Project 1: Chem 537 Spring 2022

Due date: 3/18 (Friday of spring break so I can grade over the weekend)

The goals of this project are to ensure that you can go through the process of finding and justifying a classical force fields, go through the equilibration process (testing different aspects of equilibration and algorithms that you use), and to analyze the equilibrium ensemble and compare to known data (from experiment or prior simulations).

IMPORTANT NOTE ABOUT RESOURCES: Please restrict yourselves to submitting no more than 2 jobs at a time, using all of the resources of a single node.

Step 1: Choose a chemical system – these will be simulations of a bulk liquid using cubic periodic boundary conditions. You may choose one of the three following systems:

a) Liquid water at 298K and 1 atm pressure
b) Liquid methanol at 298K and 1 atm pressure
c) Liquid hexane at 298K and 1 atm pressure

Step 2: Choose 2 different box sizes – look through the literature and find examples of the radial distribution function for the relevant pairs of atoms in your chemical system. Based upon the radial distribution function choose 2 box sizes – one where you anticipate the box will be too small and introduce finite size effects and one where you believe the box will be large enough to capture all correlations. To keep some computational expediency, please do not use more than 2000 atoms in a box. The pdf's of the literature RDF papers will be included in the document you turn in.

Step 3: Choose 3 different force fields – look through the literature and find 3 different force fields that describe the intra and intermolecular interactions of these systems. You will include the pdf's of these reference force field literature in the document that you turn in. I suggest sticking with the LJ+Coulomb type for the intermolecular interactions, but you are free to choose others as well. Make sure that for these reference force fields you have radial distribution functions and other properties associated with the force fields so that you can make sure you can reproduce those data after equilibration.

Step 4: Develop 3 different equilibration protocols. The equilibration protocol is defined by the timestep chosen, the specific cycle of ensembles chosen (NVT, NPT, NVE) and their duration. The protocol is also defined by the criterion you develop for determining if the system is equilibrated – you must decide and justify what level of fluctuations are acceptable in each of the variables for thermomechanical equilibrium (V, T, P, E). The different protocols you develop must compare and contrast the effect of 2 different thermostats and 2 different barostats. You will need to discuss how these thermostats and barostats work in your document that you turn in. They must also compare and contrast the effects of different number of and organization of cycles between ensembles. THE GOAL IS TO GET TO EQUILIBRATION AND SO YOU MAY NEED

TO ADAPT YOUR PROCEDURES TO ENSURE THEY ACTUALLY LEAD TO AN EQUILIBRATED SYSTEM.

Step 5: Go through your equilibrations and analyze the performance of the equilibration procedures AND the fidelity of the different force fields you have chosen and box sizes you have chosen.

Step 6: To be turned in for this project will be a word document (probably about 5 pages) that is organized as follows:

Overview:

A. Description of chemical system (this includes the box sizes, number of molecules in each box (in a table) and the force fields described). You will describe the features of the force field chosen, and include in a table the terms and values for the force field.
B. Description of the equilibration procedures.
C. Description of the analyses performed and criterion set out for equilibration. Include any jupyter notebooks used in your analysis when you upload onto your github.

Results and Discussion:

A. For each chemical system and equilibration procedure (of each box size and force field chosen) – demonstrate that the chemical system is at equilibrium. You may want to label them – for example: Chemical System 1, XXX Force Field, Equilibration Procedure 1.
B. Using literature RDF's and other physical properties identify which set of box sizes, force fields and equilibration procedures align most closely with experimental data or prior simulation data. Show the RDF's and tabulate any other properties calculated for comparisons with the experimental data. If one equilibration procedure was more computationally expedient please note it. This means that you should keep track of how long it takes for a specific simulation to run given the resources you have requested.