Name: PHY401 (Spring 2013), 04/18/13

Homework Assignment #9

(*Due Date*: Monday, April 29, 12noon, in MPHY-313)

9.1 *Molecular Dynamics of Noble Gas* (cf. textbook Ex. 9.1) *(2+8 pts.)*
Write a FORTRAN program to perform molecular dynamics simulations for neon atoms ($m = 20u$) interacting via the Lennard-Jones potential,

$$V(r) = 4\epsilon \, [\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}] \tag{1}$$

with $\epsilon/k_B = 37K$, $\sigma = 2.8\mathring{A}$ in a 2-D 25×25 box using periodic boundary conditions. Initialize the simulation with 100 particles and initial speed of v_0=5 for each particle (pointing in a random direction, with positions slightly varied around 2σ apart).

(a) Work out the basic units of time and speed, and calculate temperature, density and pressure of the equivalent 3-D system (V=25^3 with 1000 particles) using the ideal-gas law.

(b) Perform numerical simulations with about 10000 time steps (with $\Delta t = 0.01$) and extract 3 speed distributions by averaging over t=25-50, 50-75, and 75-100. Eyeball-fit a Maxwell distribution to each set of points separately to estimate the temperature, and evaluate the average temperature. Compare to the theoretically expected value for an ideal gas.