Homework 5

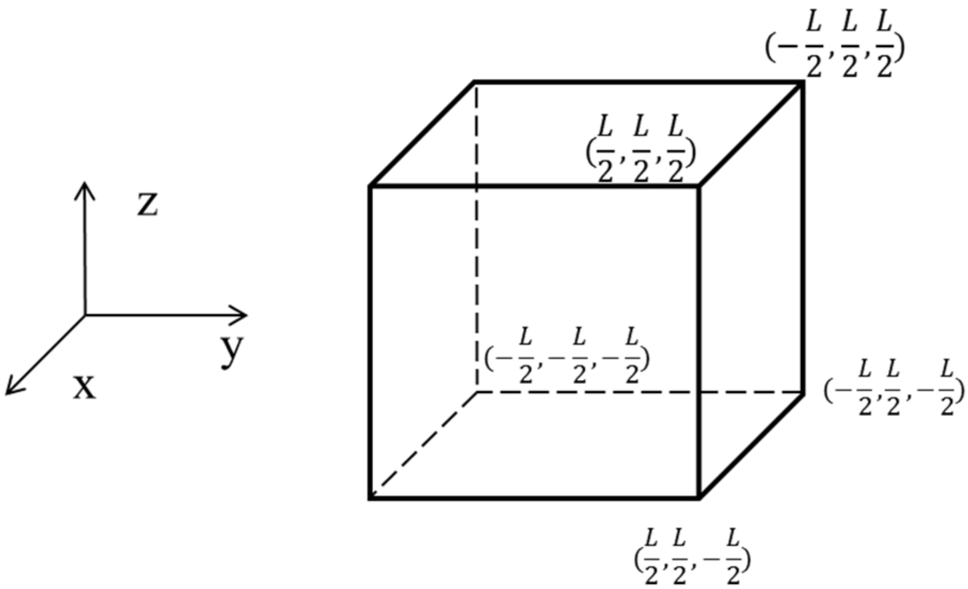
Due Date

2016/06/29(Wednesday), 23:59 ◦ LATE submission is NOT ALLOWED.

In this assignment, you should be able to accomplish a program to simulate particle collision with REFLECTIVE BOUNDARY CONDITION. In terms of solving the differential equation, you are allowed to use verlet method, Euler Method, Higher Order Tylor Method or any combination of them. In case you adopt one method not listed, please describe the detail of the algorithm you use. Please be advised that no grade will be given if the function to solve differential equation is not crafted by yourself. In addition to using Matlab, it is encouraged to finish the main program by C or C++. If the task is accomplished by C or C++, the data shall be recorded in files for later use of plots or animations in Matlab.

Problem :

Assume that there are two argon(^{40}Ar) atoms in a square cubic box. The length of each side of the box is $4.0 \times 10^{-9} m$ box. Assume the center of the two argons as well as the box is at the origin of a coordinate. And the two atoms are placed on the x-axis. The parameters of the Lennard-Jones Potential for argon atom are as follows: $\epsilon = 1.66 \times 10^{-21} J \; and \; \sigma = 3.4 \times 10^{-10} m$. Based on the facts, a simulation program should be ready for running as soon as the initial conditions are given.



Assume that N Argon atoms in a square cubic box. The length of each side of the box is 2×10^{-7} m. Let $\vec{r}_i$ and $\vec{v}_i$ denote the position and the velocity of each particle. Although we had no chance to discuss Kinetic Theory of Gas in the class, you should have been familiar with the concept from high school textbook. In Kinetic Theory of Gas, temperature T is defined by the TOTAL KINETIC ENERGY of the system via

$$\sum_{i=1}^{N} \frac{1}{2} m |\vec{v}_i|^2 = \frac{3}{2} N k_b T,$$

where k_b is the Boltzman constant: $1.381 \times 10^{-23} \, \frac{m^2 \, kg}{s^2 K}$. When you are setting up the initial velocity of all the particles, you can assume the speed of particles are identical but going to different direction. In addition to temperature, Pressure (P) is also a thermodynamic quantity of interest. In Kinetic Theory, P is defined associated the TIME AVERAGED collision of the particles on the wall. Suppose a particle hits the wall on the x axis at time t with velocity v_i, the change of the particles momentum provides a force on the wall by

$$F_x(t) = \frac{2m\vec{v}_{i,x}}{\Delta t}.$$

Then the pressure on the wall is defined by the averaged impact over a certain amount of time (τ)on the wall:

$$P_x = \frac{\sum_{t=0}^{\tau} F_x(t)\Delta t}{\tau \times A_x}.$$

Now follow the steps to check whether the law of ideal gas can be explored:

1. Set N = 500. Randomly assign $\vec{r}_i$ of the particles and be careful the overlapped particles. Subsequently, give each particle a VELOCITY by the random number generator and make the system be at temperature $T = 0^0C = 273\ K$.
2. Carefully choose a Δt , let the system run a while and record the total energy (Lenard Jones Potential Energy + Kinetic Energy), the temperature and the pressure of each wall for every several steps (say 100 steps?). Note that the pressure is an averaged quantity over the recoding period.

   If energy, temperature and pressure curve becomes stable, the system is set properly. If the energy becomes huge all of a sudden or not conserved, the problem may come from too large Δt, overlapped particles at the beginning or some unknown bugs in the code.

   (Note: you are allowed to decide how long the system should run until it is stable. Also you are allowed to set up record period for the physical quantities as long as it is reasonable)

3. Record the averaged pressure at the stable phase.
4. Change the number of particles say N = 50, 100, 150, 200, ….. and keep the system's temperature at 273K. Then repeat 1-3. And record the pressure for each different N.
5. Plot P versus N.

Note: Proper scaling may be required for this program to achieve adequate precision. Refer to http://scitation.aip.org/content/aapt/journal/ajp/83/3/10.1119/1.4901185 for the scaling information.

Contents to submit:

1. All the source codes including .m, .c, .cpp and .h, you compose for the assignment including proper COMMENTS.
   (No comment, no score)
2. A word document or a PDF includes Your Name, Your Student ID Number,
   In the document, please include all the written answers, plots (**total energy, temperature, and pressure curve versus time and the plot of N-P.)** and HOW LONG DOES IT TAKE for the program to finish the simulation.

Notice:

1. DO NOT PLAGIARIZE. You are encouraged to ask and to discuss the homework content with your fellow classmates, the TAs and the instructor. But identical core program wording is NEVER ACCEPTABLE.
2. Upload all the files without archiving. Do not upload files that don't work well. Any missing file or function that leads to fail of the execution will be regarded as a program that never works.