to simulate with water
  - For certain systems, you will need to build a membrane
- You usually need much longer simulations to get publishable results
  - GPU computing provides significant acceleration
  - Calculations will usually be done remotely
    - XSEDE supercomputer
    - Google/Amazon cloud
- We will help each group with all of these