PHY407 Lab 06

Sang Bum Yi, 1004597714

Jianbang Lin, 1004970720

The workload was distributed as followings:

- Sang Bum Yi did question 3
- Jianbang Lin did questions 1 and 2.

Question 1

Let a ball orbit around a rod, the gravitational force acting on the ball toward the rod is:

$$F = \frac{GMm}{L}\sqrt{x^2+y^2}\int_{\frac{L}{2}}^{\frac{L}{2}} \frac{dz}{\left(x^2+y^2+z^2\right)^{\frac{3}{2}}}$$ [eq 1]

Acceleration on x and y direction can be obtained from equation 1:

$$\frac{d^2x}{dt^2} = -\frac{GMx}{r^2\sqrt{r^2+\frac{L^2}{4}}}$$ [eq 2]

$$\frac{d^2y}{dt^2} = \frac{GMy}{r^2\sqrt{r^2+\frac{L^2}{4}}}$$ [eq 3]

Where G is taken taken to be 1, M is 10, L is 2, and r is defined as:

$$r = \sqrt{x^2+y^2}$$ [eq 4]

Then the motion of the ball can be simulated, with initial condition (x, y) = (1, 0) and velocity is (0, 1):

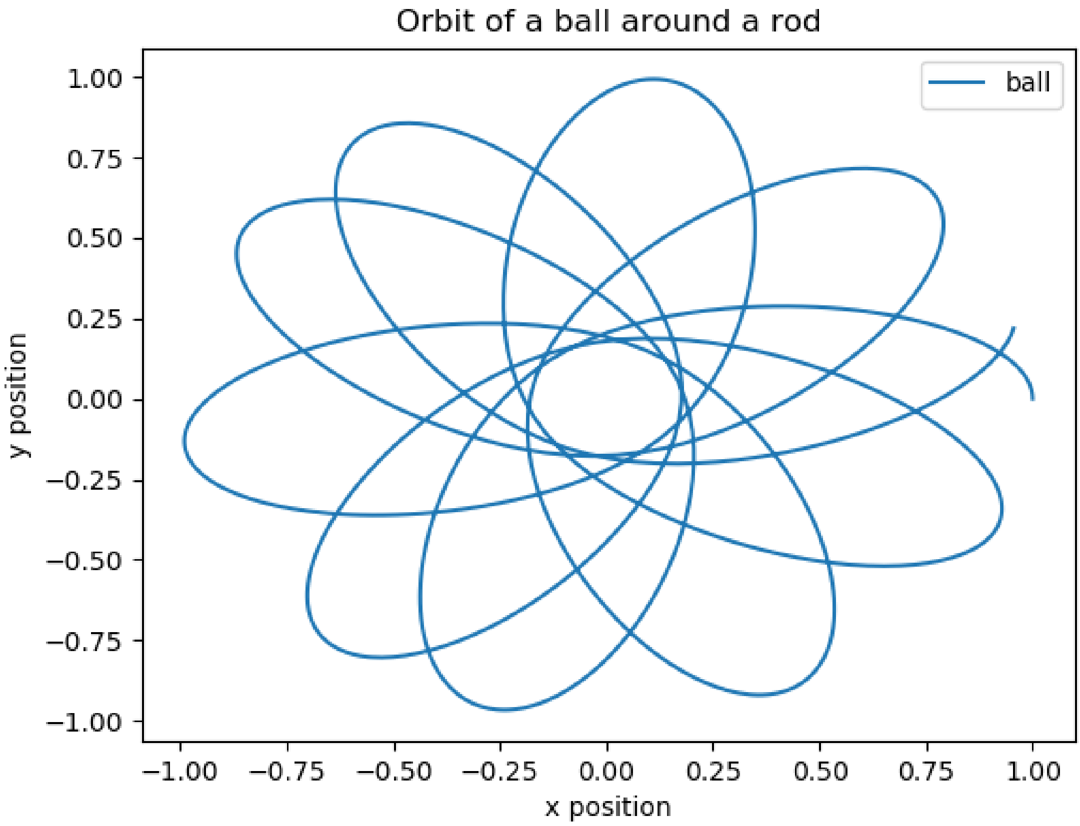

Figure 1: Motion of ball around rod due to gravitational force, total time duration is 10 with interval 0.01

This graph shows that the ball orbits around the rob, not in an elliptical shape, but a precessing orbit. That is because unlike attraction force between planets, the attraction force between rob and ball is not proportional to $1/r^2$, that is why it does not have the same motion as planetary orbit.

Question 2

Part a)

The potential energy between two particle can be described by Lennard-Jones potential:

$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \quad \text{[eq 5]}$$

Where r is the distance between them, $\boldsymbol{\sigma}$ and ε are given to be 1. The force between them can be calculated from potential:

$$F(r) = -\frac{dV}{dr} = 24\varepsilon\left(\frac{2\sigma^{12}}{r^{13}} - \frac{\sigma^{6}}{r^{7}}\right) \quad \text{[eq 6]}$$

Therefore the x and y component of acceleration are:

$$\frac{24\varepsilon}{m}\left(\frac{2\sigma^{12}}{r^{13}} - \frac{\sigma^{6}}{r^{7}}\right)\frac{x}{r}\hat{x} \quad \text{[eq 7]}$$

$$\frac{24\varepsilon}{m}\left(\frac{2\sigma^{12}}{r^{13}} - \frac{\sigma^{6}}{r^{7}}\right)\frac{y}{r}\hat{y} \quad \text{[eq 8]}$$

Where m is the mass of particles, m is taken to be 1 for simplicity.

Part b)

Equation 7 and 8 can be used to simulate motion of 2 particles, for example, if two particles are at position (4, 4) and (5.5, 4). The simulated motion is shown as following:

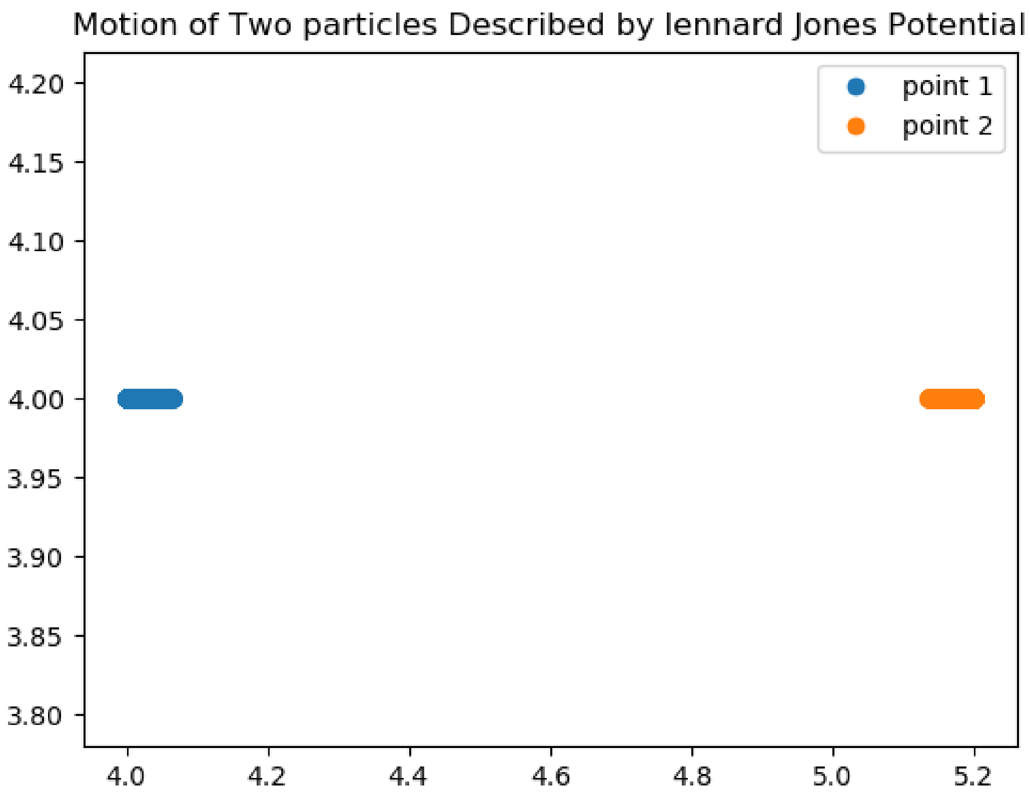

Figure 2: Motion of two particles starting at position (4, 4) and (5.2, 4) and 0 initial velocity, it consists of 1000 steps, and the time interval between each step is 0.01.

This graph shows that these two particles only move in x-direction, and the motion is not large, which implies the repulsive and attractive force almost cancels out and these particles are close to the equilibrium point.

If two particles are taken to be every close to each other, for example (4.5, 4) and (5.2, 4), then the motion can be simulated as following:

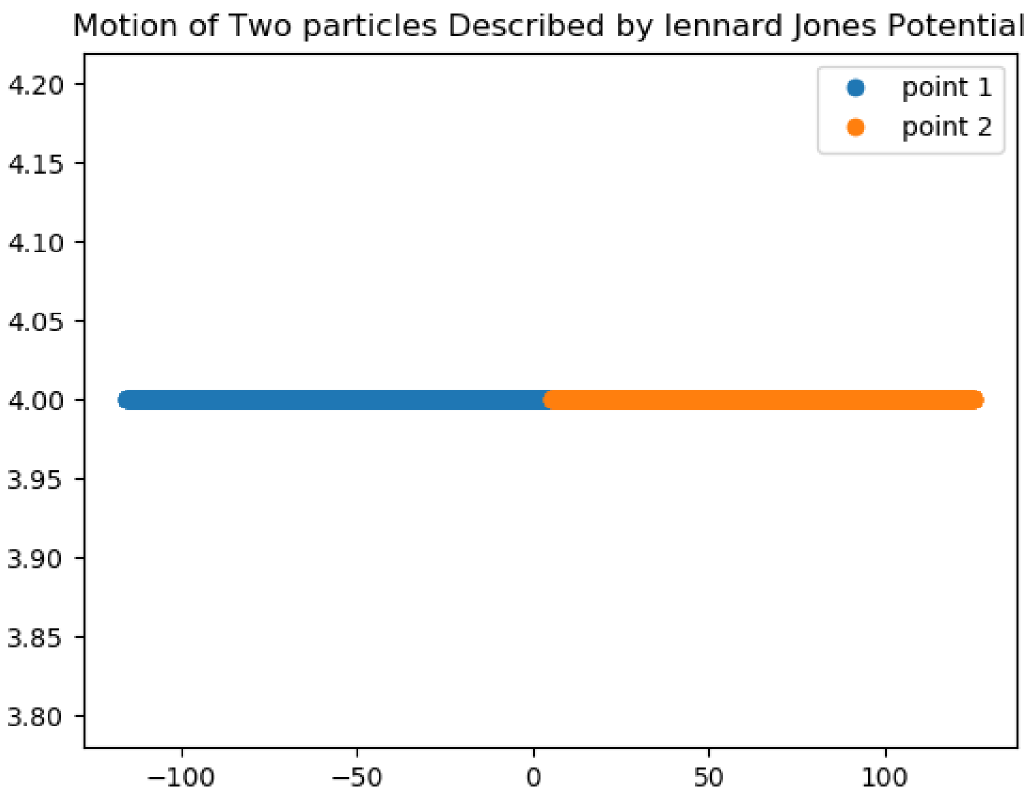

Figure 3: Motion of two particles starting at position (4.5, 4) and (5.2, 4) and 0 initial velocity, it consists of 1000 steps, and the time interval between each step is 0.01.

This graph shows that the particles move away from each other if they are placed too close, that is because when they are placed too close, the outward acceleration becomes very large, causing the outward velocity to become large as well. Therefore these two particles draft apart. However, if given enough time, the inward acceleration will bring them back again.

In previous cases, the particles only move in x-direction, because they have the same y-coordinate. If they differ in y-coordinate as well:

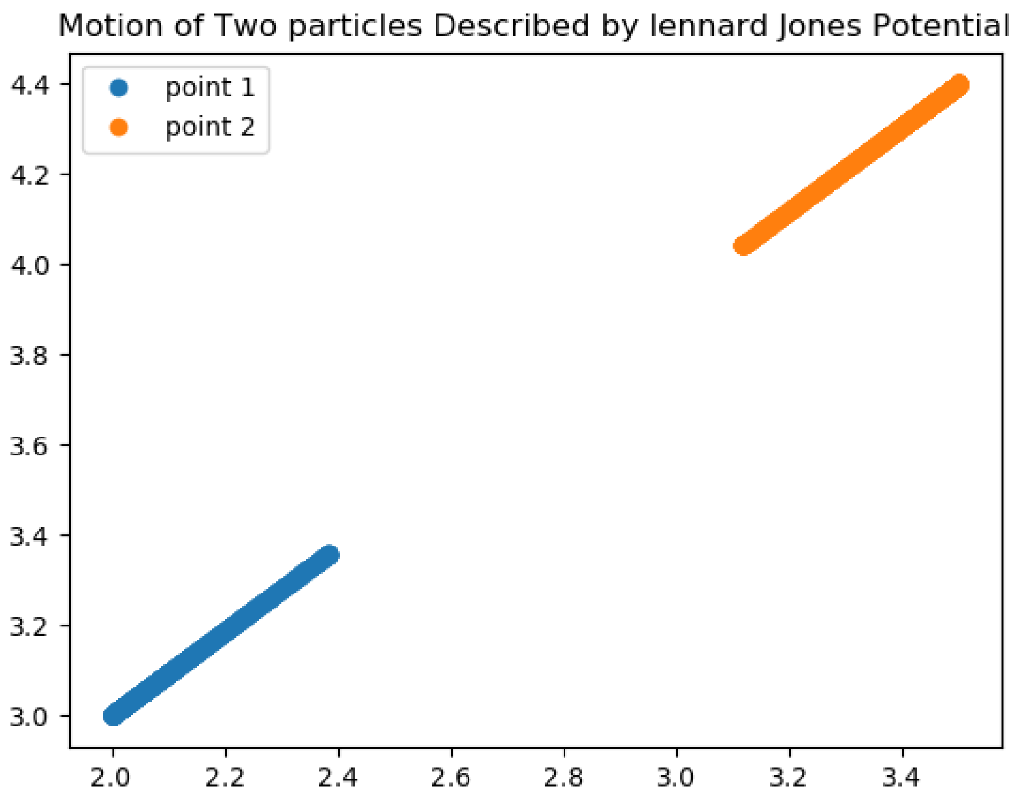

Figure 4: Motion of two particles starting at position (2, 3) and (3.5, 4.4) and 0 initial velocity, it consists of 1000 steps, and the time interval between each step is 0.01.

This graph shows that two particles will move in the same line, and the moment for these two particles is not as large as in figure 3, this means these two particles are close to the equilibrium position.

Part c)

The equilibrium separation is where the repulsive force is equal to the attractive force, and by solving equation 6, the equilibrium separation is calculated to be 1.12. Particles in figure 2 is the only set that shows oscillation, because the separation between them is 1,2, which is very close to 1.12. However, since this equilibrium is stable, the other two sets will exhibit oscillation if given enough time.

Question 3

Part a)

In Question 3, the molecular dynamics was simulated using the Verlet algorithm, which is a method to compute the position and velocity after small time steps. Equation 9 below defines the acceleration, which is a necessary component in obtaining the position and velocity.

$$\frac{d^2\vec{r}}{dt^2} = \vec{f}(\vec{r}, t) \qquad \text{[Eq 9]}$$

The first step of the Verlet algorithm computes the velocity after half time step by Equation 10.

$$\vec{v}\left(t + \frac{1}{2}h\right) = \vec{v}(t) + \frac{1}{2}h\vec{f}(\vec{r}(t), t) \qquad \text{[Eq 10]}$$

After the first step, Equation 11, 12, and 13 are repeated in each step to compute the positions and velocities in the next time steps.

$$\vec{r}(t + h) = \vec{r}(t) + h\vec{v}(t + \frac{1}{2}h) \qquad \text{[Eq 11]}$$

$$\vec{k} = h\vec{f}(\vec{r}(t + h), t + h) \qquad \text{[Eq 12]}$$

$$\vec{v}\left(t + \frac{3}{2}h\right) = \vec{v}\left(t + \frac{1}{2}h\right) + \vec{k} \qquad \text{[Eq 13]}$$

The Molecular Dynamics simulation involved a total of 16 particles with the initial velocity being zero. In other words, 16 particles were stationed at still. However, they were under the influence of Lennard-Jones potential between each other, which is expressed in Equation 14.

$$V(r) = 4\epsilon[\left(\frac{\sigma}{r}\right)^{12} - (\frac{\sigma}{r})^6] \qquad \text{[Eq 14]}$$

where ‘r’ refers to the distance between two particles

By implementing the Verlet algorithm on python, the trajectories of all 16 particles under the Lennard-Jones potential were plotted in Figure 5. The pseudo-code for the python implementation can be found in the submitted code.

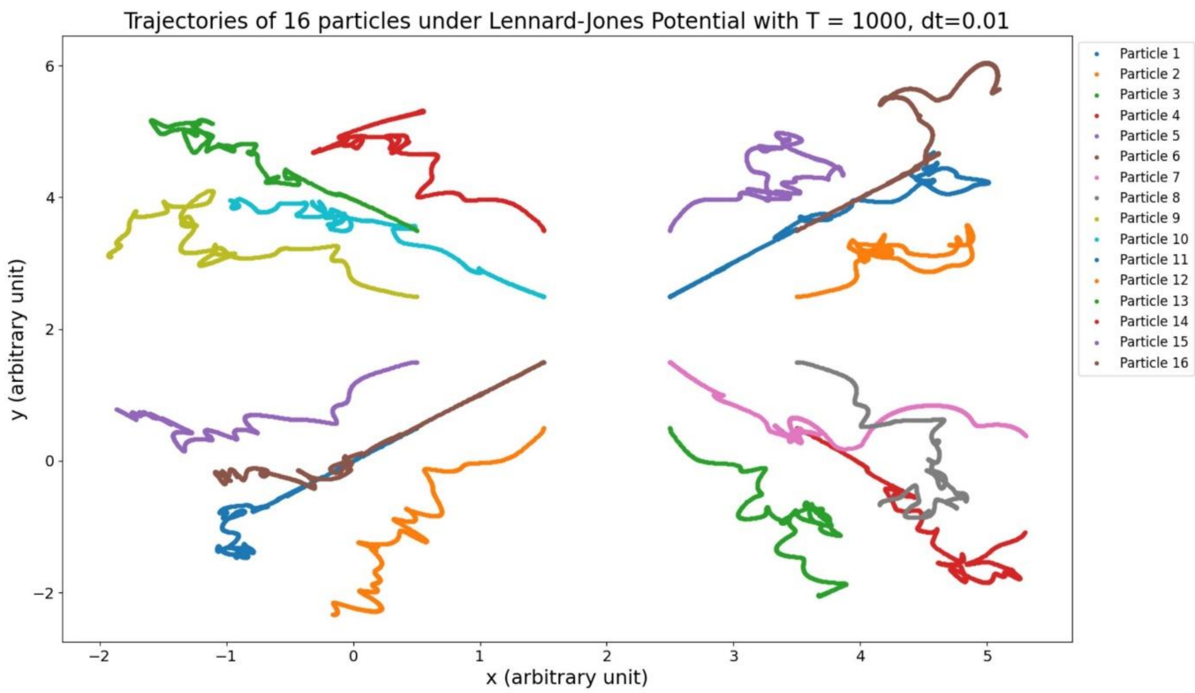

Figure 5: Trajectories of 16 particles under Lennard-Jones potential. The particles were observed to get away from the center, due to the repulsive force they experience caused by Lennard-Jones potential. It consists of 1000 time steps, with time interval between each step being 0.01.

Note that the trajectories initially showed a linear pattern, but later became irregular. In addition, the particle started getting far away from the center without any limitation as there was no periodic boundary condition applied, which will be discussed in part 'c' below.

Part b)

The Molecular Dynamics Simulation investigated in part 'a' above is in fact a conservative system. In other words, the total energy should be conserved at each time step. Therefore, when the kinetic energy increases, the potential energy should decrease, and vice versa. The potential energy and the kinetic energy are defined in Equation 14 and 15, respectively

$$K(v) = \frac{1}{2} m \vec{v}^2 \qquad \text{[Eq 15]}$$

$$\text{where } v = \sqrt{v_x^2 + v_y^2}$$

In the Verlet algorithm, the positions of particles were updated at each time step h, whereas the velocities were updated at time steps of $\frac{1}{2}$ and $\frac{3}{2}$. In order to compute the kinetic energy at the same time steps as the updated positions, the velocities are also to be computed at each time step h. The expression for such updated velocity can be found in equation 16.

$$\vec{v}(t+h) = \vec{v}\left(t+\frac{1}{2}h\right) + \frac{1}{2}\vec{k} \qquad \text{[Eq 16]}$$

As a result, the potential energy and the kinetic energy are plotted in Figure 6. Note that the graphs of potential energy and kinetic energy are symmetrical, which means the conservation of the total energy as the increase of potential energy resulted in the decrease of kinetic energy at the same time step.

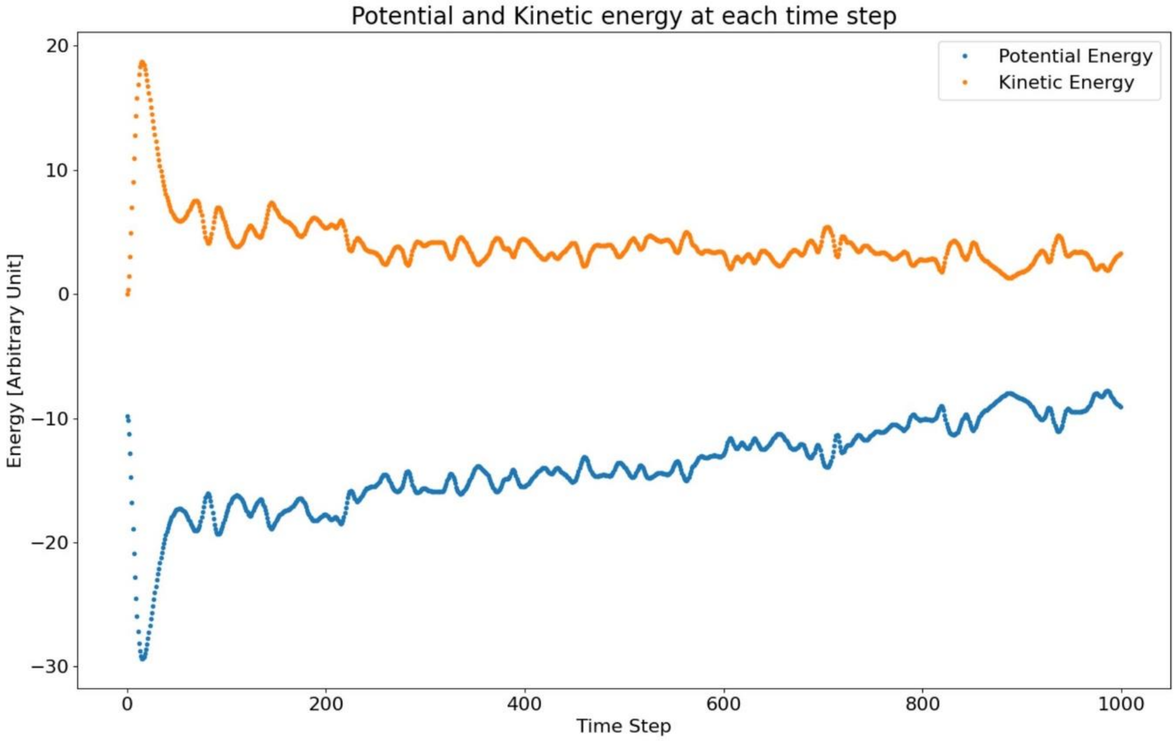

Figure 6: Potential and Kinetic energy at each time step. It consists of 1000 time steps, with time interval between each step being 0.01.

For example, the energies at the first three steps are listed in Table 1. The whole list of the energies, which is the direct output of the python computation, can be found in Appendix A. The values in Table 1 were deprecated to three decimal places for accuracy. The units of the energies are omitted as they are in an arbitrary unit.

Time step	Potential Energy	Kinetic Energy	Total Energy
t = 0	-9.791	0.0	-9.791
t = 1	-10.172	0.377	-9.795
t = 2	-11.249	1.446	-9.803

Table 1: The potential, kinetic, and total energy at the first three time steps.

The table 1 shows that the total energies were conserved to within about 1%, as expected.

Part c)

The periodic boundary condition was applied to the Molecular Dynamics Simulation. In other words, two changes were made to keep the particles inside the box [0.0, 4.0] x [0.0, 4.0]. First, the particles that exit this box in Figure 5 were moved back to the appropriate position inside the box, by applying numpy.mod() function. This makes the particle that exited appear on the other side of the box.

Furthermore, it was assumed that there are identical particles in all 8 sides outside this box. In other words, the box at each time step was replicated to form a total of 9 tiles, meaning that there are 9 identical systems now. Then, instead of just N-1 particles inside the box, additional 8N number of particles outside the innermost box were considered in the calculation of forces and acceleration. As a result, figure 7 shows the trajectories of 16 particles with the periodic boundary condition.

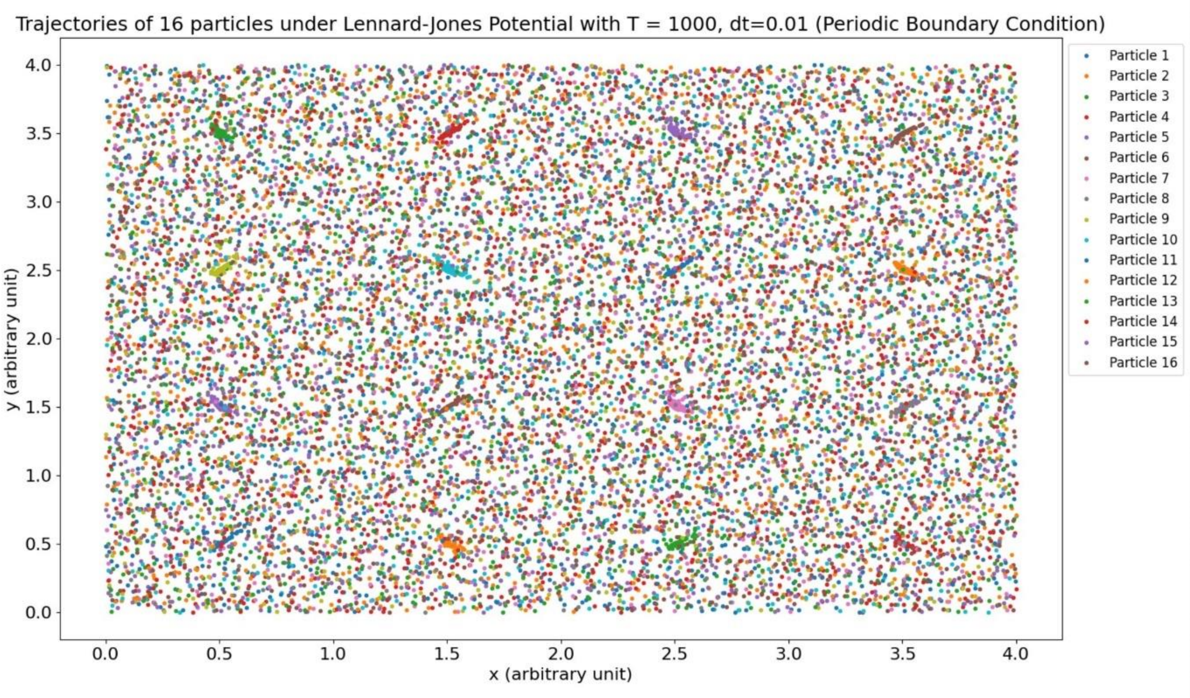

Figure 7: A reproduction of figure 5 with the periodic boundary condition. It consists of 1000 time steps, with time interval between each step being 0.01.

Note that each particle shows a concentrated movement at their original starting point before it starts to travel. With the particles all confined to [0.0, 4.0] x [0.0, 4.0] box, the trajectories show a chaotic behavior. However, a closer look at specific particles reveals a periodic behavior of their trajectories such as Figure 8 and Figure 9, which show trajectories of Particle 1 and 8, respectively.

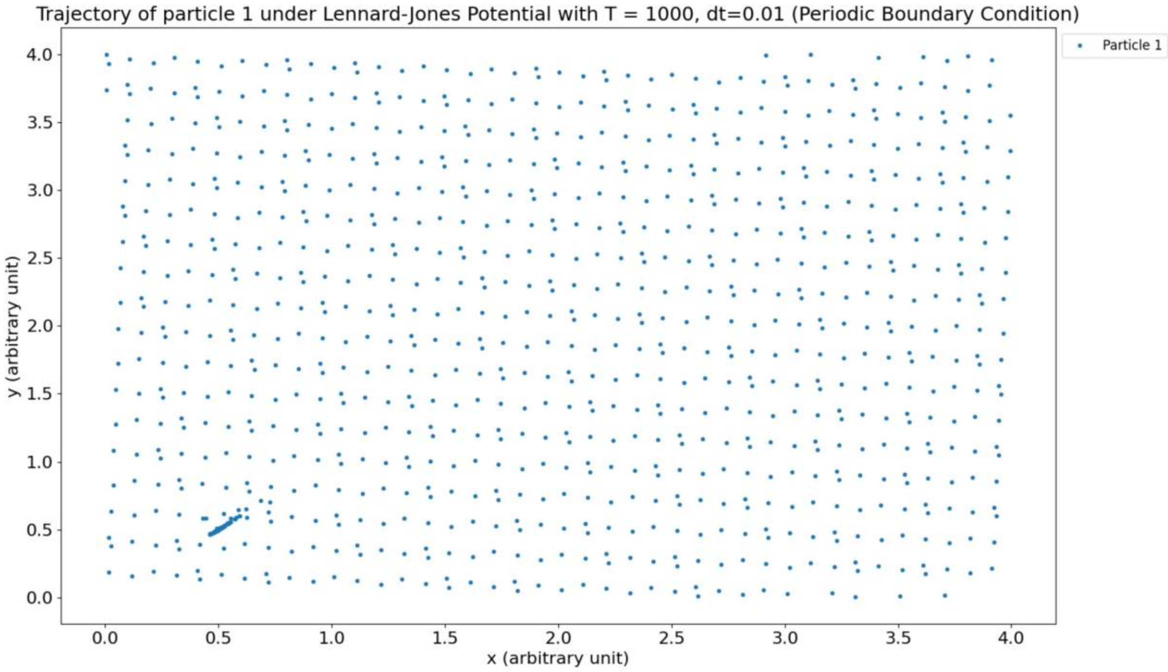

Figure 8: The trajectory of Particle 1 with Periodic Boundary Condition.

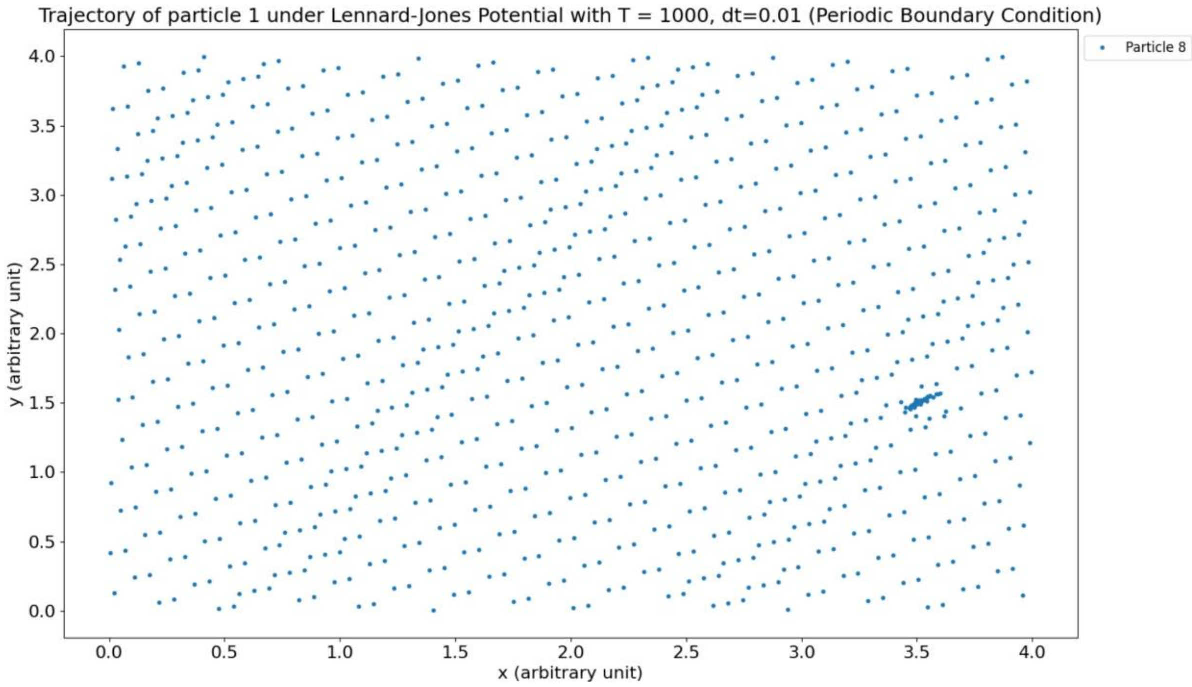

Figure 9: The trajectory of Particle 8 with Periodic Boundary Condition

Note that the same concentration at their starting point can also be observed in the close-up graphs in Figure 8 and 9.

Appendix A – Printed Output of Potential and Kinetic energies for Q3.b

Potential Energy

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