Homework 4

Due Date

2017/06/25 (Sunday), 23:59。

Create a matlab script and change the filename to F7xxxxxxx_hw4.m. Link all the programs to solve following problems to this script. Make sure once type the filename' F7xxxxxxx_hw4', the results of the following problems will pop-up automatically in order. Remember not to type any 'clear all ', 'close all' command in any of the codes.

In this assignment, you should be able to accomplish a program to simulate two body interactions in two or three dimension with reflective boundary condition. Verlet method, Euler Method, Higher Order Tylor Method or any combination of them are allowed to solve the differential equations. In case you adopt one method not listed, please describe the detail of the algorithm. Please be advised that no grade will be given if any MATLAB's embedded function for solving differential equation is found.

Special Notice: Not everyone is required to write this homework. Problem 1 and Problem 2 are mainly designed for those who would like to amend their homework records. If you are already satisfied with your homework/quiz scores, you are not required to work with problems 1 and 2. Problem 3 has been a bonus problem for 2 years but unfortunately no one has ever acquired full score yet. For those who prefer some challenge, you are encouraged to give it a try and upload your solution. The points of Problem 3, unlike the others will be averaged, will be added directly to the final score.

[50%] Problem 1:The mission of the triplet Jay, Jake and Jim. (The blue birds) [F7xxxxxxx_hw4_prob1.m]

The triplet Jay, Jake and Jim have identical weight of 0.1 kgw. In a rescue mission, they were launched 20cm from ground zero at a speed of 20m/s and a shooting angle of 50^0 . They were ordered to split 2 seconds after taking off. Assume that they were in line formation (Jay-Jake-Jim). During separation, they pushed each other horizontally with a constant force for 0.1 second. The force was 1.0N between Jay and Jake and 2.0N between Jake and Jim. Start the simulation and answer the following questions:

(a) Plot the trajectory (x-y) of the center of mass from launching until they landed.
(b) Estimate how far from the catapult would Jim be when it was landed.
(c) Estimate the speed of Jake right before landing.
(d) Estimate the kinetic energy of the triplet right before landing.

[50%] Problem II: Simple Molecular Dynamics

[F7xxxxxxx_hw4_prob2.m]

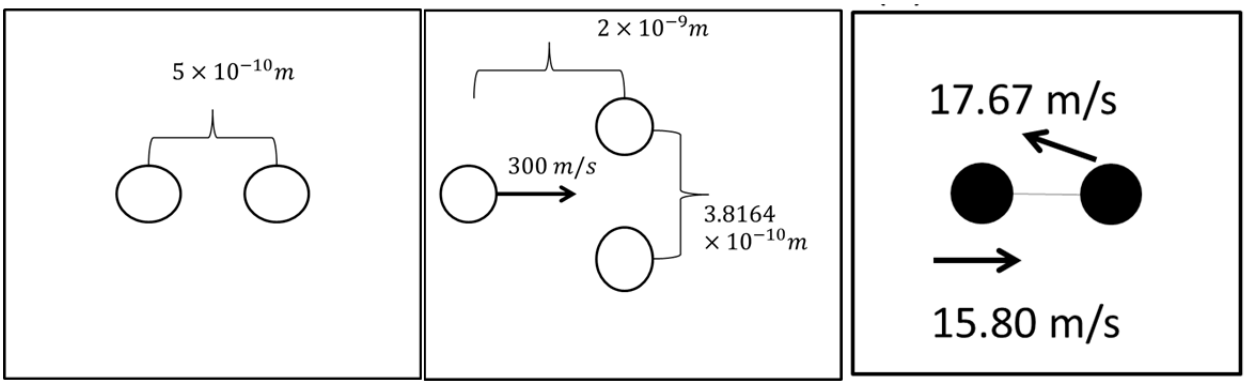
Assume that there are argon(^{40}Ar) atoms in a square cubic box. The length of each side of the box is $4.0 \times 10^{-9}m$ box. Assume the center of the two argons as well as the box is at the origin of a coordinate. And the two atoms are placed on the x-axis. The parameters of the Lennard-Jones Potential 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.

Use each of the given initial conditions to simulate the dynamic system for $0 \leq t < 10 \times 10^{-10} \; sec$. For each initial condition, you should (1) specify the time step Δt you use in the program for the simulation, (2) plot the total energy versus time of the system and choose the time step for the plot properly, and (3) record the locations of the atoms and make a movie to show how the atoms move. Save the movie in avi format. You may need the functions "getframe" and "movie2avi" to accomplish the task. Choose frame rate wisely to demonstrate the particles' motion within reasonable show time.

(a) Suppose two atoms are found rest and separated by 5×10^{-10}m at t = 0. In addition to the three results to present, which type of phase (gas, liquid and solid) do you think this state is if more than two atoms of the same state are put together?

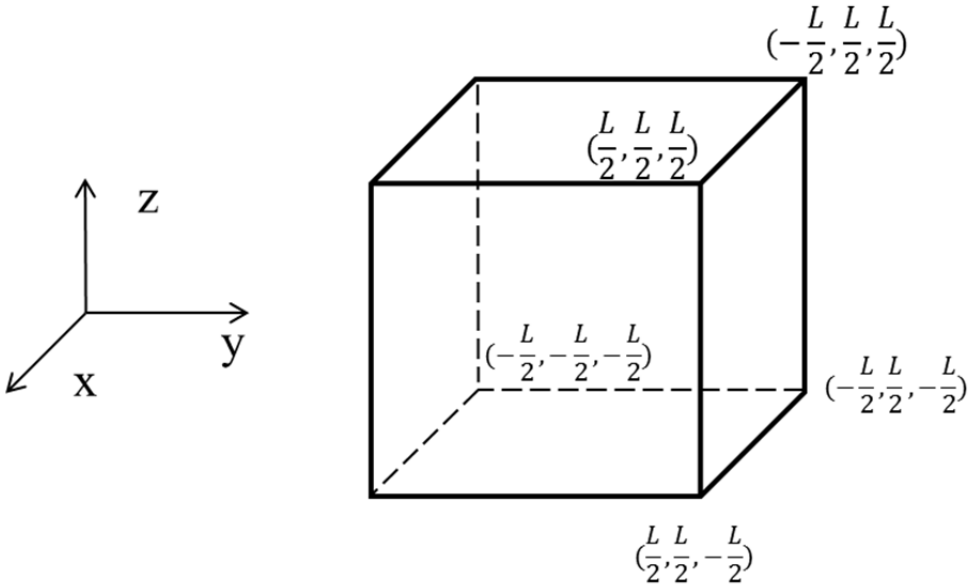
(b) Suppose at t = 0, two atoms are found rest and separated by 3.8164×10^{-10}m. Another one is flying toward the center of these two atoms at a speed of $300 \; m/s$ from a distance of 2×10^{-9}m.

(c) Suppose at t = 0, the two atoms are found separated by 5×10^{-10}m. One atom is moving toward the second one at $15.80 \frac{m}{s}$, while the second one is moving with a velocity of 17.67 $\frac{m}{s}$ toward the first one at an angle of 26.56^0



[Final Bonus : (5 points in final bonus)] Problem 3:

[F7xxxxxxx_hw4_prob3.m]



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 familiar the concept from high school textbook and General Physics (I). In Kinetic Theory of Gas, temperature T is defined to be associated with 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 following procedure to check whether you can explore the law of ideal gas.

1. Set N = 500. Randomly assign $\vec{r}_i$ of the particles and be careful not to let the particles overlapped. Subsequently, give each particle a randomized VELOCITY but make the system be at temperature $T = 0^0 C = 273\ K$.

2. Carefully choose a Δt and 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 of your 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. (Don't forget the axis and the unit of P and N)
6. Reminder: This problem may require very long execution time in Matlab. If you know how to program it in C code, feel free to write it in C and record the results in a text file. Then write a matlab program to read the record and plot them out. If the main code is written in C, please write a make file or clarify how to compile all the source codes and link them properly.

Contents to submit:

1. All the m-files + C codes if any you compose for the assignment.
2. All the m-files should include proper COMMENTS.
   (No comment, no score)
3. **Problem II: The avi file or gif file for each cases and the answer of II(a).**
4. A PDF includes Your Name, Your Student ID Number,
   In the document, you will need to include all the written answers and plots.

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.