Melting and Hysteresis

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1 Main Exercise

1. Perform simulations of a Lennard Jones crystal with 864 particles at different temperatures from 0.01 to 3.0. The temperature can be controlled using the Langevin Thermostat. What happens to the crystal as temperature increases?

2. Compute the average total energy at different temperatures. How does the energy depend on the temperature? Also compute the heat capacity of the system for different temperatures. (hint: the heat capacity can be computed as $C_v = (< E^2 > - < E >^2)/T^2$.)

3. Repeat the exercise starting from a structure that has been equilibrated for a long time at T=3. (hint: simpleMD writes the final coordinates on a file. You should start from that configuration). Are the average energy and the heat capacity the same as in the previous points of the exercise? For which temperatures do you observe more difference?

2 Bonus Exercise

1. Modify the function *compute_forces* in simpleMD to simulate a GEM4 fluid. The new potential is given by

$$v(r) = \exp(-r^4), \tag{1}$$

and the force is given by

$$f(\mathbf{x}) = 4x^2\mathbf{x}\exp(-x^4). \tag{2}$$

2. Equilibrate 300 particles in a cubic box of size 3 starting from a random configuration at T=0.1. What happens to the system at low temperature? Is this the same phase one finds in the Lennard Jones fluid?

3. Build a phase diagram of the GEM4 fluid by changing the temperature and the box size. (hint: you can find the approximate position of the transition line by looking at the heat capacity dependence on the temperature at fixed volume).