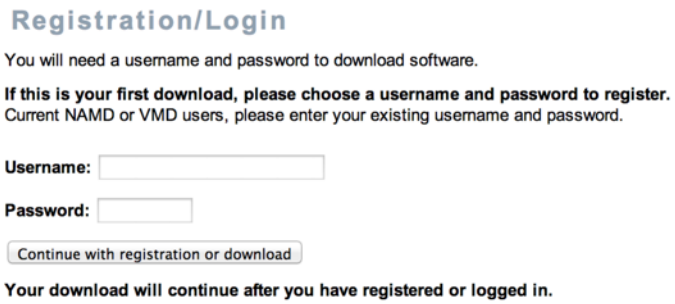
Converting a Binary Trajectory to the Multi-Frame PDB Format using Visual Molecular Dynamics

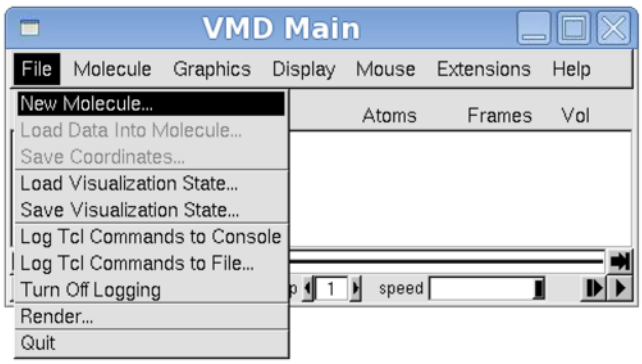
Many programs are capable of saving trajectories to the multi-frame PDB format. One free option is Visual Molecular Dynamics (VMD), produced by the Theoretical and Computational Biophysics Group at the University of Illinois at Urbana-Champaign.

Download VMD for free from http://www.ks.uiuc.edu/Research/vmd/. Note the download section on that page:

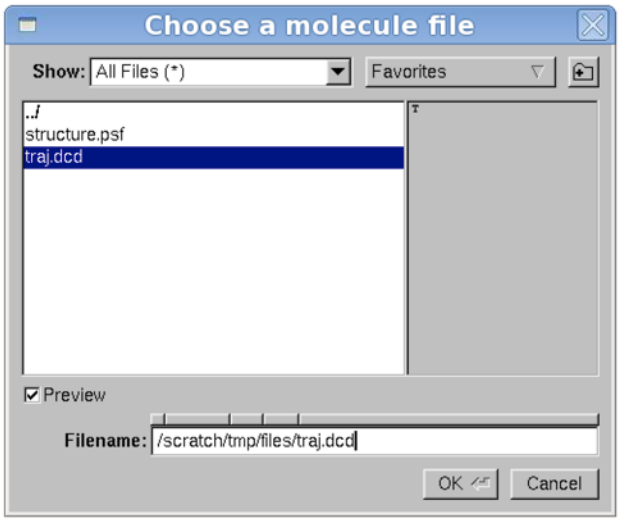
After selecting your operating system, a brief registration is required:



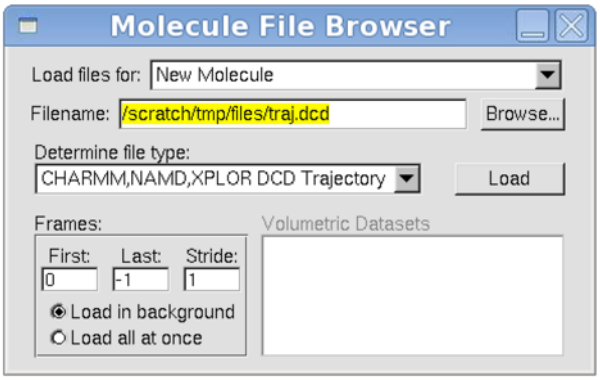
2. After downloading, installing, and running VMD, load your binary trajectory files. For this tutorial, I'll use a CHARMM PSF file, which contains information like atomic connectivity and partial atomic charges, and a CHARMM DCD trajectory, which contains atomic coordinates.



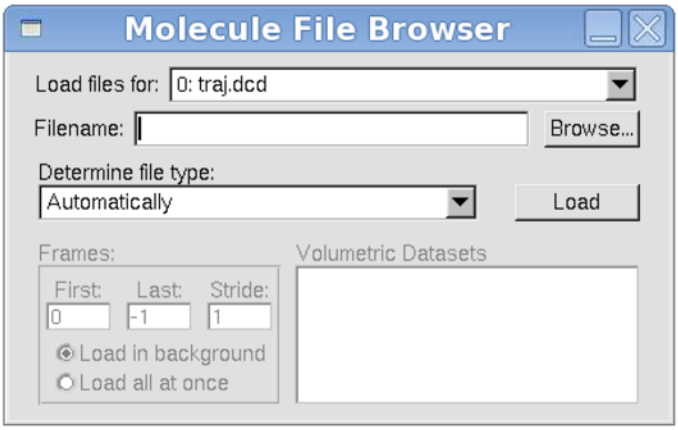
Click the browse button, select the first file (DCD in this case), and press “OK”.



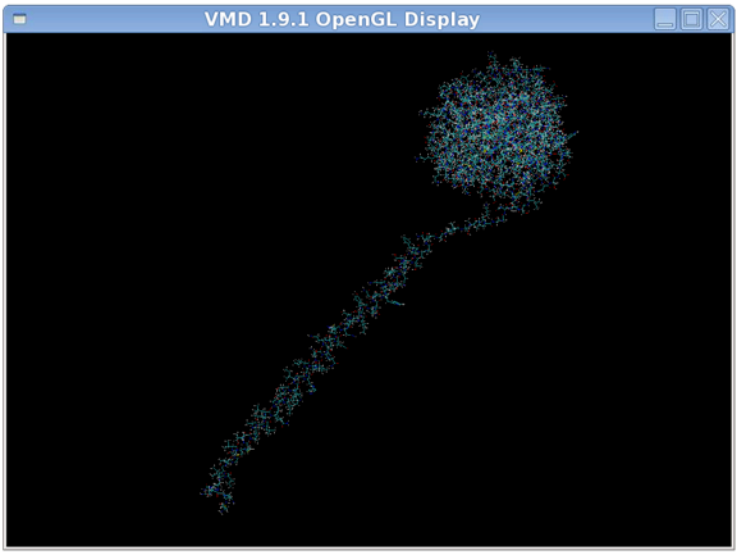
Now click the “Load” button to load the specified file into VMD.



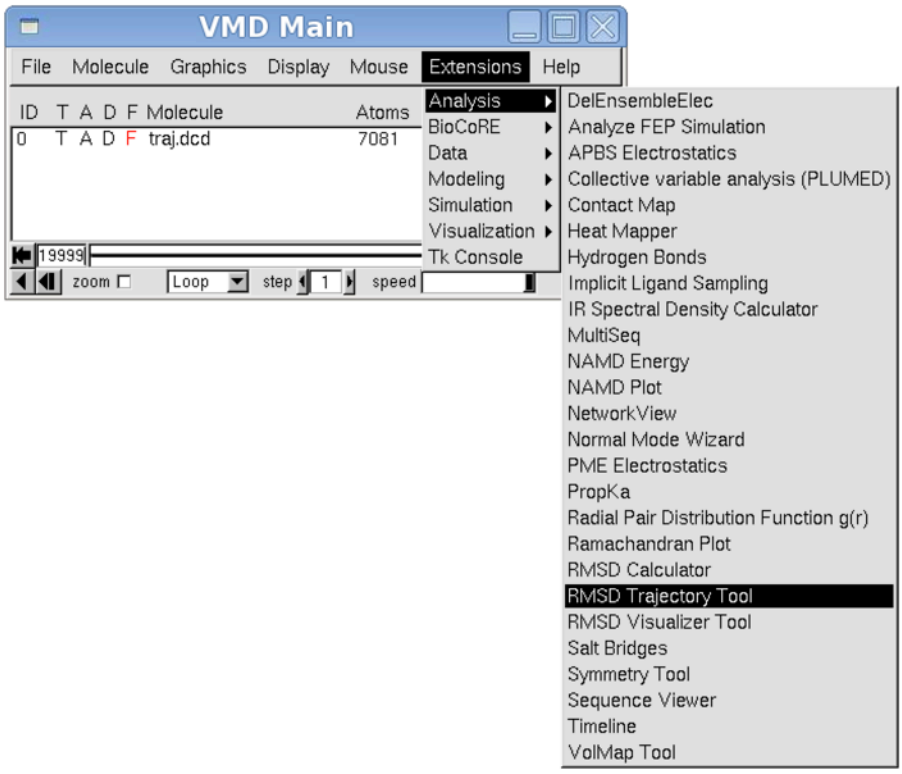
Making sure the “Load files for” field specifies the DCD file now in memory, click on “Browse” again.



Select the PSF file, press “OK”, and press “Load”, as before. You have now specified both the atomic coordinates and connectivity of your system, so it will appear in VMD’s main visualization menu:

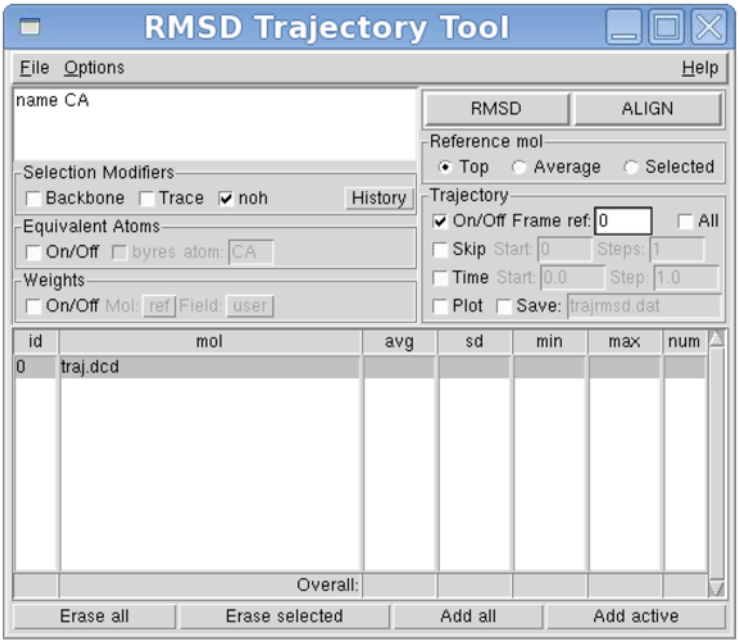


If you haven’t already done so with another program, align all the frames of your MD trajectory. In the main VMD window, click on Extensions → Analysis → RMSD Trajectory Tool.



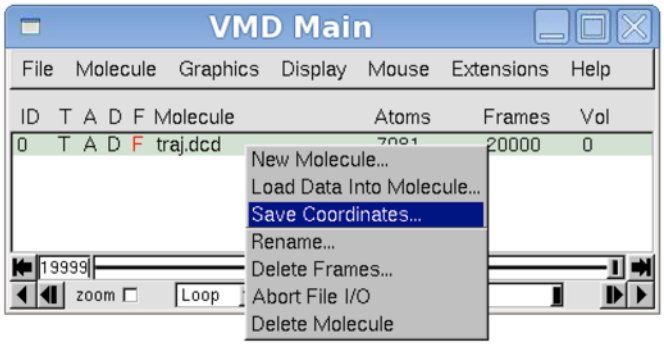
In the main text box, use a VMD atom selection to specify which atoms to use in the alignment. You can learn more about VMD atom selections here: http://www.ks.uiuc.edu/Research/vmd/vmd-1.3/ug/node132.html

For the purposes of this example, I'll align by all protein alpha carbons.

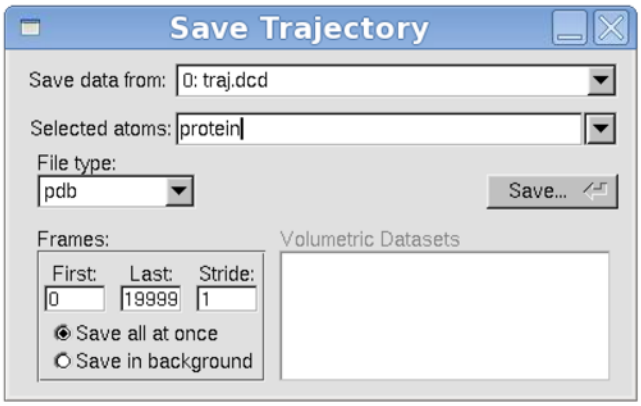


Click the "ALIGN" button to perform the alignment.

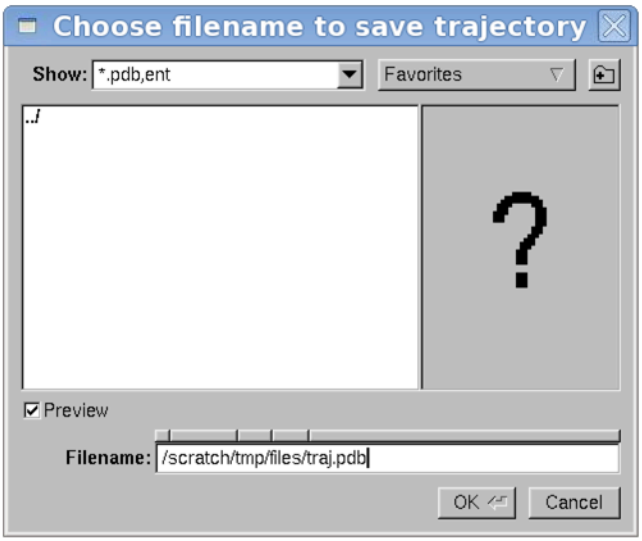
With your trajectory aligned, you're now ready to save it in the multi-frame PDB format. In the main VMD menu, right click on the file and select "Save Coordinates…"



In the "Selected atoms" field, use a VMD atom selection to specify which atoms to save to the multi-frame PDB trajectory. Given that you wish to measure pocket volume, be sure not to include non-receptor atoms that might occupy the pocket. The selection "protein" is often ideal, since it excludes other system components like solvent molecules and counter ions.



Note that the "File type" is "pdb" by default. Click Save, specify the file name, and press "OK".



Your aligned, multi-frame PDB trajectory is now ready for POVME analysis.