PHY407 Lab06

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1 Modeling space garbage

1.a

Defining

$$\frac{dx}{dt} = v_x$$

and

$$\frac{dy}{dt} = v_y,$$

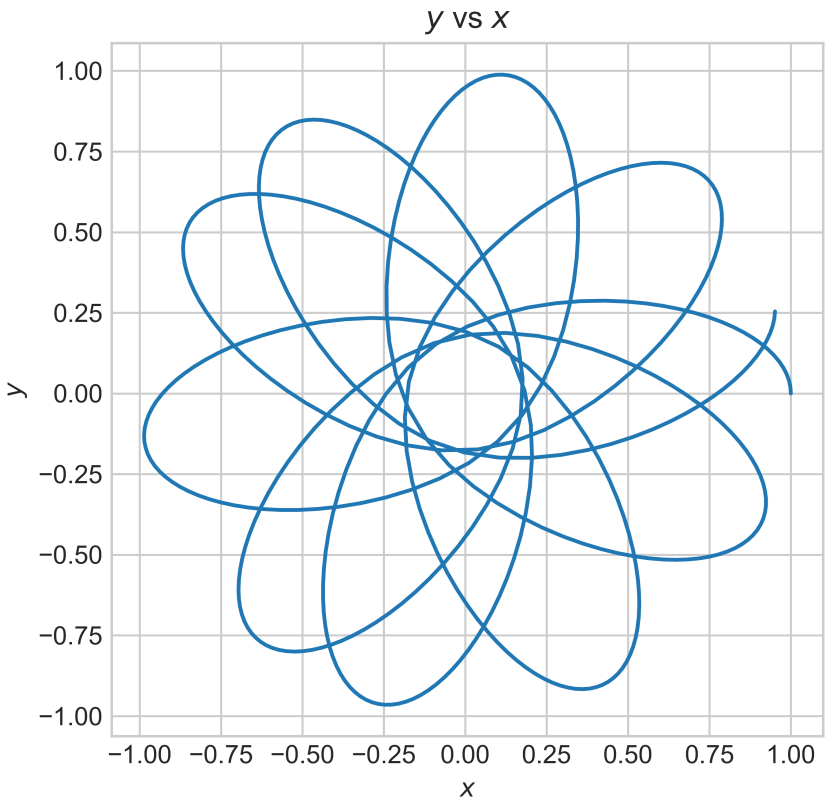
the four set of equations that define the motion of a ball bearing in the xy-plane around a rod of mass M and length L is:

$$\frac{dx}{dt} = v_x, \quad \frac{dv_x}{dt} = -GM\frac{x}{r^2\sqrt{r^2 + L^2/4}}$$

$$\frac{dy}{dt} = v_y, \quad \frac{dv_y}{dt} = -GM\frac{y}{r^2\sqrt{r^2 + L^2/4}}$$

1.b

For $G = 1$, $M = 10$, $L = 2$ and initial conditions $(x, y) = (1, 0)$; using these equations to solve for x and y points with the RK4 method, we get the below figure below:



As can be seen, it has a precessing orbit. It is not a circle nor an ellipse. This shows that the acceleration on the ball is not a simple $1/r^2$ function.

2 Molecular dynamics simulation, Part 1

In this section we will be using the Lennard-Jones potential to plot time steps of the interactions between two particles with different initial conditions. To update the position on each time step we will use the Verlet algorithm.

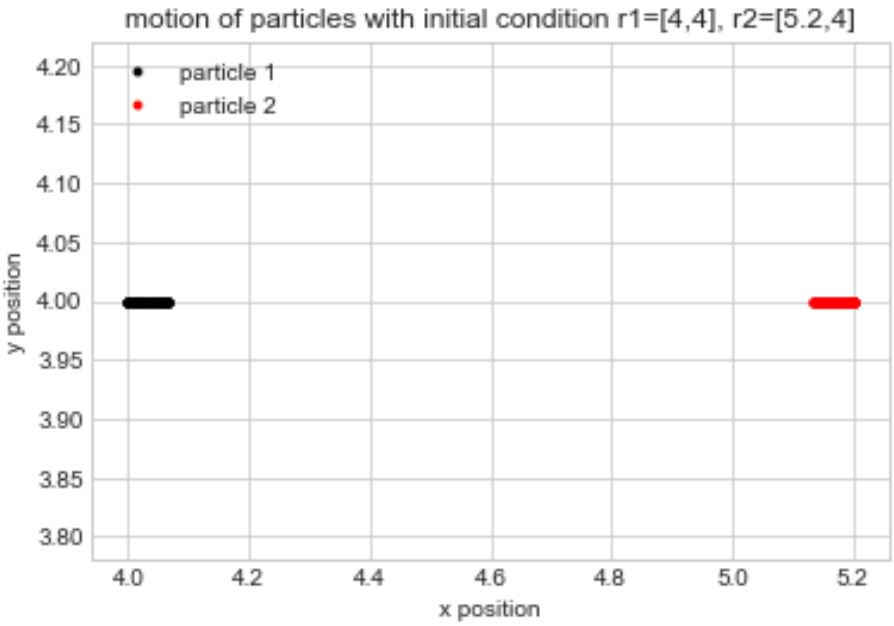
2.a

[Nothing to submit]

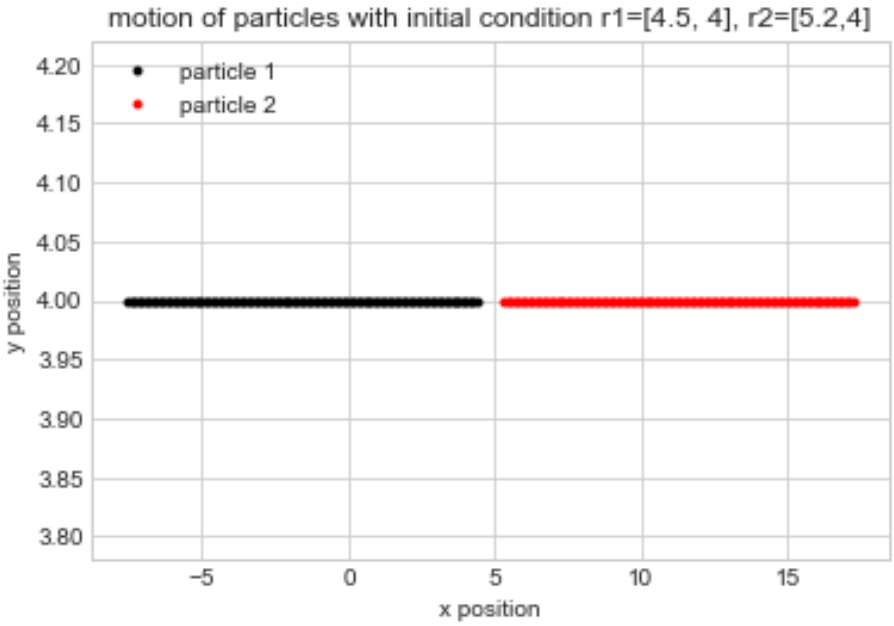
2.b

begin Pseudo-code:
-set up an acceleration function that takes the position of two particles and outputs the acceleration they cause on each other
Pseudo-code for the Verlet algorithm:
- set constants for time step and total time
-set initial velocity for particle one and particle two
-set initial position
- begin a loop that updates the position of both particles by adding the initial velocity multiplied by the timestep to the initial position, and then updates the velocities by adding the acceleration multiplied by the time step to the previous velocities, and then sets the previous positions to the new positions. essentially follows this pattern:
$v_{initial}$=0+h*a$acceleration_{initial}/2$
$r_{initial}$=initial positions of the two particles
begin loop:
$r_{updated}$=$r_{initial}$+h*$v_{initial}$
k=h*$acceleration_{updated}$
$v_{updated}$=$v_{initial}$+k/2
$v_{initial}$=$v_{updated}$

below we graphed three graphs that plot the trajectory of two particles that are experiencing the Lennard-Jones potential from different initial conditions: with particle one's initial position being (4,4) and particle two's initial position being (5.2,4), we get this first graph:

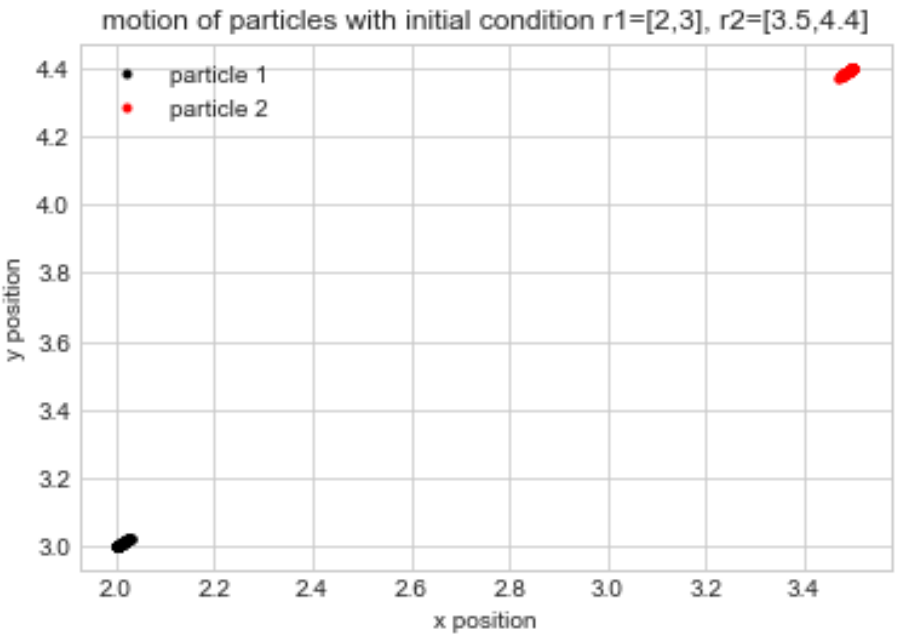


with particle one's initial position being (4.5,4) and particle two's initial position being (5.2,4), we get this second graph:



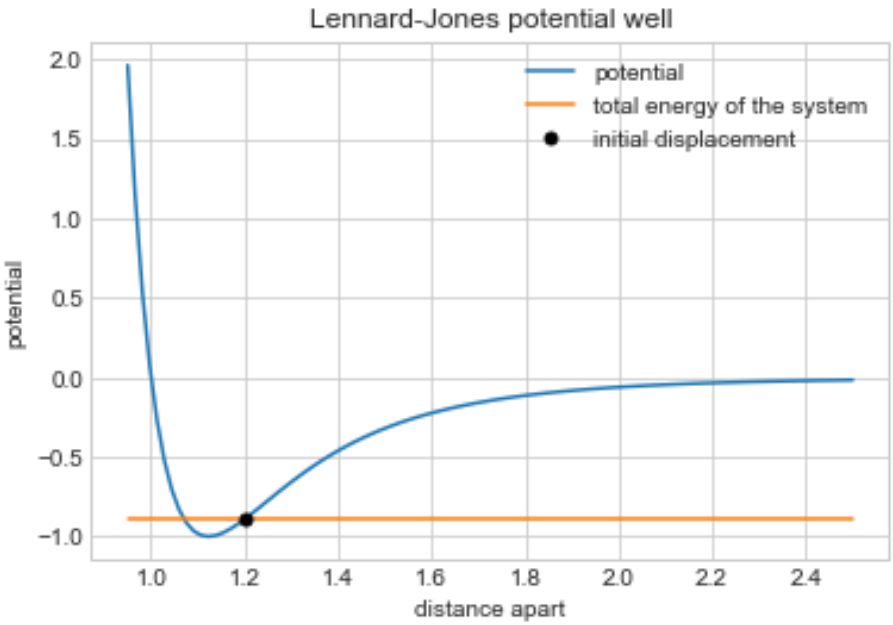
with particle one's initial position being (2,3) and particle two's initial posi-

tion being (3.5,4.4), we get this third graph:

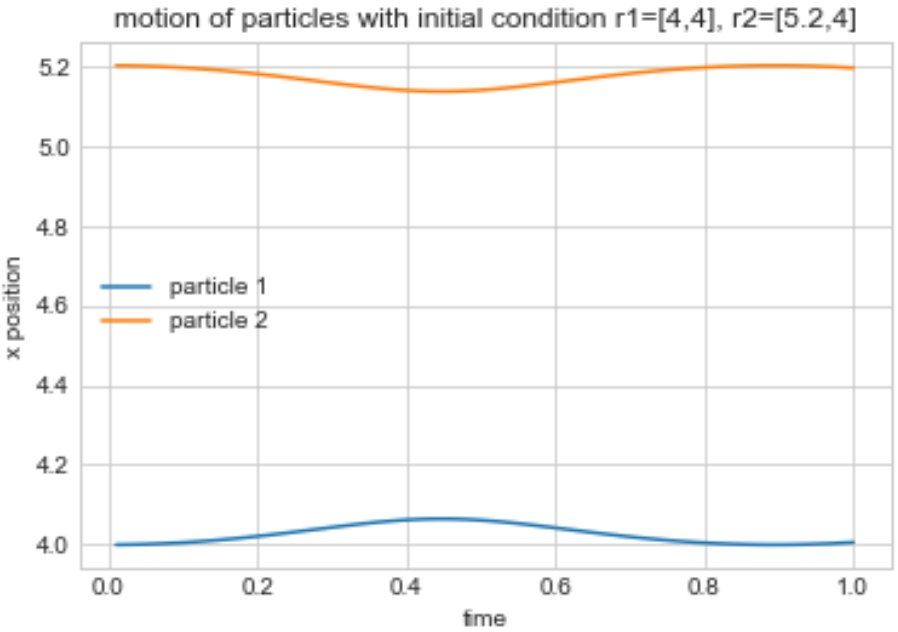


2.c

The initial condition that leads to oscillatory motion for both of the particles is initial positions (4,4) and (5.2,4). this condition leads to oscillatory motion because the initial potential energy of the system (since velocity=0 initially, this is the total energy of the system) is less than the walls of the potential well the system is in. Since there is no damping force, and since energy is conserved, the particles will remain in oscillation forever. The graph below shows the potential well and the total energy of the system:



The graph below shows the oscillation that both of the particles experience in the x direction (note that there is no motion in the y direction because the y position is the same in the initial position of both particles):



3 Molecular dynamics simulation, Part 2

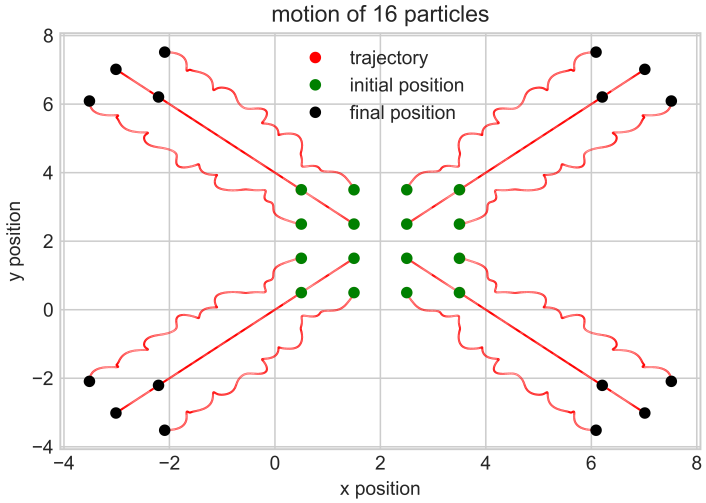
In this section We will use the Lennard-Jones potential to simulate the motion of 16 particles interacting with each other at the same time. We will then plot the total kinetic and potential energy of the system and check if energy is conserved, and finally implement periodic boundary conditions.

3.a

The multi-particle verlect algorithm is similar to the two particle verlet algorithm but with a few extra things we need to account for:

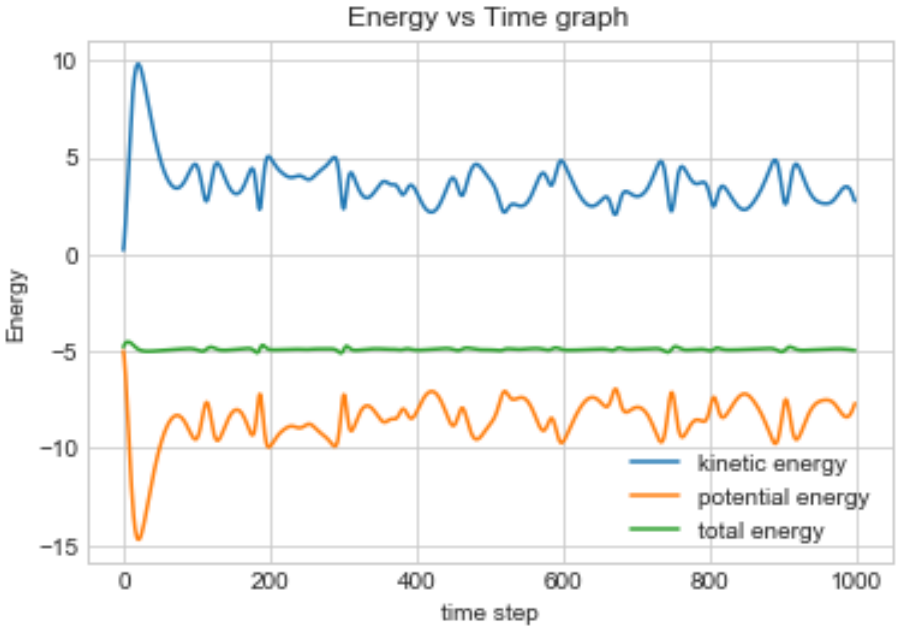
begin Pseudo-code:
-set up a distance function that takes the position of each particle and outputs the distance between each particle
-set up an acceleration function that takes the position of multiple particles and outputs the acceleration they cause on each other by incorporating the distance function
Pseudo-code for the Verlet algorithm:
- set constants for time step and total time
-set initial velocity for the multiple particles
-set initial position for multiple particles
- begin a loop that updates the position of both particles by adding the initial velocity multiplied by the time step to the initial position, and then updates the velocities by adding the acceleration multiplied by the time step to the previous velocities, and then sets the previous positions to the new positions. essentially follows this pattern:
$v_{initial}$=0+h*a$acceleration_{initial}$/2
$r_{initial}$=initial positions of the two particles
begin loop:
$r_{updated}$=$r_{initial}$+h*$v_{initial}$
k=h*$acceleration_{updated}$
$v_{updated}$=$v_{initial}$+k/2
$v_{initial}$=$v_{updated}$

Below we graphed the trajectory of 16 particles that are experiencing the Lennard-Jones Potential:



3.b

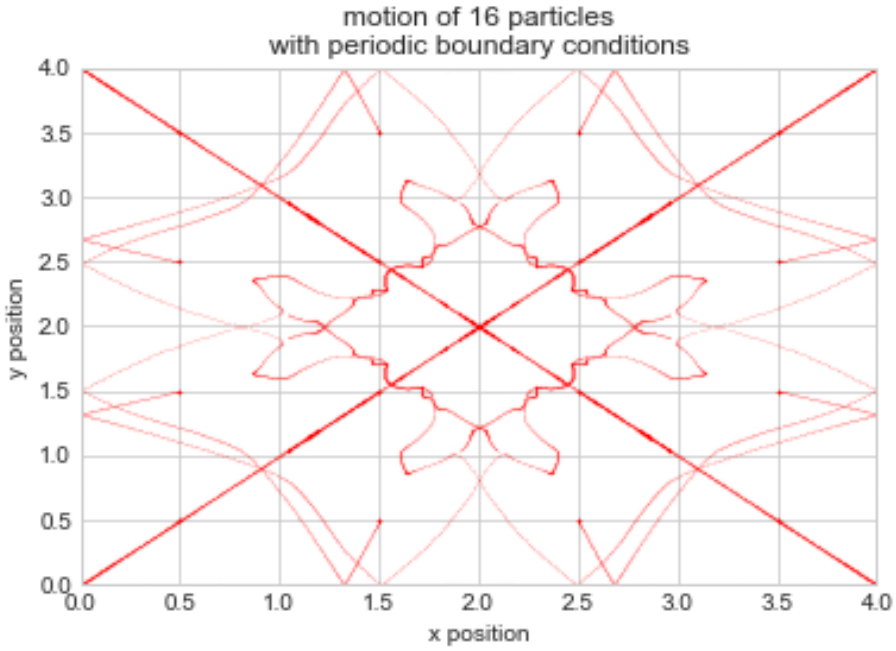
The graph below plots the total kinetic and potential energy at each time step of question 3a, as well as the total energy at each time step:



As shown in the graph, energy is conserved.

3.c

now we will implement periodic boundary conditions to the system of particles in



q

the particles say in a bound of x=0 to x=4 and y=0 to y=4. The trajectory is symmetric. When compared to the results of 3.a, we see that the trajectories are now not that much distinctive. This is because in this part we applied the boundary conditions and also the particles outside of this tile (our domain of concern) are also affecting the accelerations of our particles.