Computational Physics Homework Assignment #5

May 13, 2019; Due June 03, 2019

Reading Assignment

1. Read Textbook Chapter 8 and understand program "md.f90". Prepare your own MD program with any languages you prefer.

Laboratory Assignments (Total Points: 50 + 30), on May 20, 2019

1. **Approach to equilibrium** (Points: 10,10,10,10,10)

   (a) The system is $L_x \times L_y = 6 \times 6$ and $N = 16$. Set $\Delta t = 0.01 or 0.005$ and run the program "md.f90" to make sure it is working properly. The total energy and total momentum should approximately conserved.

   Calculate temperature $T(t)$ and pressure $P(t)$ as functions of time t. Compare your estimate for P to the value for an ideal gas.

   (b) Suppose that at $t = 0$, the box is changed from $L_x \times L_y = 6 \times 6$ to $L_x \times L_y = 12 \times 6$. (You should do a little thinking on how to make such a change.) Run the program again and check the total energy and total momentum.

   (c) Compute $n(t)$, the number of particles in the left half of the cell, and plot $n(t)$ as a function of t. What is the qualitative behavior of $n(t)$? Also compute the time average of $n(t)$, and plot it as a function of t. What is the mean number of particles on the left half after the system has reached equilibrium? Compare your qualitative results with the results of last lab.

   (d) The system is $L_x \times L_y = 6 \times 6$ and $N = 32$. Repeat calculations in part (a) and compare the results. (How will you set up the initial conditions?)

   (e) Now, let the box size to be $L_x \times L_y = 12 \times 12$ and the number of particles to be $N = 64$. Repeat calculations in part (a) and compare the results.

2. **Distribution of speeds and velocities** (Points: 10+10+10, optional)

   (a) Write a subroutine to compute the equilibrium probability $P(v)\Delta v$ that a particle has a speed between v and $v + \Delta v$. You should first estimate the value of the maximum speed, v_max, and then select Δv which should not be too small. Now you count number of particles whose speed is within $[v, v + \Delta v]$. Your results depend on the value of Δv.

   (b) Plot the probability $P(v)$ versus v. What is the qualitative form of $P(v)$? What is the most probable value of v? What is the approximate width of $P(v)$? Compare your result to the theoretical form (Maxwell-Boltzmann distribution) in two dimensions:

   $$P(v)dv = Aexp(-mv^2/2k_BT)vdv$$

   (c) Determine the probability density for the x and y components of the velocity. What is the most probable value of x and y velocity components? What are their average values? Plot $P(v_x)$ versus v_x.