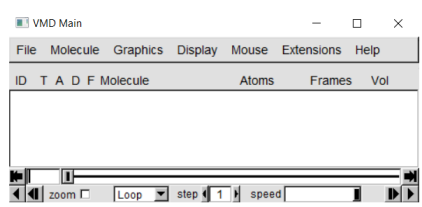
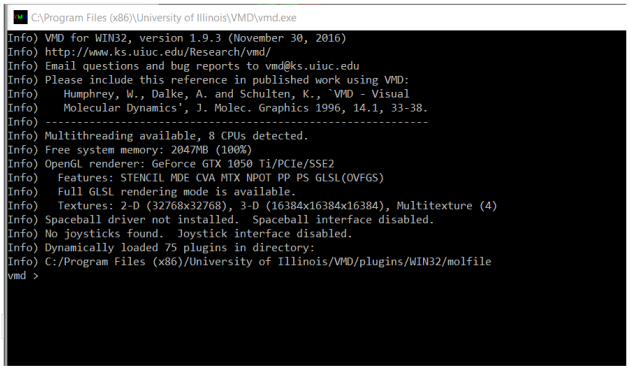
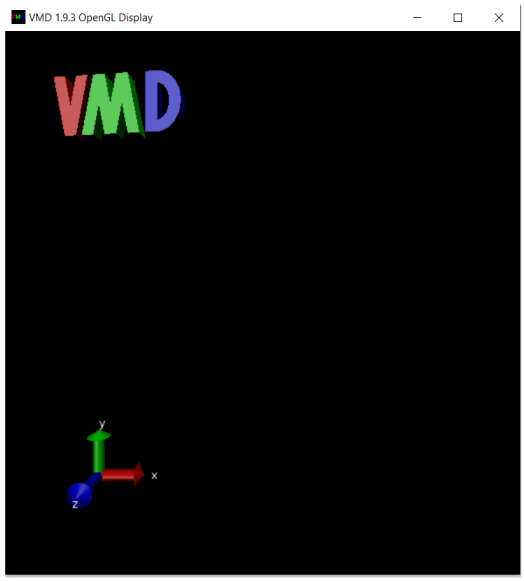
How to use VMD:

Before anything you have to install the program. Please go to https://www.ks.uiuc.edu/Research/vmd/ and download (Download VMD – on the left) the appropriate version of the program for your operating system. Registration is free. IF you are having issues, I have provided movies (mp4) of the simulations, however, using VMD will be much more informative and will also give you some hands-on experience with a useful tool for visualizing PDB (Protein Databank) structures. Other programs are available that can accomplish this task, however VMD is one of the most widely used in the molecular dynamics communities.

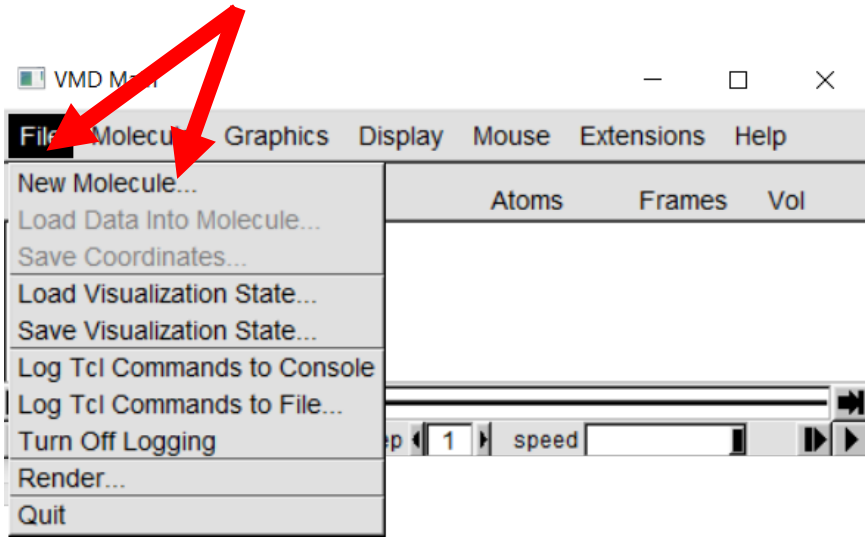
Start the VMD program and you should have three windows pop up. The main window (top left) is where you will do most of the work, the terminal window (bottom left) is where you would load commands and scripts if you were performing analysis and the display window (right) is where simulations will be visualized.



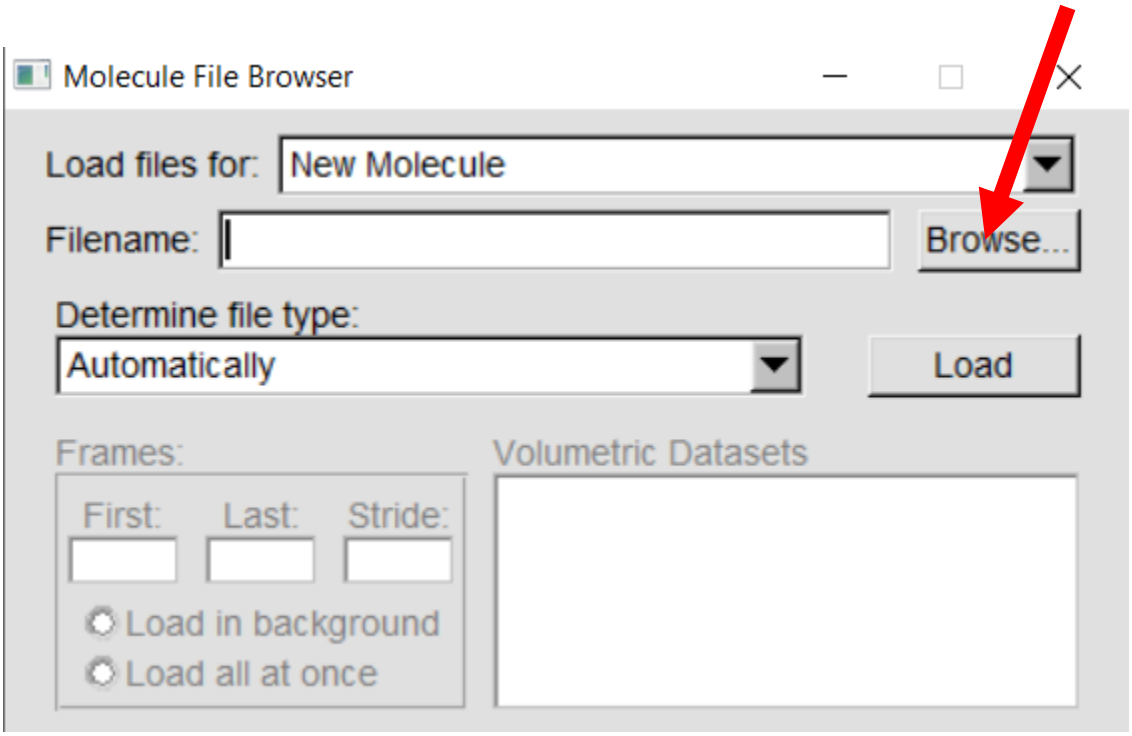




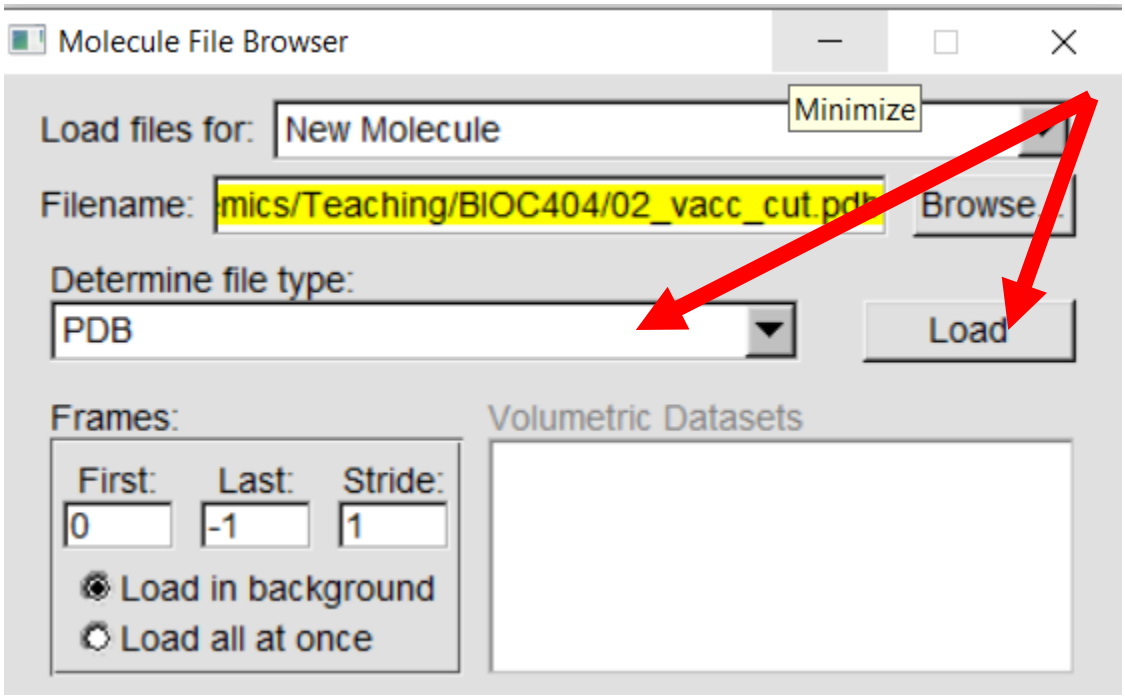
Next you will want to load a new molecule (PDB)



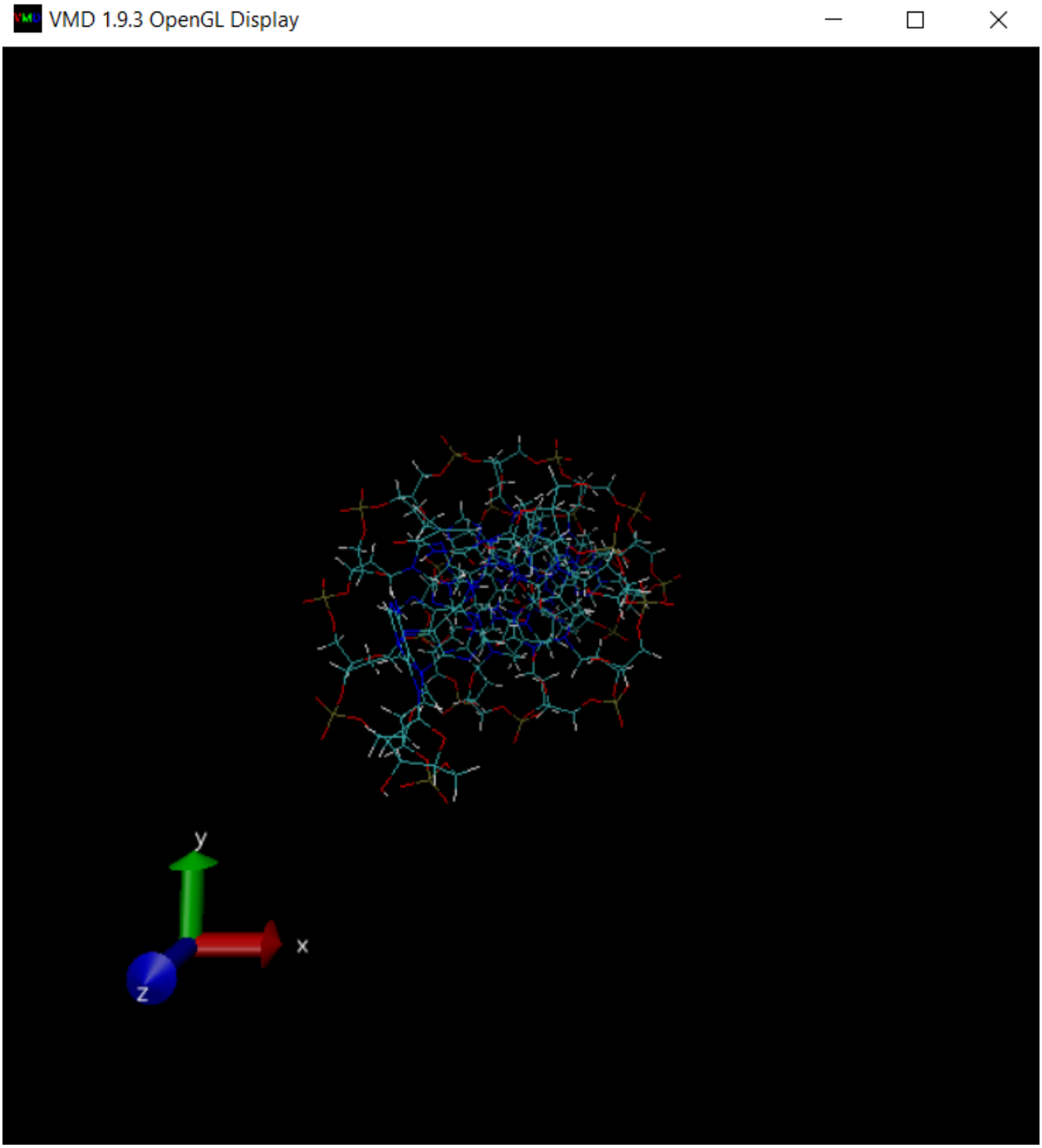
Then you will want to click Browse



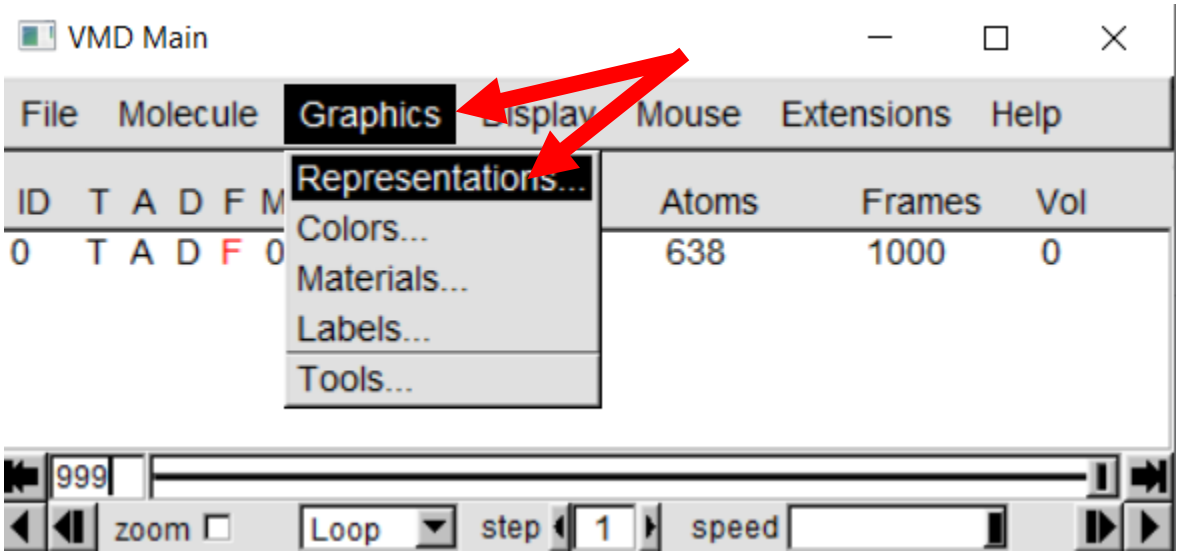
Find the PDB file you want to load and click 'Okay'. Then make sure the file type is what you want it to be (VMD can handle a wide range of inputs from different programs) then click load.

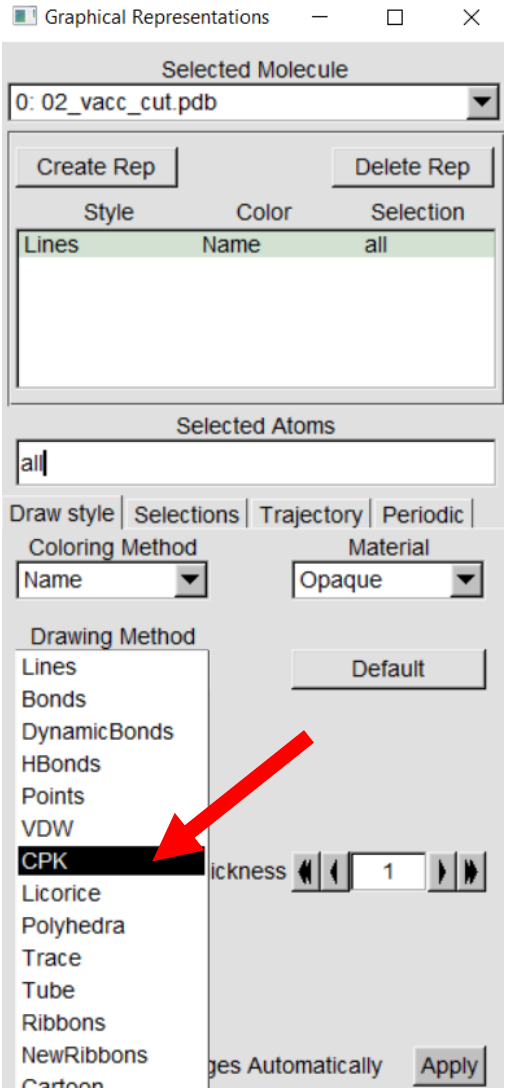


The trajectory should not load and you will see it playing in the display window. You can manipulate the speed as well as play it again using the controls on the main window



I also recommend that you adjust display settings (Also, personal preference, Display -> Orthographic)





Play around with the different styles and see what you like. Finally, It can be very informative to use the Query tools to look at distances, angles, and dihedral (torsions) in the simulations.