HOMEWORK 7A: MC AND MACROMOLECULES

Due electronically April 18 at midnight

In this homework, you will revisit your lattice sums codes in order to create an atomic scale Monte Carlo simulation, which you will compare to a LAMMPS result from Homework 6. You will also explore MD for a polymer molecule. For this homework, you will need:

- **atommc.py**: python file where you will implement the atomic MC code.
- **mcinput.json**: json file containing a sample input deck for atomic MC code.
- **polymer.zip**: LAMMPS files for simulating deformation of polyethylene molecule.
- You will also recycle some codes and files from HW5.
- For general clarification questions, please ask publicly on Piazza. For private questions about the specifics of your code, please email your code to the TA's.

1. In HW6 problem 4, you used MD to study melting of FCC Lennard-Jonesium. We know that MC and MD can model the same phenomena. We will demonstrate this by performing an atomic MC simulation of the same system.

   (a) (4 pts) Implement an atomic scale MC code for FCC Lennard-Jonesium as directed in the prompts in **atommc.py**. Note that you will use codes you wrote for HW5 for the interatomic potential evaluation and lattice sum, as well as the atomic position files. Turn in your completed **atommc.py** file with your solutions filled in.

   - You may verify your code using the default parameters in the **mcinput.json** file. The average system potential energy should be about $\langle U \rangle \sim -88 \pm 4$ and the attempt success fraction should be about $f \sim 0.47 \pm 0.04$. (Remember that MC simulations are statistical; you may need to perform more than one run to test your code.)

   (b) (2 pts) Run 1000 MCS on a 2 x 2 x 2 unit cell simulation with with $\varepsilon = \sigma = 1$, a cutoff radius $r_c = 2$, density = 0.55, temperature $kT = 0.8$, and maximum displacement $D = 0.08$ (that is, the box around the atom has side length $2D$). Report the average system potential energy $\langle U \rangle$ and the attempt success fraction, f.

   (c) (2 pts) Modify the maximum displacement D to achieve approximately $f = 50\%$ successful attempts. Report $\langle U \rangle$ and D. Does it make sense that $\langle U \rangle$ has not changed significantly?

   (d) (2 pts) Note that D is a function of system size and other parameters like kT and density. Keep the same parameters, but find the optimal D for a 3 x 3 x 3 system. Report $\langle U \rangle$ and D. (Note: You may wish to use fewer MCS here.)

   (e) (4 pts) According to the Lennard-Jones phase diagram, the system you are simulating should melt (as you saw using MD last week). Attach a plot of the system potential energy vs. time. Does the system appear to be equilibrated? Attach a 3D plot of the atomic positions in the 3 x 3 x 3 system after 500 MCS. (You can use Ovito, or any plotting program you prefer.) Does the structure show evidence of disordering?

(f) (2 pts) Now, simulate the same system, but with a density = 1.0 and a cutoff radius r_c = 1.58; this system should remain crystalline. For $f \sim 50\%$ successful attempts, report D. Attach a plot of the system potential energy vs. time. Does the system appear to be equilibrated? Attach a plot of the atomic positions. Does this system appear to remain crystalline, as predicted? Does the difference in potential energy between the liquid and the crystal make sense?

2. In this problem, we will solidify your familiarity with LAMMPS and provide you a polymer data set to have in your toolbox. Included with this homework is a ZIP file (**polymer.zip**) containing the LAMMPS files to simulate the deformation and rupture of a single polyethylene molecule. This is a complete atom simulation that uses the Modified Embedded Atom Method (MEAM) interatomic potential for C and H.

Your job is straightforward: Unpack the ZIP file, use the contents to run a LAMMPS simulation, and supply the following information:

(a) (2 pts) How many monomers are in this polyethylene molecule?

(b) (2 pts) Attach an OVITO snapshot of the initial, minimized configuration of the molecule. Be sure to include covalent bonds.

(c) (2 pts) What does this simulation do? Which group of atoms does not move? Which group of atoms moves fastest? What is the final outcome?

(d) (2 pts) Attach an OVITO snapshot of the final configuration of the molecule, and indicate where rupture occurred.

(e) (2 pts) Modify the input deck so that the system compresses the molecule rather than extends it. How does the behavior change? Attach an OVITO snapshot of the final configuration.