Computational Assignment 4: The Andersen Thermostat

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This assignment's computational exercise will be an extension of the previous Lennard-Jones system, so you should modify your code file to include some new computations. In your last assignment, you must have seen that you cannot arbitrarily set the temperature of your system, only the total energy. As a result, you cannot study a lot of the thermodynamics of this system, since that would require one to "heat" the system, which is not possible since your last simulation was essentially a *microcanonical* simulation. In this exercise, we will first see how to implement setting a target temperature for our Lennard Jones simulation, and then see how the pressure, another thermodynamic quantity, can be computed from your simulation.

In order to set a desired temperature T, we use an algorithm called the *Andersen thermostat*, where the velocities of randomly selected particles of your simulation are replaced with random velocities drawn from a Maxwell-Boltzmann distribution corresponding to the desired temperature T . This resembles the system's coupling to an infinite heat bath at temperature T. Note that in our simulation, the natural temperature scale in the problem is some T_0, which we have chosen to be 1. Therefore, all values of T are essentially multiples of T_0.

(a) Implement an Andersen Thermostat in your code. The algorithm to do this is the following:

  (i) At the *end* of each time-step (after all the positions and velocities have been updated) loop over all particles in your system.

  (ii) For each particle, with some probability $\nu\Delta t$, assign it a new velocity drawn from the Maxwell-Boltzmann distribution associated with the target temperature T. ν is a collision *rate* with the heat-bath: choose it to be 0.1. You can vary this rate later and see what effect it has on your simulation.

  (iii) Repeat this until the system settles into a new equilibrium.

  Plot the resulting speed distribution and verify that it is indeed the correct one. [4]

(b) Run your code to create an equilibrium configuration and determine how the energy of your system depends on the temperature (i.e., determine $T(E)$) in the range $T \in (0.5, 2)$.

  Is T a monotonically increasing function of E? Try to find C_V for this system. Why is an accurate determination of C_V difficult to achieve? [4]

(c) Go through Section 8.7 (*Thermodynamic Quantities*) of *An Introduction to Computer Simulation Methods* by Harvey Gould, Jan Tobochnik, and Wolfgang Christian. Use the formula given there to compute the mean pressure for such a Lennard Jones system.

  Use your code to determine $P(T)$, the pressure as a function of temperature of your system, for the same temperature range given above. [2]