Molecular Dynamics at constant temperature

December 19, 2014

1. Perform a simulation of a Lennard Jones crystal with 864 particles. Temperature should be controlled using the Langevin thermostat at temperature $T = 2$. Try with different values of the friction γ (e.g. 0.01, 0.1, 1.0, 10.0) and look at the difference in the behavior of the potential energy.

2. Compute the average potential energy for different values of the temperature (ranging from 0.1 to 3 in Lennard Jones units) using a fixed friction (e.g. $\gamma = 1$). Also compute the specific heat using energy flucutations and look at how the specific heat depends on the temperature. Remember that you should discard the initial equilibration.

3. Repeat the same calculation but starting from a structure that has been equilibrated for a long time at temperature T=3. (hint: simplemd writes the final coordinates on a file, you should restart from that configuration). Are the value of average and fluctuations of U equal or different with respect to previous points? For which values of T do you observe more difference?

4. At fixed T=1, look at how specific heat depends on system size (try e.g. 256, 500, and 864 particles).

5. Modify the routine thermostat() so as to implement velocity rescaling. Compute average and fluctuations at fixed T and compare with results obtained with Langevin thermostat