Chemistry 438/550: Computational Chemistry, Spring 2020

Homework #6, due 1 April

This project will walk you through establishing a computer environment suitable for molecular visualization, especially for looking at the results of MD simulations that we will be carrying out soon.

1. *Install Chimera on a laptop or desktop computer.* One of the disadvantages of computing remotely on a server like Amarel is that the interface is inherently text-based, and doesn't allow things like interactive visualization. To understand what is going on in molecular simulations (especially in biomolecular simulations) one needs to be able to visualize the results in an interactive manner. This requires a local machine (to carry out the graphics) but any reasonably modern desktop or laptop computer should be fine. We are going to use the Chimera program, which is both powerful and well-integrated with MD programs like Amber.

   (a) Please visit www.cgl.ucsf.edu/chimera/. Click on the Download menu item on the left, choose your operating system (MacOSX, Windows, Linux), and download the current production release (version 1.14). Install this in the usual way.

   (b) Send email to me (david.case@rutgers.edu) if you encounter problems.

   (c) [Aside: you will find out later that the Amber tutorials are built to use VMD (Visual Molecular Dynamics), which is a similar program. Unfortunately, VMD can not run on the current version of MacOS (10.15, aka Catalina). If you have a working version of VMD, don't discard it. But it is still worth your time to learn Chimera.

2. *Learn how Chimera works.* Go back to the Chimera home page, and click on "Getting Started". There are four sections here, two on "working with menus" and two on "working with commands". Like many good user interfaces, you can do most things either way. Menus are great when you are just learning what is going on, and commands become more and more useful as you become more experienced. Take the time to work your way through all of these sections; you don't have to literally do everything that is suggested, but explore enough to get a basic understanding of how things work.

3. Learn how to analyze and compare structures. On the Chimera home page, click on "Tutorials", and choose item 4, "Structure Analysis and Comparison". Go through the first three topics: "Background and Setup", "Distances, H-bonds, Contacts", and "Angles, Rotamers, Clashes".

4. From the "Distances, H-bonds, Contacts" portion, find all H-bond distances between Ser21 and the FPS ligand. Put this information (the two heavy atoms involved in the H-bond, and the distance between them) into a file called *lastname.txt* on Amarel. (It's a very small amount of information, so you can just login to Amarel, open a new file with a text editor, and type in the relevant results you see in the Reply Log in Chimera.) "Hand this in" in the usual way:

   ```
   cp lastname.txt /home/dacase/ccb550/homework6
   ```

   (OK: this is a pretty trivial thing to "hand in". The point is to make sure you are actually doing the tutorial. Chimera is an amazingly powerful program, and taking the time to really learn your way around it will pay good dividends for a long time.)