Chemistry 438/550: Computational Chemistry, Spring 2020

Homework #9, no due date! nothing to turn in!

We've talked a lot in this course about how to prepare systems and how to run simulations. But we haven't spent much time on analysis tasks. In this assignment, I'd like you to get a basic familiarity with Amber's cpptraj program, which is devoted to this task. Work throught the following two tutorials:

An Introduction to cpptraj

RMSD analysis in cpptraj

Note that the tools here can be used to analyze simulations carried out in many programs, such as Amber, CHARMM, gromacs, LAMMPS, OpenMM, etc. Many parts of *cpptraj* (although not the ones in these first tutorials) require just one or more PDB files as input, so getting familiar with this program may help you with many structural analysis tasks, even those that don't involve MD trajectories.

To give you more time to devote to working on your term papers, I'm not asking anything to be handed in for this assignment.