PHY407 Lab-06 Report

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[1] *Q1 - Molecular Trajectories Simulations*
[2] *Q2 - Molecular Dynamics Simulation*

1. Q1 - MOLECULAR TRAJECTORIES SIMULATIONS

For the pseudo-code and code for this and all is consecutive sub-questions please refer to the python script `Lab05_Q1.py`. The function used to perform the Verlet methods is in the python script labeled `MyFunctions.py`.

1.1. *Q1a - Acceleration of Particles Due to Lennard-Jones Potential*

For this simulation we will be looking at a conservative system of 2 particles, that is not subject to any external forces. For such scenario we can express the potential between the particles through the Lennard-Jones potential described as follows.

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

For our derivation we will center our origin at the position of one of the particles such that we can express the distance between the particles in a cleaner manner i.e $r^2 = x^2 + y^2$. We proceed to compute the force acting on the particles by taking the negative gradient in spherical coordinates of the potential.

$$\vec{F} = -4\epsilon\left[\frac{-12\sigma^{12}}{r^{13}} + \frac{6\sigma^6}{r^7}\right]\hat{r} \tag{2}$$

We can express this force in Cartesian by noting that $x = r\cos\theta$, $y = r\sin\theta$

$$\begin{aligned}
\vec{F} &= F_r\cos\theta\hat{x} + F_r\sin\theta\hat{y} \\
\vec{F} &= \left[\frac{48\epsilon\sigma^{12}}{(x^2+y^2)^{13/2}} - \frac{24\epsilon\sigma^6}{(x^2+y^2)^{7/2}}\right]\cos\theta\hat{x} + \left[\frac{48\epsilon\sigma^{12}}{(x^2+y^2)^{13/2}} - \frac{24\epsilon\sigma^6}{(x^2+y^2)^{7/2}}\right]\sin\theta\hat{y} \\
\vec{F} &= x\left[\frac{48\epsilon\sigma^{12}}{(x^2+y^2)^{13}} - \frac{24\epsilon\sigma^6}{(x^2+y^2)^{7}}\right]\hat{x} + y\left[\frac{48\epsilon\sigma^{12}}{(x^2+y^2)^{13}} - \frac{24\epsilon\sigma^6}{(x^2+y^2)^{7}}\right]\hat{y}
\end{aligned} \tag{3}$$

We can use this result to express the Cartesian components of the acceleration for each particle. We just need to consider one last detail, instead of setting our origin on the position of one of the particles we will now let this second particle be located at some point (a, b). Which means the respective acceleration for the the particle located at (x, y) is given by.

$$\vec{a}_x = \frac{(x-a)}{m}\left[\frac{48\epsilon\sigma^{12}}{((x-a)^2+(y-b)^2)^{13}} - \frac{24\epsilon\sigma^6}{((x-a)^2+(y-b)^2)^{7}}\right]\hat{x} \tag{4}$$

$$\vec{a}_y = \frac{(y-b)}{m}\left[\frac{48\epsilon\sigma^{12}}{((x-a)^2+(y-b)^2)^{13}} - \frac{24\epsilon\sigma^6}{((x-a)^2+(y-b)^2)^{7}}\right]\hat{y} \tag{5}$$

The same is true for the second particles only that we switch the order of the subtraction.

1.2. *Q1b - Implementing Verlet Method to Simulate System*

In order to simulate the system described in subsection 1.1 we will need to implement the Verlet method to solve the coupled 2^{nd} ODE that are eq.4 and eq.5. The Verlet method is a form of leapfrog method which allows simulations of conservative systems such as this one. Using the stated method to compute the trajectories of the particles from 0 to 1s with a time step of 0.01s, and $\epsilon = \sigma = m = 1$ we get the following plots. Figure 1 is consistent with the ODE's presented in eq.4 and eq.5. And its most visible for the first simulation where we see the repulsion term dominate when the particles are close and the attraction term dominates when the grow further apart.

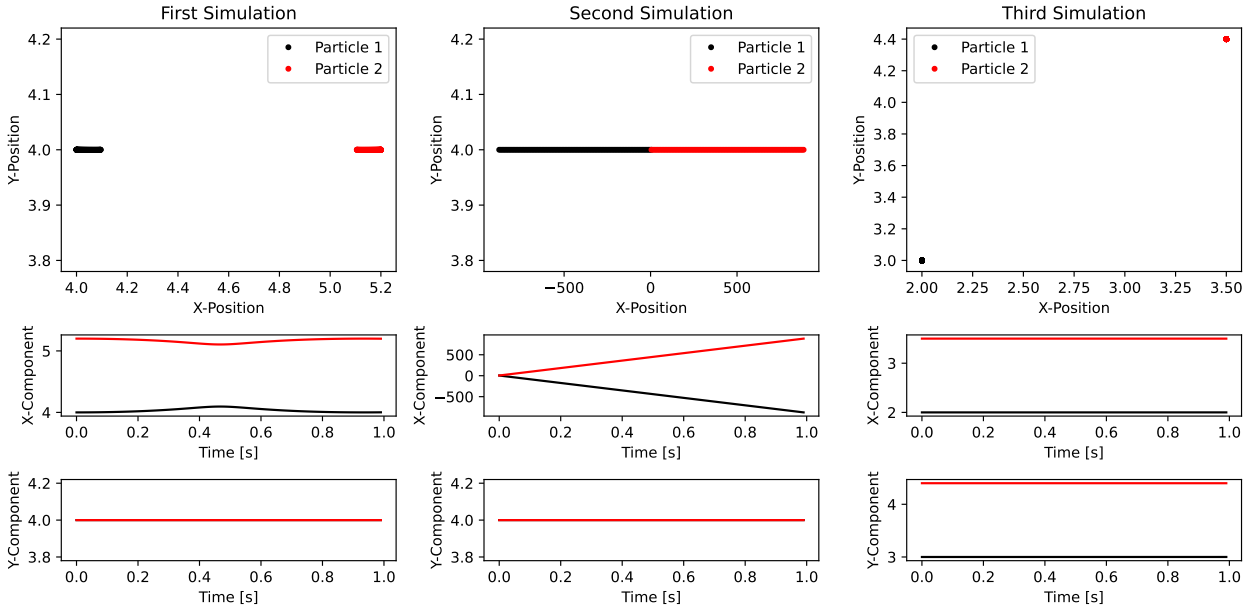

Figure 1: Molecular trajectory simulation for 2 particles subject to Lennard-Jones potential. The first simulation has initial conditions $r_1 = (4, 4)$, $r_2 = (5.2, 4)$. The second simulation $r_1 = (4.5, 4)$, $r_2 = (5.2, 4)$. And the third simulation $r_1 = (2, 3)$, $r_2 = (3.5, 4.4)$ where the subscript represent the particle index.

1.3. *Q1c - Physical Interpretation of Results*

The natural question to ask after performing these simulations is if our results make physical sense for a isolated system where no external forces are acting on the particles. As previously stated at the end of subsection 1.2 the oscillations observed in the x-component plot of simulation 1 is due to the alternating dominance of the attractive $1/r^7$ force and the repulsive $1/r^{13}$ force. The straight oscillation seen in figure 2 represents energy conservation because the

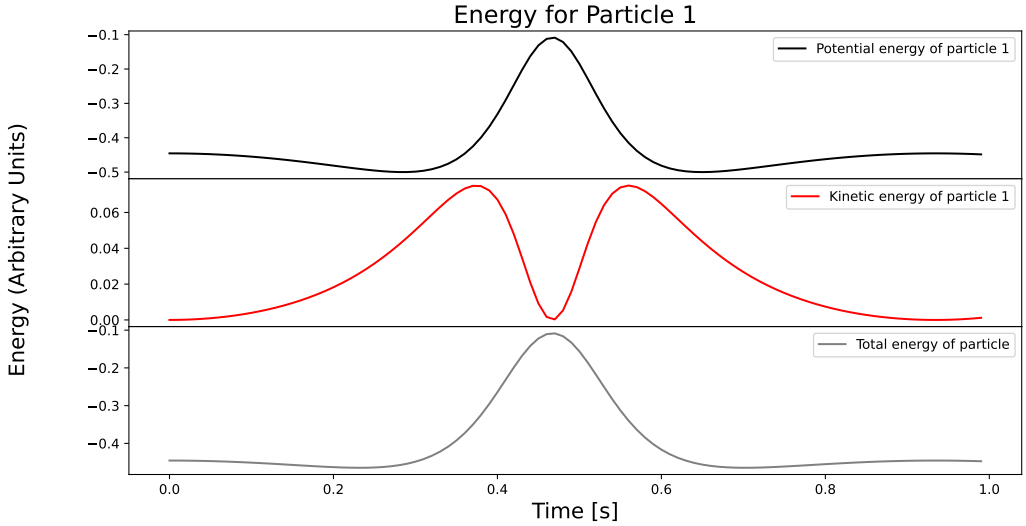

Figure 2: Potential, kinetic and total energy of particle 1 from top to bottom respectively.

particles are oscillating with respect to their equilibrium point instead of displacing further or closer to one another, meaning that there is no energy drift in the total energy.

2. Q2 - MOLECULAR DYNAMICS SIMULATION

For the pseudo-code of all the sub-question please refer to the python script titled `Lab06_Q2.py`.

2.1. *Q2a - 16 particles simulation*

In this question, we simulated the dynamic interaction of 16 particles with Lennard-Jones potential, where the initial conditions are that the particles are located on the xy-plane evenly spaced out and the initial velocity of all 16 particles are set to zero. Using the acceleration derived in Eq.4-5 in Q1 above, we modified the Verlet method in order to simulate the subsequent behaviour of all 16 particles. Compared to the Verlet method implemented in Q1, the modified method here now has to account that for each particle i, the acceleration (i.e. force) and potential energy of i are due to all 15 other particles simultaneously; and in order to have the method work correctly, at each "time-step" we have to first calculate the positions of all 16 particles first (using Eq.9 in lab handout) before moving on to calculate $\vec{k}$ vector, half-step and full-step velocities for each particle. See the comments in the function for more detail. Figure 3 shows the trajectories of the 16 particles on the xy-plane, where we have set the center of the system at $(x, y) = (0, 0)$.

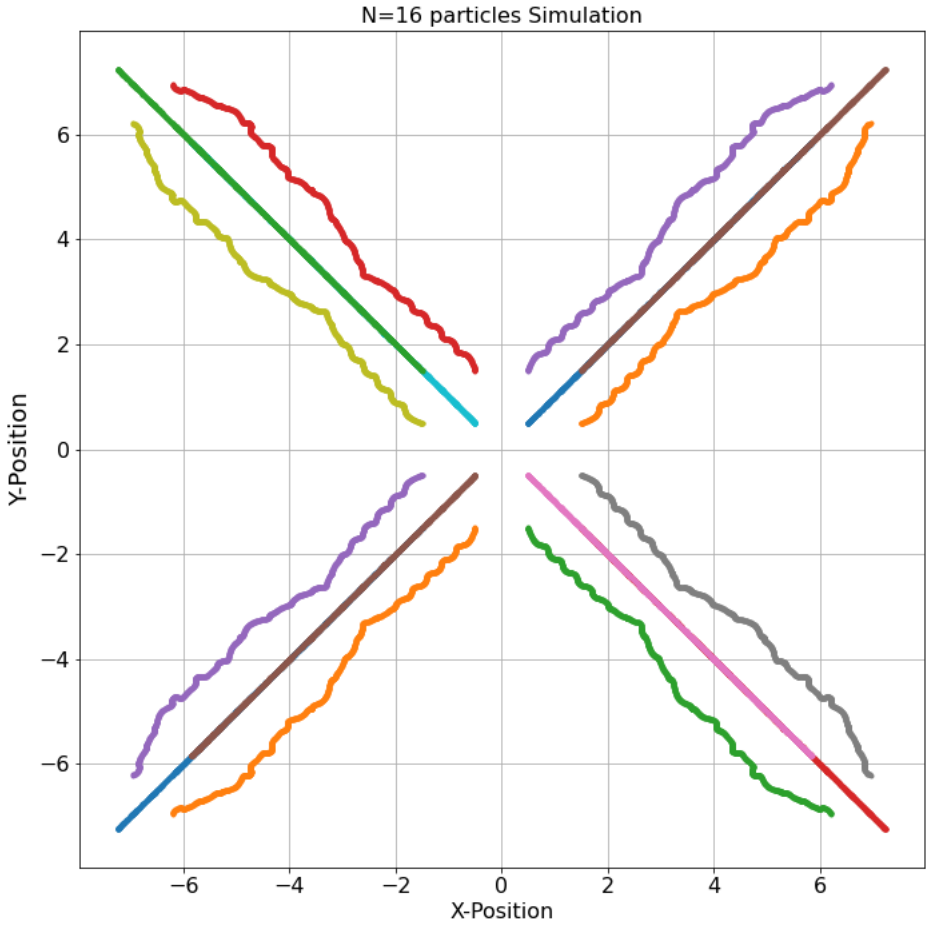

Figure 3: The trajectory of 16 particles in the simulation shown here each with a different color.

As we can see in Figure 3, the 16 particles can be group into 4 groups, where in each group two of the diagonal particles would move away from the center of the entire system in a straight line, while the other two in the group would vibrate in-and-out synchronously along the straight line.

2.2. *Q2b - Energy Conservation in the dynamic simulation*

In addition, we also book-keep the kinetic energy and potential energy in the Verlet method function, and we plotted the total energy of the system as a function of time in the graph below.

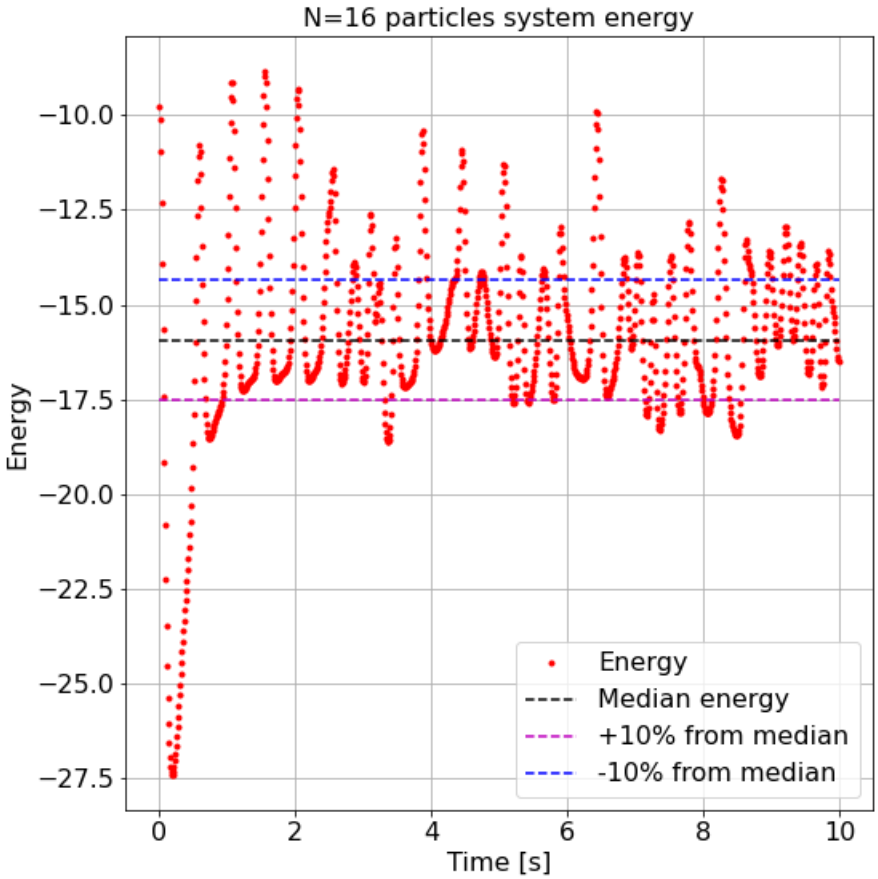

Figure 4: Total energy in the simulation indicated in red dots. The black dashed line indicates the calculated median energy. The blue and purple line indicates the upper and lower bounds of the 10% interval.

We calculated the median of the energy is -15.9 in the simulation. As we can see, there are many fluctuations throughout simulation, but we found the it eventually is "conserved" within approximately $\pm 10\%$ of the calculated median. However, we were not able to limit the fluctuation to be conserved within $\pm 1\%$ of the median as required by the question, and we are unsure of why. We think it might be due to propagation of numerical error based on how we implemented the Verlet method that is causing these huge fluctuations, but we are unable to locate the source of the problem given the due date of the lab.