PY525 Homework 3; due 10/23/18

1)(36 pts) Simulate a system of 16 Lennard-Jones particles in a 2D, periodic, 10×10 box (units $\epsilon = 1, \sigma = 1$, $\epsilon/k_B = 1$, reasonable value of the suggested timestep in these units $\delta t = 0.01$, but explore whether that's appropriate).

a)(12 pts) Assuming that particles velocity components are distributed according to the Maxwell-Boltzmann distribution, find out what is the distribution for the speed $v = |\mathbf{v}|$. After some equilibration time, compare the observed speed distribution from the simulation with your derived expression.
b)(12 pts) Evaluate $\langle|\mathbf{r}|^2\rangle(t)$ and find the diffusion constant.
c)(12 pts) Is this a liquid, a solid or a gas ?

Technical: Use L-J potential truncated at $r = 3$; initial velocities homogeneously distributed in $(-3/2, 3/2)$, (ie, $-3/2 \le v_x \le 3/2$, etc), use the version of Verlet algorithm that is more accurate for the energy conservation.

2)(36 pts) Position 16 L-J particles on a perfect square lattice with the lattice constant $a_l = 1$ in a periodic box of the size 4×4. Assign random but tiny initial velocities to the particles, eg, 0.0001 or so. Since the particles are not at the equilibrium positions, the system should evolve. Use the time step 0.005 or smaller.

a)(12 pts) What is your guess for the value of temperature (after some equilibration time and using the reduced units as defined above) ?
b)(12 pts) What is the structure of the equilibrium lattice which you see at $t > 15$ or so ?
c)(12 pts) How would you argue that the system models a 2D solid ?

3)(28 pts) Start from the resulting positions of problem 2. Gradually heat the system, ie, over a time interval of $\Delta t = 1$ increase the average temperature by small amounts ≈ 0.1 (in the units defined above).

a) Guess the melting temperature. (Consider supporting evidence in the form of graphics or displacements or pair correlations.)