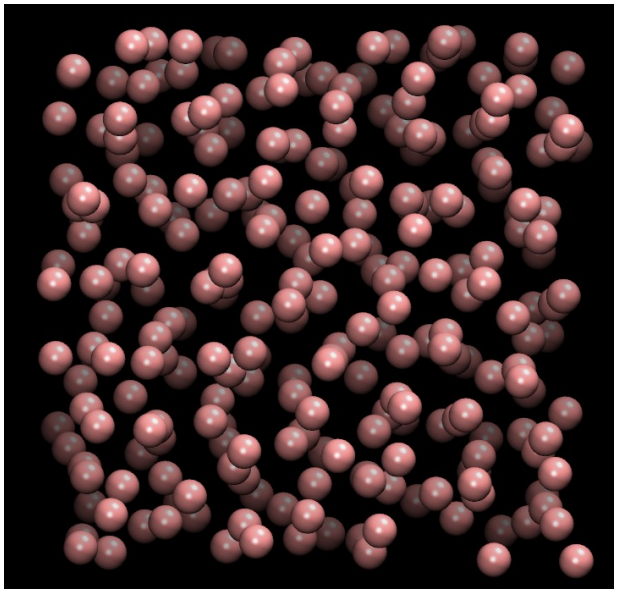
Problem 2:

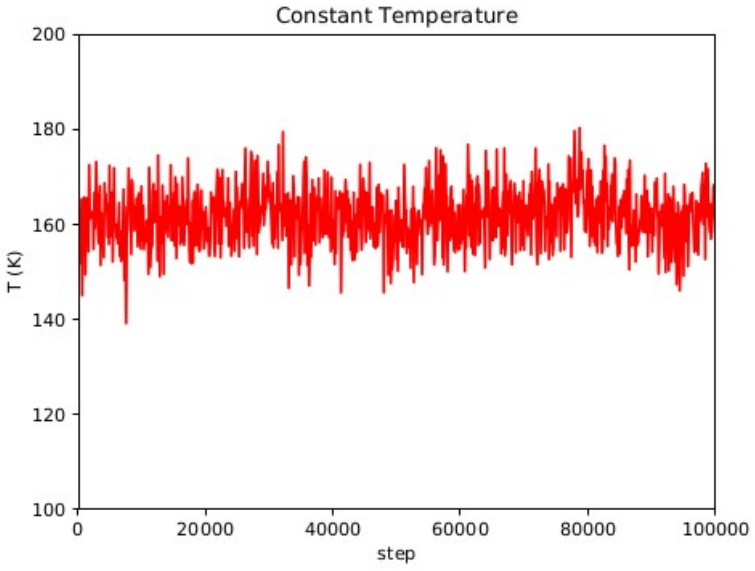
NOTE: I converted my codes to python 3! Run pbcMD.py to run the MD simulation. I have changed the duration to only 1000 steps but the files ‘full.log.MD’ and ‘full.traj.xyz’ correspond to the run for 100,000 steps. The other files ‘fine.xxxxx’ are the same simulation but thermodynamic quantities and trajectories were written every 2 steps but only for about 1,000 steps. I did this to show what happens early on during the simulation. The rest of the included files in the directory .../etc/ are just plots or scripts for plotting.

PBC can be observed by viewing one of the trajectories; you will see particles exiting one side of the box and entering another. Minimum image is imposed in the verlet lists. The radius of the cutoff sphere is the cutoff radius for the potential. The skin distance is set manually. In this simulation, the cut off distance is 2.5*sigma and the skin distance is 0.1*sigma.

For starters, here is a pretty snapshot!

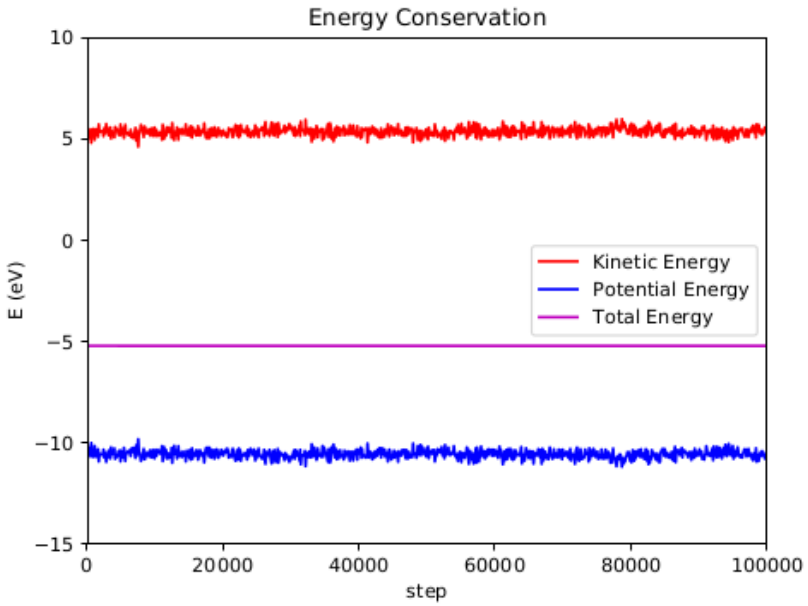


For the full simulation, here are plots of temperature vs. time:



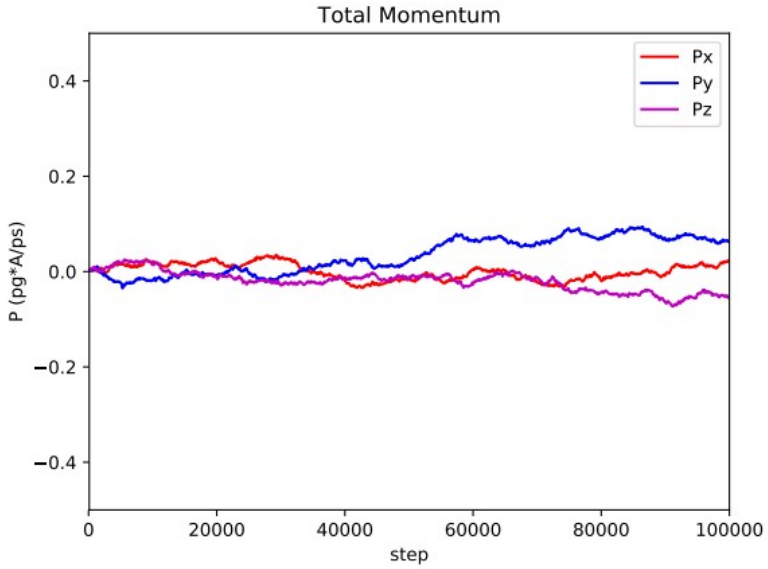
The average temperature stays fixed at it's value for the whole simulation (after the initial equilibration period discussed below), while the instantaneous temperature oscillates periodically. This is consistent with the fixed kinetic energy that oscillates slightly.

The kinetic, potential, and total energy are well conserved over time:



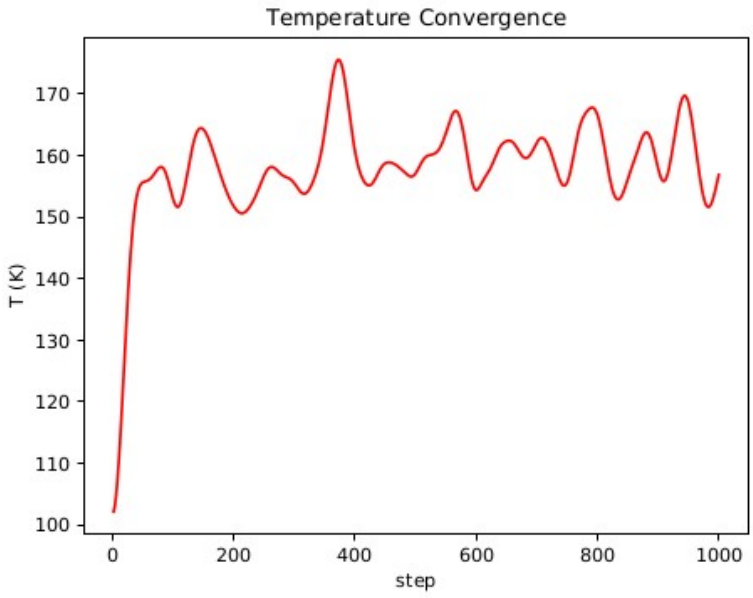
The kinetic energy and potential energy stay very close to their initial values throughout the whole simulation. The sum of the two, the total energy, is conserved quite well. i.e. total energy is a straight line on a plot vs time. This is consistent with the NVE ensemble.

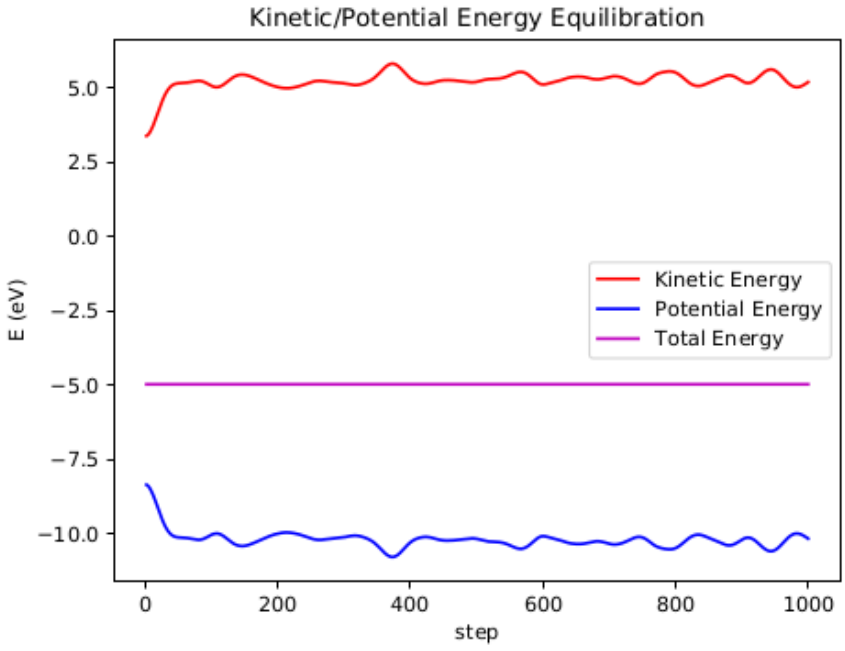
Finally, the total momentum is conserved quite well over time.



It may LOOK like momentum is not conserved, but please take note of my units.
I am expressing momentum in picograms*Angstrom/ps. I did this to keep the number digits very small. ~0.1 pg*A/ps is the largest center-of-mass momentum during my simulation. This value corresponds to about 1*10^-11 g*m/s. It's a very small value!

Some more notes:
It seems that the initial structure was equilibrated at a different temperature than 100 K. This can be seen in that the temperature rapidly changes from ~100K, the initial value, to ~165K. The equipartition theorem says that for systems at equilibrium, the average kinetic and potential energy are constant. Apparently this system wasn't equilateral at 100 K because the temperature, kinetic energy, and potential rapidly change during the first few steps until equilibrium is achieved and the average kinetic and potential energies (and the temperature!) remain constant about their average value.





EQUILIBRATED USING LAMMPS

I further verified my claim by checking two things:

First, I used LAMMPS to run a identical simulation (i.e. NVE at 100K with no thermostatting). I got very similar results, i.e. similar total energies and similar rapid change in the average temperature.

Second, I used LAMMPS to thermalize the structure you gave us at 100K for 200 ps before equilibrating it for another 200 ps. I then took the equilibrated structure and ran it in my MD code. The temperature and energies are now fixed about their initial value for the whole simulations. The temperature oscillates slightly around 100 K.

I have put the output data for the equilibrated structure in .../etc/equil