Lab 6 Report

PHY407 Week 5 Assignment

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Contribution: Landon Wang writes the entirety of question 1 and completes this document, Yinshi Liu writes the entirety of question 2.

Question 1

a)

The Lennard-Jones potential follows that

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1.1}$$

Where ϵ is the depth of the potential well, σ is the distance where the potential is zero for a specific interaction.

Since it's a potential, we can derive the force due to the potential by taking a derivative respect to r

$$\begin{aligned} F(r) &= -\nabla V(r) \\ &= \frac{d}{dr}V(r)\hat{r} \\ &= 4\epsilon\left[12\left(\frac{\sigma^{12}}{r^{13}}\right) - 6\left(\frac{\sigma^{6}}{r^{7}}\right)\right]\hat{r} \end{aligned} \tag{1.2}$$

We are asked for a acceleration, by newton's second law

$$F(r) = ma = 4\epsilon\left[12\left(\frac{\sigma^{12}}{r^{13}}\right) - 6\left(\frac{\sigma^{6}}{r^{7}}\right)\right]\hat{r} \tag{1.3}$$

We assumed $\sigma = 1,\ \epsilon = 1,\ m = 1$, therefore

$$\begin{aligned} a &= 4\left[\frac{12}{r^{13}} - \frac{6}{r^{7}}\right]\hat{r} \\ &= \frac{24}{r^{7}}\left[\frac{2}{r^{6}} - 1\right]\hat{r} \end{aligned} \tag{1.4}$$

r is defined as the distance between the two particles, therefore we can express it in terms of cartesian

$$\begin{aligned} r &= |\vec{r}_2 - \vec{r}_1| \\ &= \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \end{aligned} \tag{1.5}$$

Thus, we have the expression for acceleration

$$a = \frac{24}{[(x_2 - x_1)^2 + (y_2 - y_1)^2]^{\frac{7}{2}}}\left[\frac{2}{[(x_2 - x_1)^2 + (y_2 - y_1)^2]^3} - 1\right]\hat{r} \tag{1.6}$$

Since the acceleration has direction, we calculate the angle

$$\tan(\theta) = \frac{y_2 - y_1}{x_2 - x_1}$$
$$\Rightarrow \theta = \arctan\frac{y_2 - y_1}{x_2 - x_1} \quad 1.7$$

Now, we can separate x and y coordinates:

$$a_x = \text{acos}(\theta) \qquad a_y = \text{asin}(\theta) \quad 1.8$$

b)

Verlet Algorithm is a method for calculating conserved systems. Based on the fact that

$$a = \frac{F}{m} \quad 1.9$$

The algorithm follows that:

For first step only:

$$v\left(t + \frac{h}{2}\right) = v(t) + \frac{h}{2}a(r, t) \quad 1.10$$

Then, repeat equation 1.11-1.14

$$r(t + h) = r(t) + hv\left(t + \frac{h}{2}\right) \quad 1.11$$
$$k = ha(r(t + h), t + h) \quad 1.12$$
$$v(t + h) = v\left(t + \frac{h}{2}\right) + \frac{1}{2}k \quad 1.13$$
$$v\left(t + \frac{3}{2}h\right) = v\left(t + \frac{h}{2}\right) + k \quad 1.14$$

The $v\left(t + \frac{3}{2}h\right)$ term from equation 1.14 will be substitute the $v\left(t + \frac{h}{2}\right)$ term from equation 1.11 to repeat the algorithm.

It is quite obvious that equation 1.10 and 1.14 calculates a midpoint velocity for the further use, this means the number is not required to be saved into the data array.

To confirm the direction of the force due to the Lennard-Jones potential, first, we plot the acceleration in figure 1.1

We notice that for $x \lesssim 1.15$, the acceleration is positive, which should correspond to the repulsive force. That leaves the negative acceleration part to the Van der Waals force. This result help us to determine the direction of the force acting on the particle, we calculate the angle of the force and manually adjust with π such that sin and cos of the angle corresponds to the acuate direction.

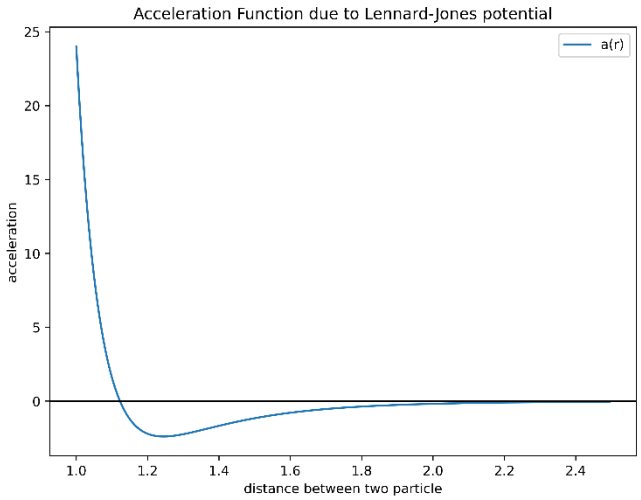

Figure 1.1 Acceleration due to Lennard-Jones Potential

Pseudocode:

1. Define the acceleration function based on the result of Q1
2. Set the initial conditions as np array
3. Set up the loop which takes the initial condition
4. Set the steps
5. Set the empty array and initialize with initial condition
6. Calculate midpoint velocity according to equation 1.10 using the acceleration function in step 1. Calculate angle θ for each particle and apply the trigonometrical correction mentioned above
7. Run a loop over each step and calculate using Verlet Algorithm according to equation 1.11 to 1.14
8. Plot the result

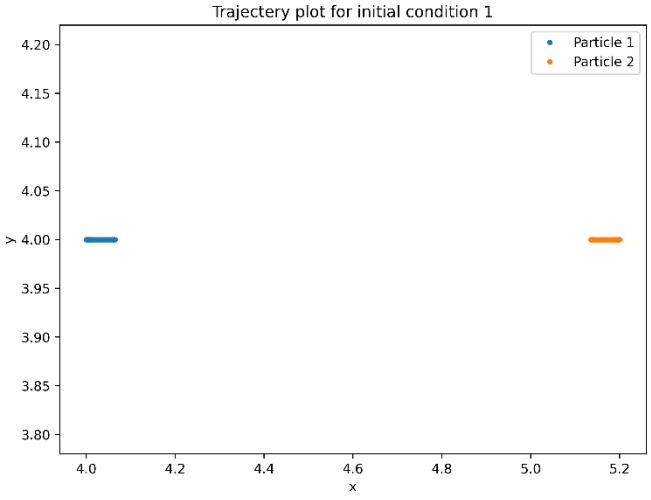

Figure 1.2 Trajectory of Particle set 1

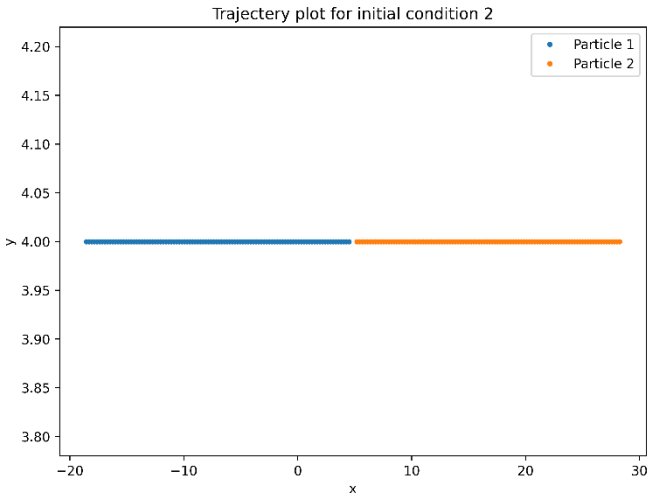

Figure 1.3 Trajectory of Particle set 2

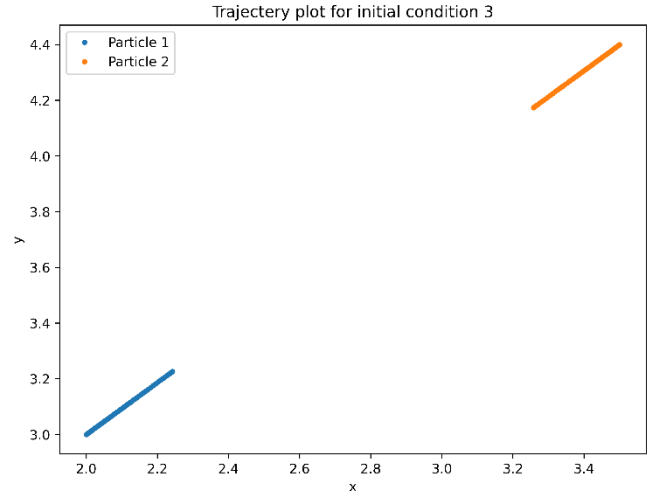

Figure 1.4 Trajectory of Particle set 3

c)

From the plots, we observed that two particles only move in 1D respect to each other which is to be expected. The movement of particles in fig 1.3 extends to a large range of x and apparently did not return which indicating a ejection. For fig 1.2 and fig 1.4, the plot apparently shows an oscillation case, but we can confirm it using potential function:

$$V(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^{6}\right] \qquad 1.15$$

This is a modified equation to 1.1 as we set $\sigma = 1,\ \epsilon = 1,\ m = 1$ for this question.

It is possible to calculate the r using the initial condition with eq. 1.5 and apply the eq. 1.15 for the potential. The result is plotted in figure 1.5

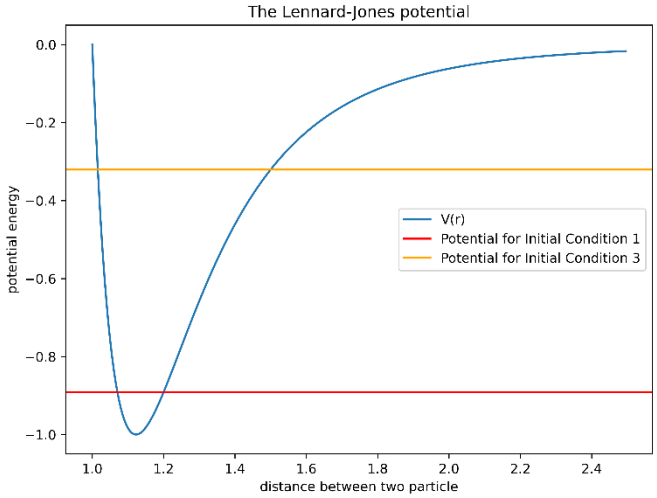

Figure 1.5 Lennard-Jones Potential plotted with Initial Conditions

Notice that initial condition set 2 is not shown in the plot as the potential is very high and affecting the viewability of the plot.

The two initial condition sets shown in the plot is in the range of the potential valley, which justified their oscillating behaviour.

Question 2

a)

Pseudocode

1. Update the code from Q1 with new initial condition of particles and adapt the code to process arrays as an input.
2. Set up the condition of the 16 particles when t = 0.

For each of the 16 particle, calculate the distance r_i from all other points.

Calculate the angle for each interaction using the np.arctan2() function to account for different quadrants. (The angle should be between $(-\pi, \pi)$)

$$\theta = \arctan\frac{dist\ x}{dist\ y} \tag{2.1}$$

Calculate the acceleration on each particle due to other particles using the LJ acceleration function

$$a(r) = 4\left[\frac{12}{r^{13}} - \frac{6}{r^{7}}\right]\hat{r} \tag{2.2}$$

since the particles should repel each other when they are close and attract when they are far, $\hat{r}$ should be negative. Break down the acceleration in to its respective x and y components and perform vector addition.

Calculate the midpoint velocity using:

$$v\left(t + \frac{h}{2}\right) = v(t) + \frac{h}{2}a(r, t) \tag{2.3}$$

for each component.

3. For each additional iteration:

Update the position using eqn. 1.10.

Calculate the acceleration components for each particle using the loop in step 2.

Calculate k using eqn. 1.12.

Update velocity and new midpoint velocity using eqn. 1.13 and 1.14.

Iterate for every time step.

4. Since the result is a nested list, extract the result using the following code:

$$\begin{aligned} x_i &= [item[i-1]\ for\ item\ in\ x] \\ y_i &= [item[i-1]\ for\ item\ in\ y] \end{aligned} \tag{2.4}$$

5. Plot the result.

Code Output

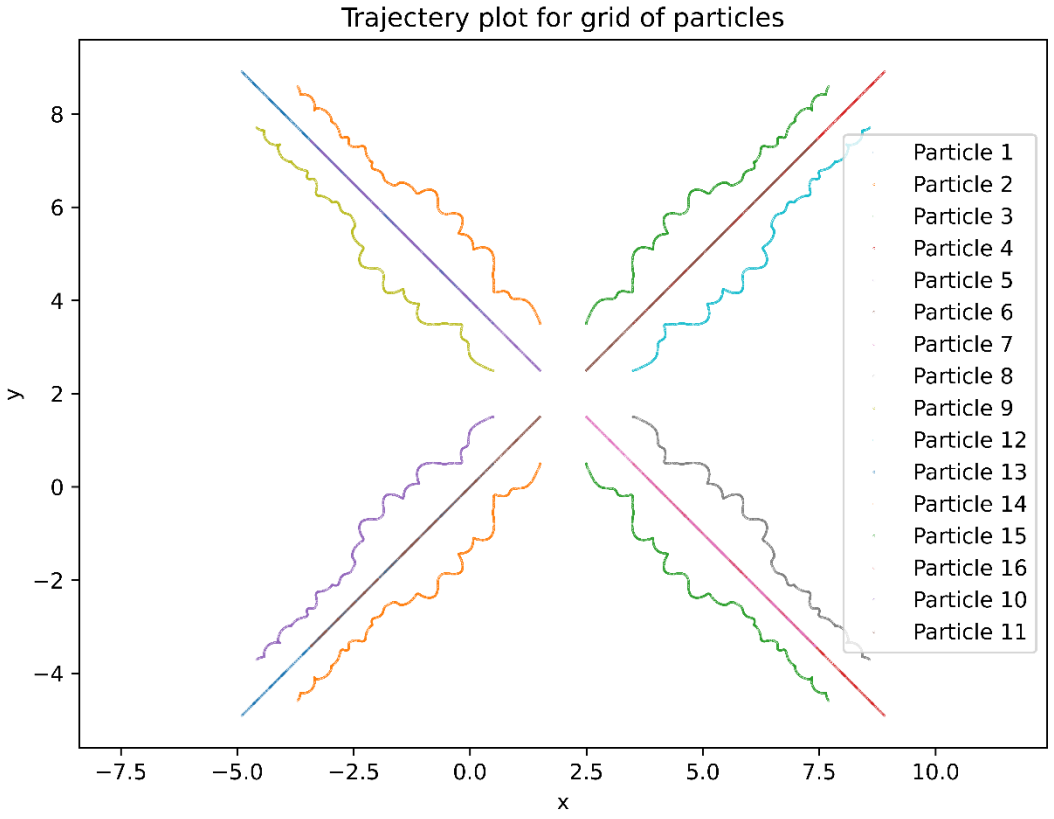

Figure 2.1 Trajectory of 16 particles

According to Figure 2.1, this initial distribution of particles is unstable. The 4 particles on the corner (Particle 1, 4, 13, 16) started to move away immediately, with the central particles (particle 6, 7, 10, 11) following the same trajectory. This agrees with the shape of the LJ potential, as they were placed very close to each other. The particles on the side (particle 2, 3, 5, 8, 9, 12, 14, 15) is seemingly attracted to the central/corner particles, and moved along the trajectory in a semi-regular pattern.

We noticed that for conner and center particles, the velocity of moving outward changes regularly. The marker size for the plot is set below 1, which creates circle with central dot shape. This creates a transparency effect in macroscopic perspective, the lighter the colour, the faster the particle travels and vise versa.

We can hardly understand the behavior shown in the plot initially and assumed that it was an error in our code, specifically with the calculation of a(r). However, after recalculating the acceleration to each particle for the t = 0 case manually, no error was found.

NOTE: High definition figure 2.1 is uploaded separately.

b)

Pseudocode

1. Update the Q2a code with empty arrays representing potential and kinetic energy.
2. Calculate the total potential energy of the system at t = 0

Since the distribution is symmetric, we can generalize the potential of each particle into 3 different categories, with particle in the same category having the same potential energy. For the particles on the corner:

$$\begin{matrix} v(3) & v(\sqrt{10}) & v(\sqrt{13}) & v(3\sqrt{2}) \\ v(2) & v(\sqrt{5}) & v(2\sqrt{2}) & v(\sqrt{13}) \\ v(1) & v(\sqrt{2}) & v(\sqrt{5}) & v(\sqrt{10}) \\ 0 & v(1) & v(2) & v(3) \end{matrix} \tag{2.5}$$

Given that potential field is a scaler field, the potential energy of a particle on the corner at t = 0 would be:

$$\begin{aligned} \mathrm{V_0} = 2\mathrm{v}(1) + 2\mathrm{v}(2) + 2\mathrm{v}(3) + \mathrm{v}(\sqrt{2}) + \mathrm{v}(2\sqrt{2}) \\ + \mathrm{v}(3\sqrt{2}) + 2\mathrm{v}(\sqrt{5}) + 2\mathrm{v}(\sqrt{10}) + 2\mathrm{v}(\sqrt{13}) \end{aligned} \tag{2.6}$$

The same idea applies to ones on the side and ones in the center as well, with the following distributions respectively:

$$\begin{matrix} v(\sqrt{10}) & v(3) & v(\sqrt{10}) & v(\sqrt{13}) \\ v(\sqrt{5}) & v(2) & v(\sqrt{5}) & v(2\sqrt{2}) \\ v(\sqrt{2}) & v(1) & v(\sqrt{2}) & v(\sqrt{5}) \\ v(1) & 0 & v(1) & v(2) \end{matrix} \tag{2.7}$$

$$\begin{matrix} v(\sqrt{5}) & v(2) & v(\sqrt{5}) & v(2\sqrt{2}) \\ v(\sqrt{2}) & v(1) & v(\sqrt{2}) & v(\sqrt{5}) \\ v(1) & 0 & v(1) & v(2) \\ v(\sqrt{2}) & v(1) & v(\sqrt{2}) & v(\sqrt{5}) \end{matrix} \tag{2.8}$$

Therefore, the total energy in this system would be:

$$\mathrm{V_{0total}} = 4V_{0corner} + 8V_{0side} + 4V_{0centre} \tag{2.9}$$

3. Collect the Potential energy and velocity of the system in the time evolution loop outlined in Q2a. Then calculate the potential energy and kinetic energy of the system for each particle using:

$$\mathrm{PE_i} = \frac{\mathrm{V_i}}{2} \tag{2.10}$$

$$\mathrm{KE_i} = \frac{1}{2}\left(v_{xi}^2 + v_{yi}^2\right) \tag{2.11}$$

4. Extract the energy for each particle and plot the result. Check the energy conservation of the system using:

$$\mathrm{E_{total}} = \sum_{n=1}^{16} KE_i + PE_i \; = 4E_{corner} + 8E_{side} + 4E_{centre} \tag{2.12}$$

$$\mathrm{E_{conservation}} = \frac{\left(\max(E_{total}) - mean(E_{total})\right)}{mean(E_{total})} \tag{2.13}$$

Code Output

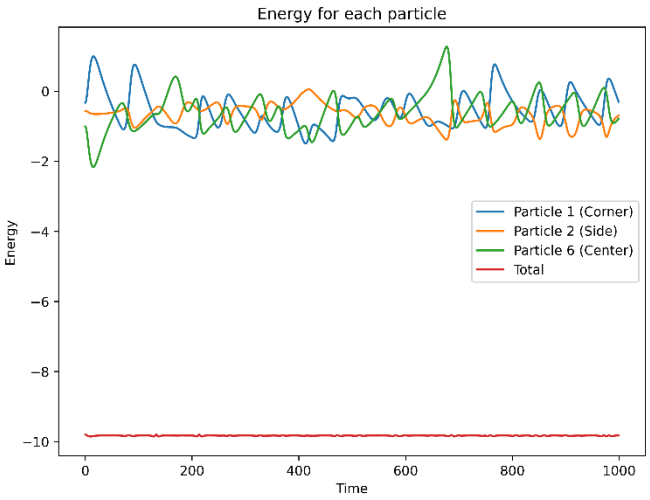

Figure 2.2 Energy of each particle

Energy conservation of the system

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energy is conserved within 0.24811056924791025 %
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Which is smaller than 1%.

According to figure 2.2, the total energy within the system remains constant. The energy of each individual particle varied as time evolved. This means that as time goes on, the interactions between particles has exchanged energy with each other. Since the total energy is conserved, this means that the Verlet method is an accurate way to numerically calculate ODE systems.