Chemistry 438/550: Computational Chemistry, Spring 2022

Homework #7, due 8 April

The goal of this homework project is to have you work through the beginning parts of of Amber tutorials 5.5, which can be found at ambermd.org/tutorials/basic/tutorial3/index.php. This will guide you through creating a protein system and minimizing its energy.

1. Login to amarel, and execute the following to load the Amber module:

   ```
   module load gcc/7.5  mvapich2/2.3.6  cuda/10.0
   module load amber/20
   ```

   (*Aside*: here's how I figured out the above comands: First, type `module spider amber`, to find information about Amber modules; that tells you that there are three such modules. Then type `module spider amber/20` to see how to load the most recent module.)

2. After doing this, you should be able to confirm that programs like *tleap* and *sander* are now in your PATH, e.g.:

   ```
   $ which tleap
   /opt/sw/packages/gcc-7_4/mvapich2-2_3/cuda-10_0/amber/20/bin/tleap
   ```

   If this has worked, you can type `tleap` on the command line, which will respond with a ">" prompt. Then, if you type `help`, you will get a list of commands that *tleap* understands.

3. Once you have done this, go to tutorial 5.5, at ambermd.org/tutorials/basic/tutorial3/index.php. This tutorial walks you through a protein folding simulation on a fairly short peptide called the *Trp cage*. But I just want you to follow the tutorial up through the minimization step, to the end of section 3. Please modify the tutorial by changing the second amino acid in the peptide from leucine to isoleucine. Build the system as in Section 2, and minimize as in section 3. For the minimization, reduce the number of steps from 1000 to 200. Note that, since you are logged in remotely, you must use tleap (text-based LEaP) rather than xleap (GUI-based LEaP) to carry out the assignment.

4. "Hand this in" by doing the following:

   ```
   cp min1.pdb lastname.txt
   cp lastname.txt /projects/community/classes/ccb550/homework7
   ```

   (Again this is a pretty trivial thing to "hand in". The point is to make sure you are actually learning how to prepare systems in *tleap*. If you have some time, try continuing the tutorial. Note that any long simulations should be submitted through the `sbatch` system.)