

Homework 4

Due Date

2016/06/25 (Saturday), 23:59 • LATE submission is NOT ALLOWED.

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.

Problem 1: Motion of Planet (Numerical Proof of Kepler's Laws of Planet from Newtonian Dynamics)

Assume that a $2 \times 10^{30} \text{ kg}$ Sun rests at the origin and a $6 \times 10^{24} \text{ kg}$ planet is found at distance $r_0 = 1.5 \times 10^{11} \text{ m}$ from the sun while the planet is moving at speed v toward the direction perpendicular to the segment connecting the center of the two objects. As the mass of the sun is much larger than the planet, the gravitational effect towing the Sun is negligible while you are encouraged to include the force imposed on the Sun.

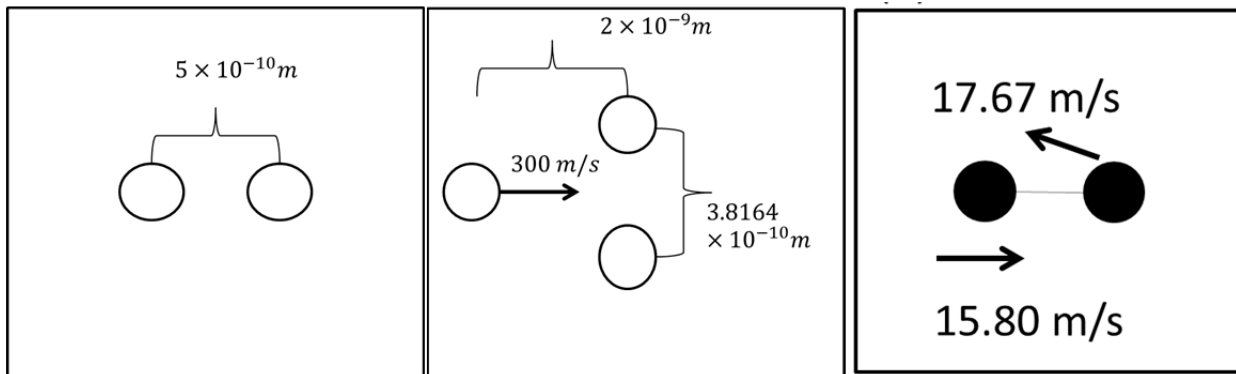
- (a) Write down the equation of motion of the planet. (ex: $\frac{d^2 x_p}{dt^2} = \dots, \frac{d^2 y_p}{dt^2} = \dots$.)
- (b) You should be familiar to calculate the speed for the planet to remain on a circular orbit around the sun if the displacement of the sun can be ignored. Assume that the speed is v_c , find v_c
- (c) Use $v = v_c$ as the initial condition in addition to the distance provided then solve the differential equation of (a) numerically for at least one orbital period and generate three plots: (1) the trajectory (x-y), (2) the x-location (x-t) and (3) the y-location y(t) of the planet. And Find the period of the planet.
- (d) If the initial conditions become $v(0) = 0.7 v_c \hat{j}$, re-calculate the location of the planet from the beginning for at least an orbital period and plot the results similar to those of (c).
- (e) Verify that the trajectory of the planet in (d) is an ellipse and find the length of the semi-major axis and the period of the planet in (d).
- (f) You should have notice that the trajectory and the period of the planet changes with the initial condition $v(0) = k v_c \hat{j}$. Now change k from $k = 1/5$ to $k = 1$ and record the length of the semimajor axis (R) and the orbital period (T) of each condition and verify that $R^3 \propto T^2$ (i.e. make a plot of $R^3 - T^2$ from the data and check if they can be fit on a line);

Problem II: Simple Molecular Dynamics

Assume that there are argon(^{40}Ar) atoms in a square cubic box. The length of each side of the box is $4.0 \times 10^{-9} \text{ m}$ 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: $\epsilon = 1.66 \times 10^{-21} \text{ J}$ and $\sigma = 3.4 \times 10^{-10} \text{ m}$. 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 $0 \leq t < 10 \times 10^{-10} \text{ sec}$. 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.

- Suppose two atoms are found rest and separated by $5 \times 10^{-10} \text{ m}$ 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?
- Suppose at $t = 0$, two atoms are found rest and separated by $3.8164 \times 10^{-10} \text{ m}$. Another one is flying toward the center of these two atoms at a speed of 300 m/s from a distance of $2 \times 10^{-9} \text{ m}$.
- Suppose at $t = 0$, the two atoms are found separated by $5 \times 10^{-10} \text{ m}$. One atom is moving toward the second one at $15.80 \frac{\text{m}}{\text{s}}$, while the second one is moving with a velocity of $17.67 \frac{\text{m}}{\text{s}}$ toward the first one at an angle of 26.56°



Contents to submit:

- All the m-files you compose for the assignment.
- All the m-files should include proper COMMENTS.
(No comment, no score)
- Problem II: The avi file or gif file for each cases and the answer of II(a).**
- A PDF includes Your Name, Your Student ID Number,**

In the document, you will need to include all the written answers and plots.

Notice:

- 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.
- 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.