Molecular Dynamics

Extended System

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February 11, 2025

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1 Introduction

The aim of this assignment is to write a simple Python program to study and analyze the basic dynamics of an extended molecular dynamical system.
The Lennard-Jones (LJ) potential was used to calculate the potential and force between the atoms, while the velocity verlet method was used to compute the time evolution of the positions and velocities, which were then plotted and analyzed.
In addition to the previous assignment, we now implement the minimum convention method to allow periodic boundary conditions in order to visualize the atoms interacting through the boundaries of the system.

2 Theory

2.1 PBC, Minimum image covention

Simulating an infinitely large system is computationally expensive, Periodic Boundary Conditions (PBC) are used to reduce those costs [1]. PBC assumes the system is enclosed in a box that repeats infinitely in all directions, allowing atoms leaving one side to re-enter from the opposite side.
The Minimum Image Convention (MIC) is a commonly used method to apply PBC, in which each individual particle in the simulation interacts with the closest image of the remaining particles in the system. That can be done by applying a simple formula to the particle's position:

$$D = D - L \cdot round(D/L) \tag{1}$$

Where D is the position and L is the side length of the box.

2.2 Initial conditions

2.2.1 Initial Positions, Cubic lattice

To provide a structured starting configuration, atoms are initialized in a simple cubic lattice, where the number of atoms, N, is determined as:

$$N = n^3 \tag{2}$$

and the size of the box, L:

$$L = n \cdot d \tag{3}$$

Where d is the density.

2.2.2 Initial Velocities, Drift removal and rescaling

Velocities were first randomly assigned from a normal distribution, then adjusted to remove drift by subtracting the center-of-mass velocity [2]:

$$v_i^{'} = v_i - \frac{1}{N}\sum_{j=1}^{N} v_j \tag{4}$$

and lastly, they were rescaled to match the desired temperature, T, using the equipartition theorem:

$$v_i^{''} = v_i^{'} \cdot \sqrt{\frac{T'}{T}} \tag{5}$$

3 Results and Discussion

3.1 Two-particle dynamics, PBC

In a similar way as in assignment 1, the LJ force and potential for two atoms separated by 4 Åwere calculated and the values were used to obtain a simple simulation of the positions and velocities of the atoms over time, and also PBC was implemented to see how the atoms behave at the boundaries.
Plots of $x(t)$ and $v_x(t)$ were analyzed to check for bouncing behavior:

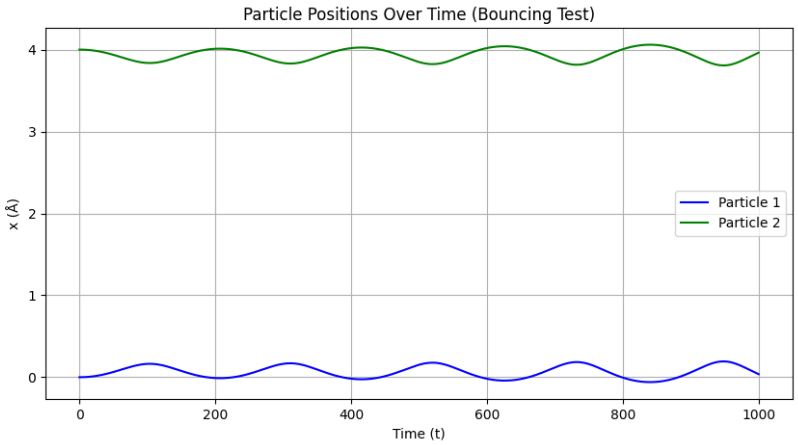

Figure 1: The position of the two atoms as a function of time.

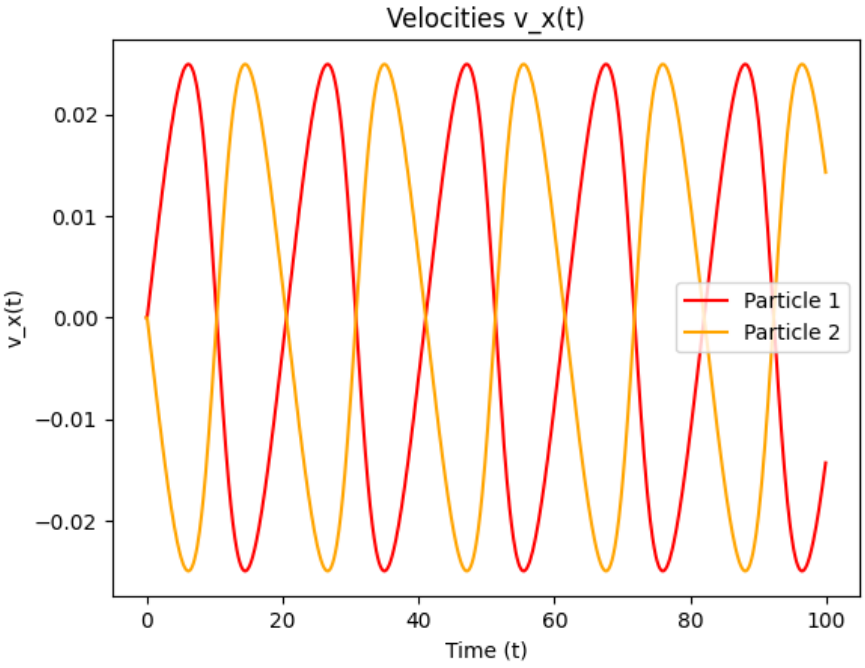

Figure 2: The velocities of the two atoms as a function of time.

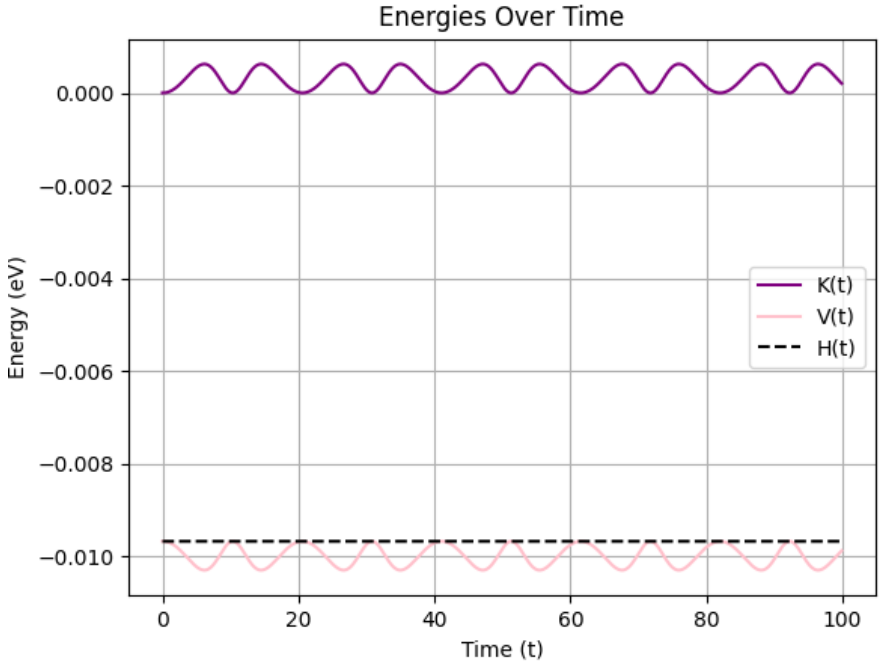

Figure 3: The potential, kinetic and total energy over time.

As shown in the figures above, the plots agrees with the ones we got without implementing PBC, i.e the particles are interacting in the same way through the boundaries, which confirms that our implementation is working correctly.

3.2 Extended system

Lastly, the same process was repeated for an extended system consisting of $N = n^3 = 5^3$ atoms, with density $\rho \approx 1.4$ g/cm^3 and temperature $T \approx 95$ K. Plots of $x(t)$ and $v_x(t)$ for the first atom are shown below:

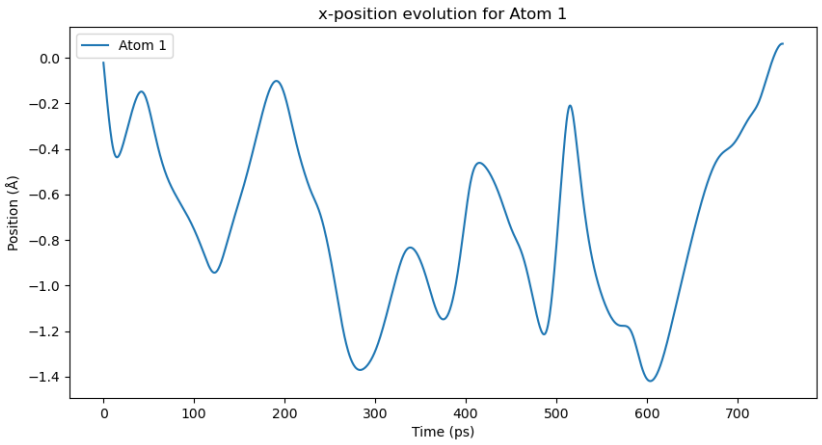

Figure 4: The position of atom 1 as a function of time.

We can observe in Figure 4 that the trajectory exhibits smooth oscillations, indicating the atom motion within the periodic box and confirming that the implementation of PBC is correctly implemented. The observed oscillatory behavior suggests that the atom is experiencing forces due to nearest neighbors, leading to bounded motion, but in contrast to the previous assignment, the atoms now are not moving

in a perfectly sinusoidal motion since they are feeling forces from a larger number of atoms.

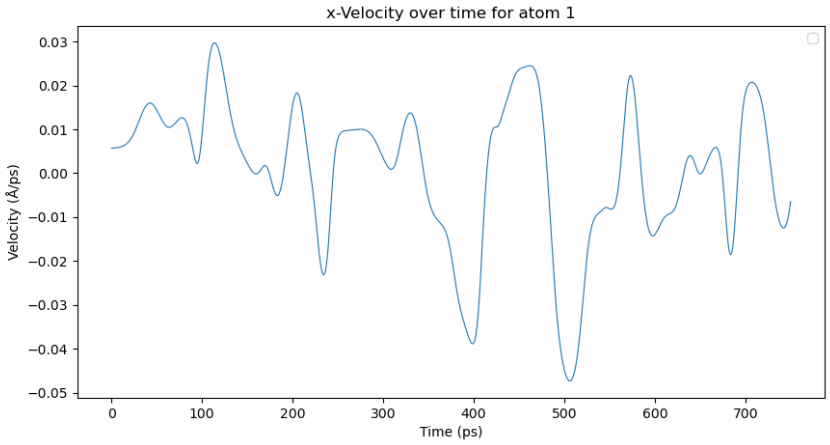

Figure 5: The velocity of atom 1 as a function of time.

Similarly, the amplitude of the velocity oscillations varies over time indicating that the atom experiences different force magnitudes throughout the simulation, which is expected in a multi-atom system, where local density fluctuations and atomic collisions affect the overall velocity distribution.

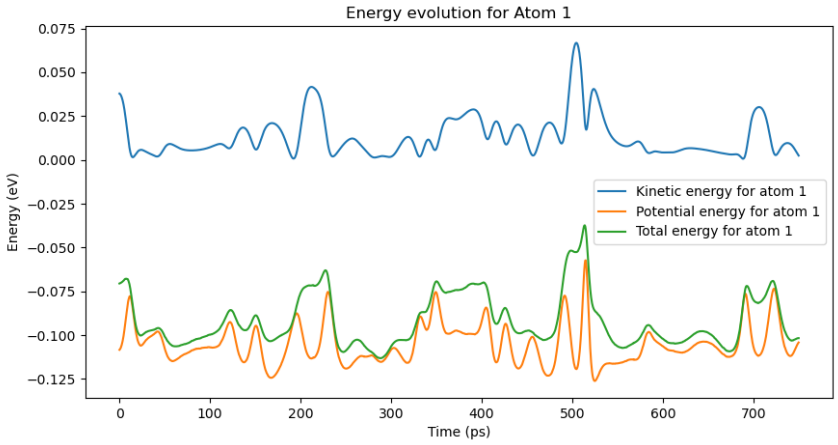

Figure 6: The energies of atom 1 as a function of time.

In Figure 6, one can observe how the velocities fluctuation aligns with the changes in potential energy, where an increase in velocity corresponds to a decrease in potential energy. The total energy exhibits minor fluctuations, but remains relatively conserved throughout the simulation.

Lastly, some plots for the first 10 atoms are included:

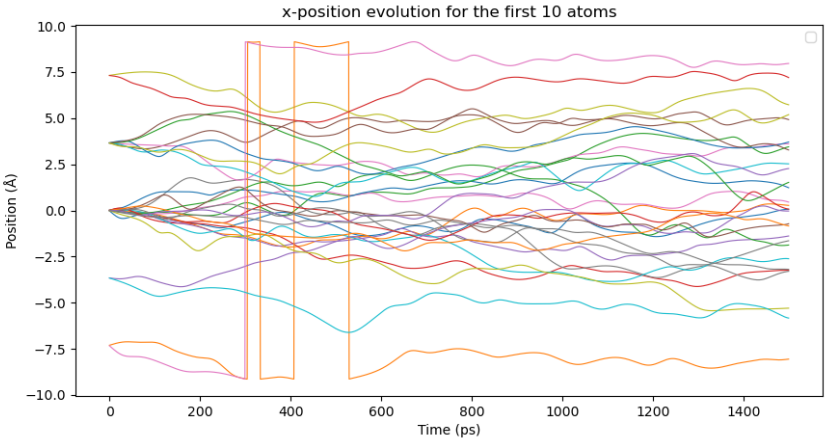

Figure 7: The position of the first 10 atoms as a function of time.

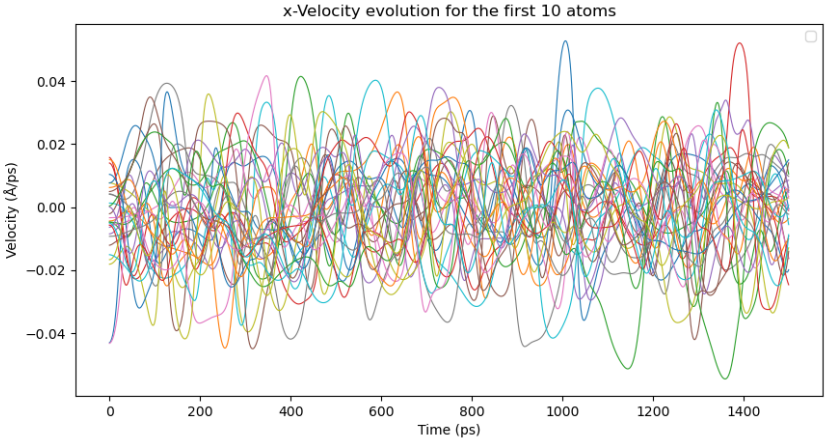

Figure 8: The velocities of the first 10 atoms as a function of time.

3.3 Conclusions

Overall, the results obtained in this lab successfully modeled an extended molecular system. These findings together with the results obtained in assignment 1 confirm our correct implementation of LJ-potential, the velocity Verlet method and PBC, providing physically meaningful results and highlighting the power of numerical methods in Molecular dynamics.

References

[1] J. Öström, *Compendium on Methods: Simulation Methods in Statistical Physics*, (Stockholm University, 2022), Section 3.

[2] J. Öström, *Compendium on Methods: Simulation Methods in Statistical Physics*, (Stockholm University, 2022), Section 4.