Simulation Methods in Statistical Physics (FK 8028)

Programming project report 1: Dynamics

Submitted by Mikhail Ivanov

Introduction

For the first part of this programming project, some of the basic features of the molecular dynamics code for the Lennard-Jones fluid simulations were developed using the *Python 3* programming language. The main implemented features include the calculation of the potential energy of the system of N particles interacting via Lennard-Jones potential, calculation of the force acting on each particle in the system, as well as the velocity Verlet algorithm for the integration of the equations of the particles' motion.

Initial conditions (number of particles, coordinates, velocities), forcefield and integration parameters (σ, ε, number of time steps, time step length) are read from the input data files. Computed values (trajectory, velocities, forces and energies) are written to the output data file and plotted by the auxiliary *Python MatPlotLib* programs. Trajectory visualisation is performed using the *VMD* molecular visualisation program.

Developed code was thoroughly tested by simulating a few basic atomic systems using different integration parameters and checking if the obtained properties are correct. It is shown that for the system of two oscillating argon atoms as well as eight colliding argon atoms, the total energy is conserved for as long as 10^5 time steps with 2 fs time step.

Results and discussion

Here the results of the first part of the programming project will be presented and discussed.

1. Lennard-Jones (LJ) energy and forces for a pair of particles

The crucial part of the molecular dynamics code is the correct computation of the potential energy and the force, acting on each particle. Potential energy and force computations were initially checked for a system of two argon atoms, separated along the X-axis. The first particle was located at the origin, while the second particle was moved away from the first particle from 2.5 Å to 7.0 Å with a distance step of $3.405 \cdot 10^{-3}$ Å (0.001 σ). The resulting potential energies and forces are presented in *Figure 1*.

The potential is zero at a distance equal to 3.405 Å (1 σ) and -ε ($1.654 \cdot 10^{-21}$ J, or ≈0.0103 eV) at the ≈3.822 Å ($2^{1/6}$ σ). At this distance, the force is zero, as this separation corresponds to the minimum of the potential. Both the potential and the force approach zero with the increasing separation.

From this data, it is possible to conclude that the potential energy and the force are computed correctly for a system of two LJ particles.

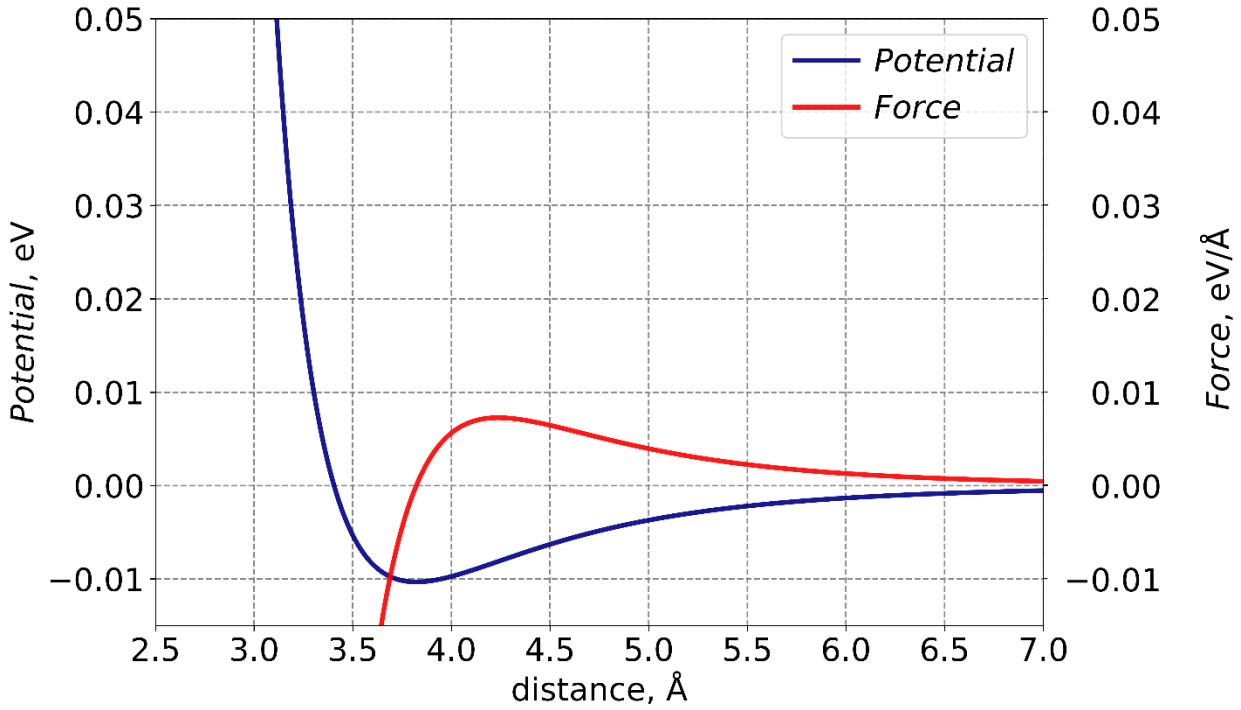

Figure 1 – Potential energy of two argon atoms (blue line) and the force, acting on one of the particles (red line)

2. Integrating the equations of motion for the system of two oscillating particles

To study the dynamics of atomic systems, one should implement a suitable integration algorithm that will ensure stable simulation with minimal integration errors. For this purpose, the velocity Verlet integration algorithm was implemented.

2.1. Choosing the time step length

To choose an appropriate time step for the integration algorithm, one should balance the integration errors and the simulation performance (i.e. simulated time per CPU time). To assess the possible integration errors, the system of two oscillating argon atoms was simulated for 500 picoseconds with eleven different time steps from the range of 1 femtosecond to 100 femtoseconds.

The total energy differences were plotted against the time step length (*Figures 2 and 3)*. The total energy difference increases monotonically with the time step and proportional to approximately Δt^4, until at some point between 62.5 fs and 100 fs time step, where the final total energy diverges from the initial total energy completely.

2 fs time step was picked for subsequent simulations, as the total energy difference between the last and the first time steps is negligible (≈0.07% of the initial total energy) while the simulation performance is adequate.

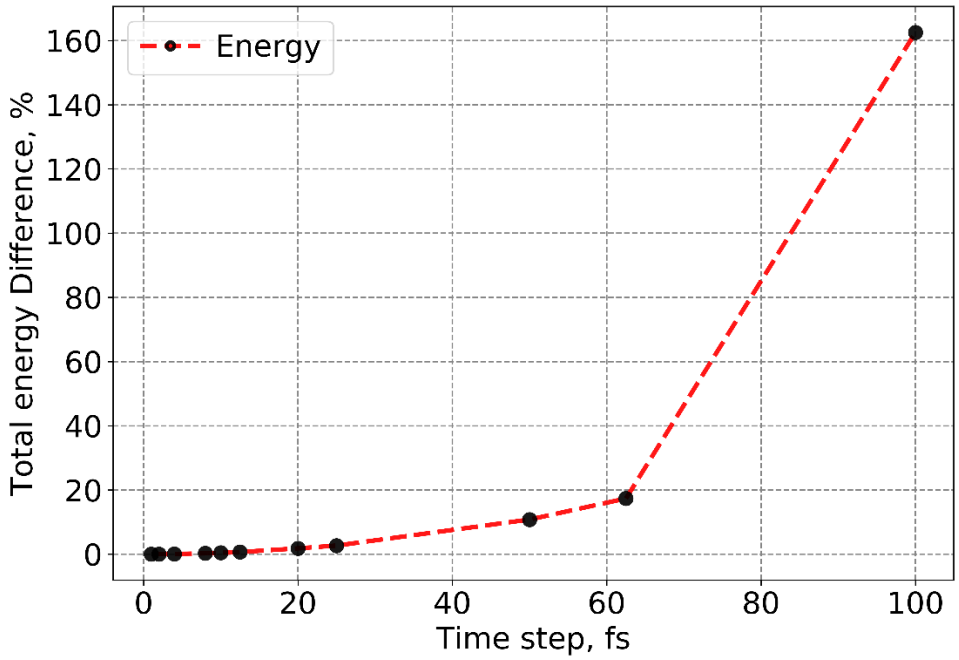

Figure 2 – The total energy difference between the last and the first time steps, expressed in per cent of the initial total energy – time step length, fs (from 1 to 100 fs)

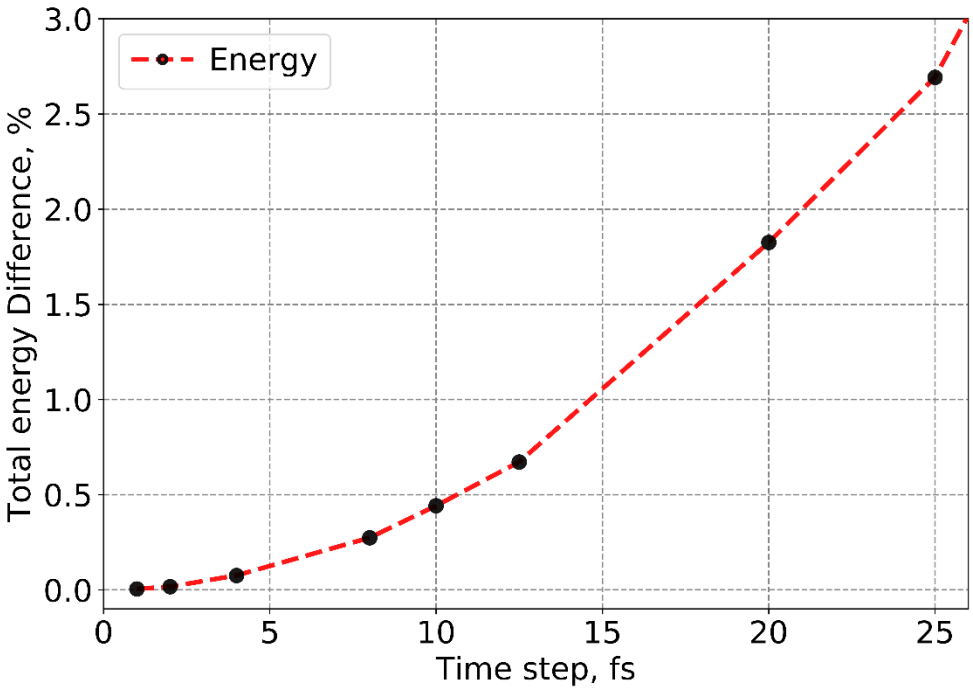

Figure 3 – The total energy difference between the last and the first time steps, expressed in per cent of the initial total energy – time step length, fs (from 1 to 25 fs)

2.2. Simulated properties

To obtain the positions, velocities, forces and energies of two oscillating argon atoms, the system was simulated for 500 picoseconds with 2 fs time step.

- Positions (*Figure 4*):

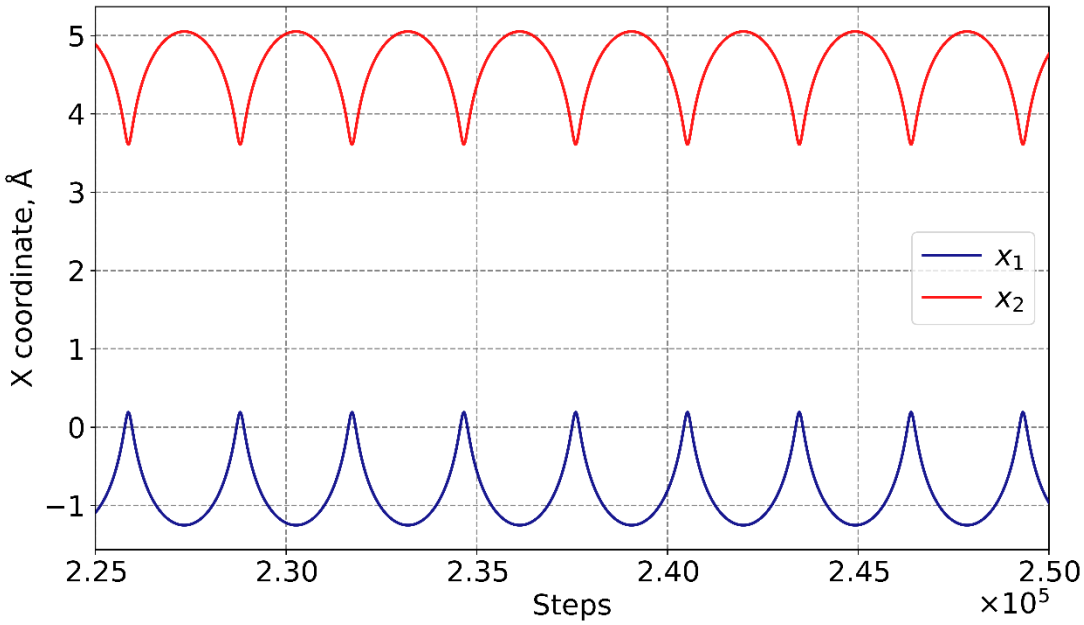

Figure 4 – The positions of two oscillating argon atoms, separated along the x-axis

- Velocities (*Figure 5*):

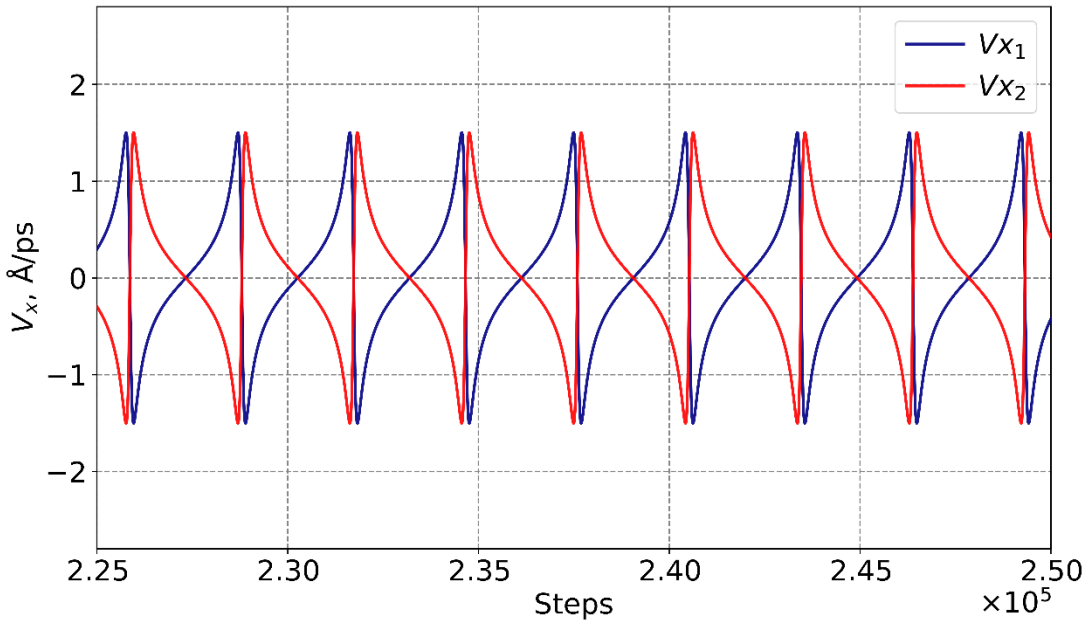

Figure 5 – The velocities of two oscillating argon atoms, separated along the x-axis

- Forces (*Figure 6*):

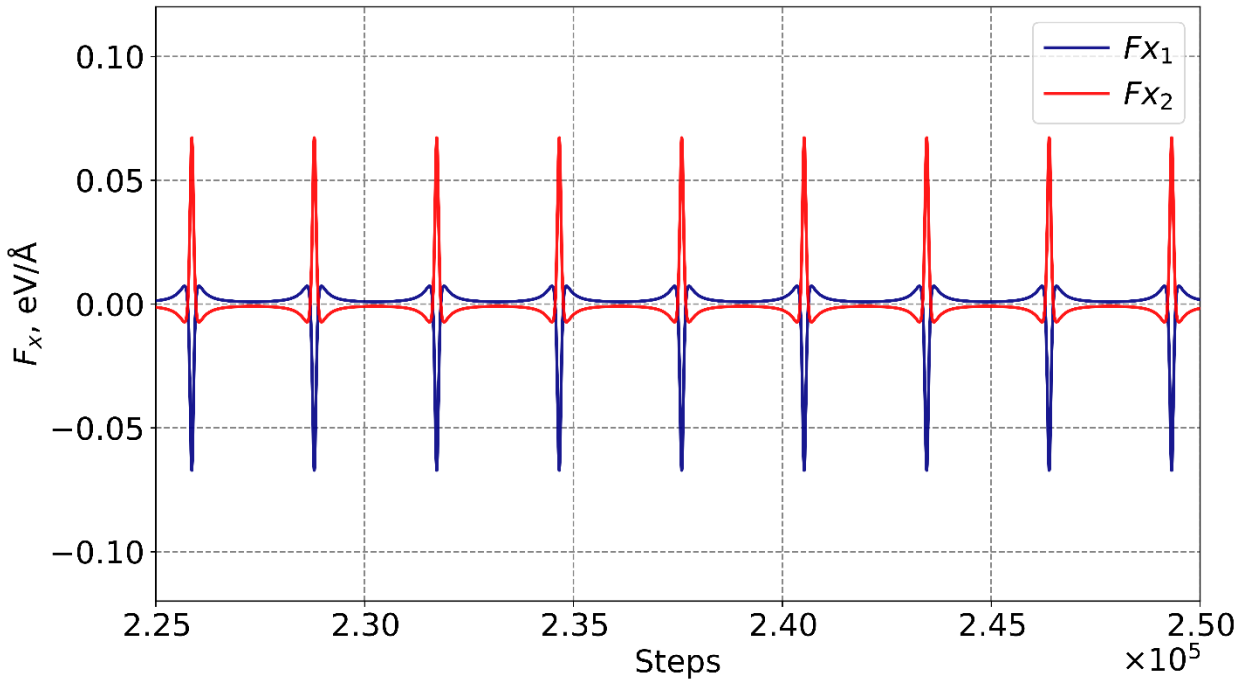

Figure 6 – The forces acting on each of the oscillating argon atoms

- Energies (*Figure 7*):

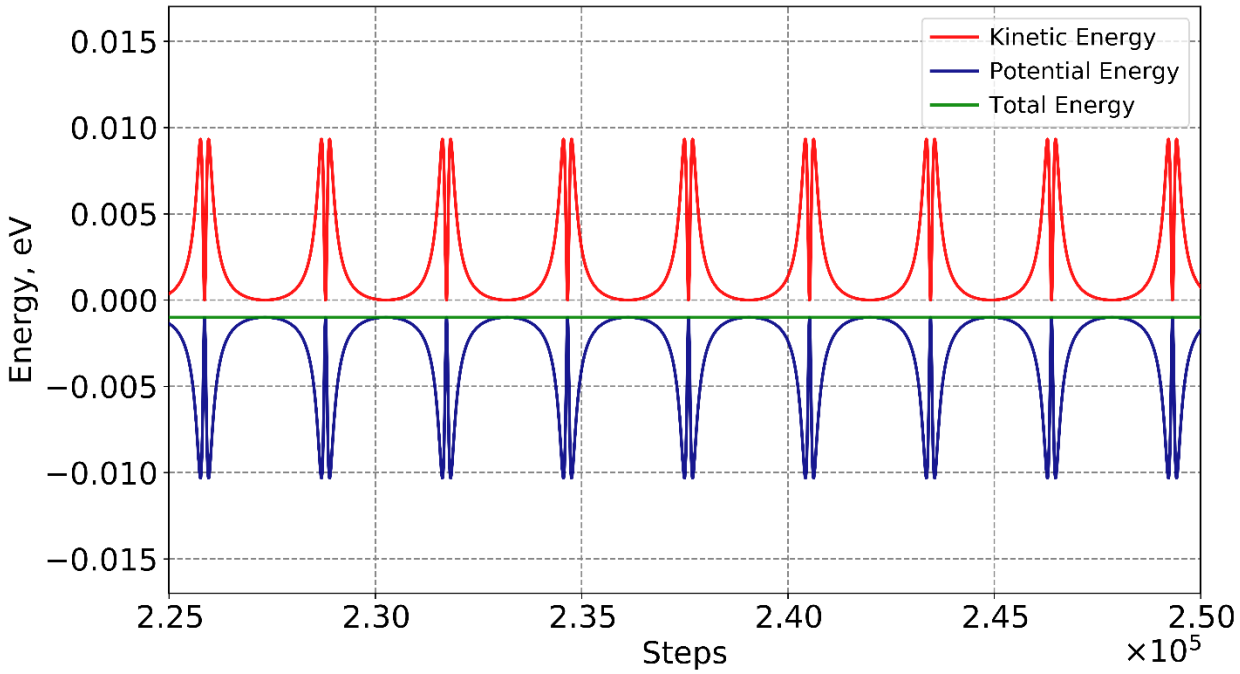

Figure 7 – Kinetic, potential and the total energy of the system of two oscillating argon atoms

- Phase trajectories (*X – Vx)* (*Figure 8*):

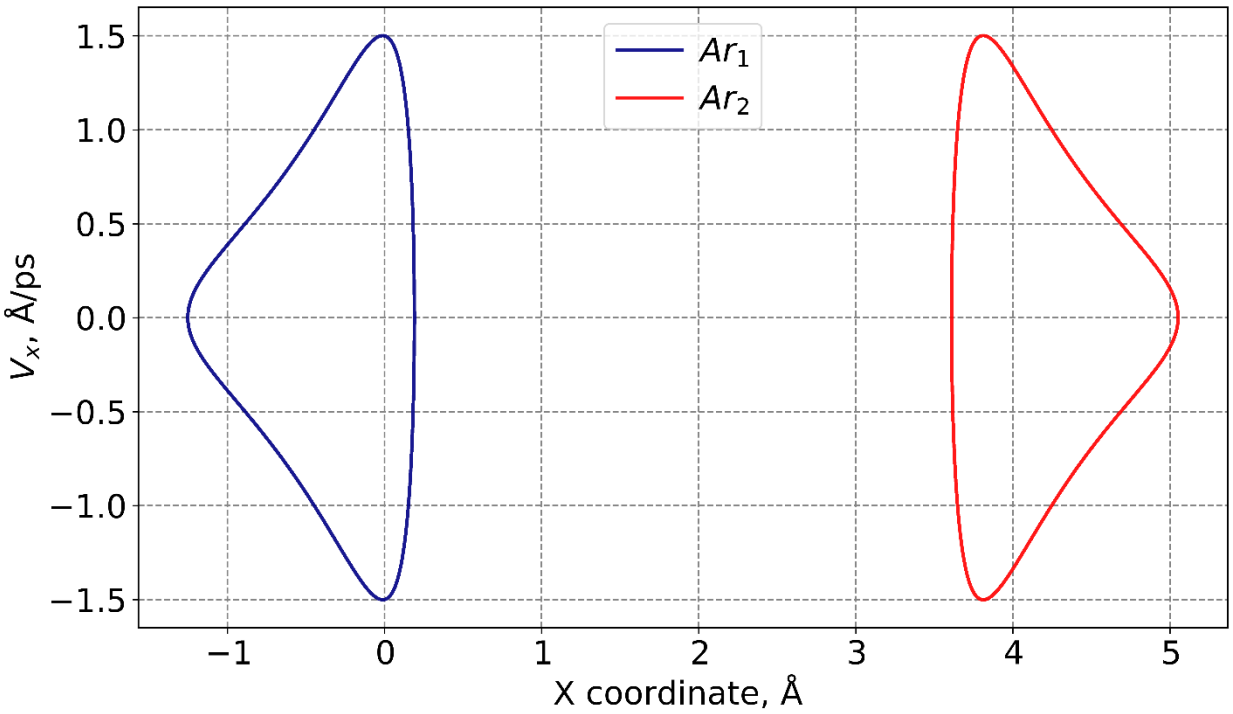

Figure 8 – The phase trajectories of each argon atom

From the figures 4-8, one can see clearly that within the simulated time, 2 fs time step ensures stable simulation with conserved total energy.

3. The total energy of the system of N particles

To check if the total energy is conserved for more than two particles, the system of eight colliding argon atoms (*Figure 9*) was simulated for 200 picoseconds with the 2 fs time step.

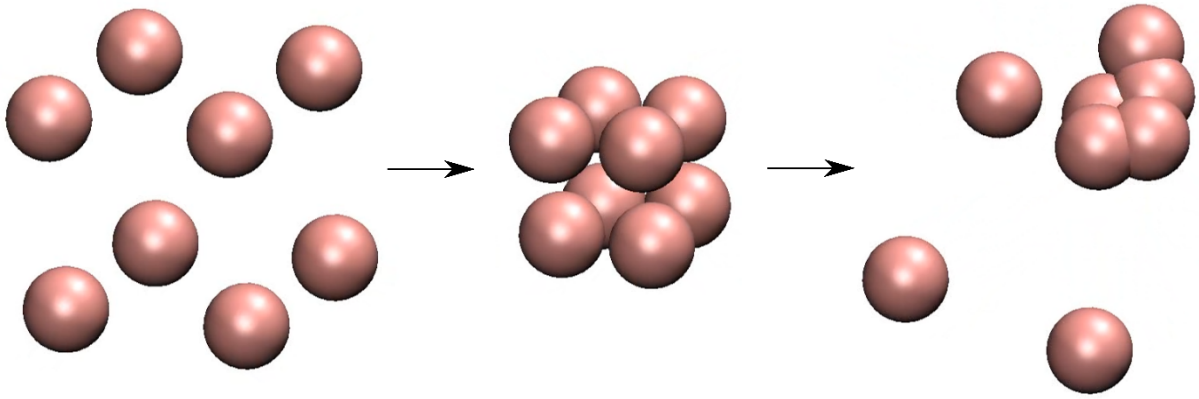

Figure 9 – The evolution of the system of eight colliding argon atoms

Starting velocities were set in such a way, that the atoms would move towards each other, but the velocities itself were a bit different. Kinetic, potential as well as the total energy of the system against the simulated time is shown in *Figure 10*.

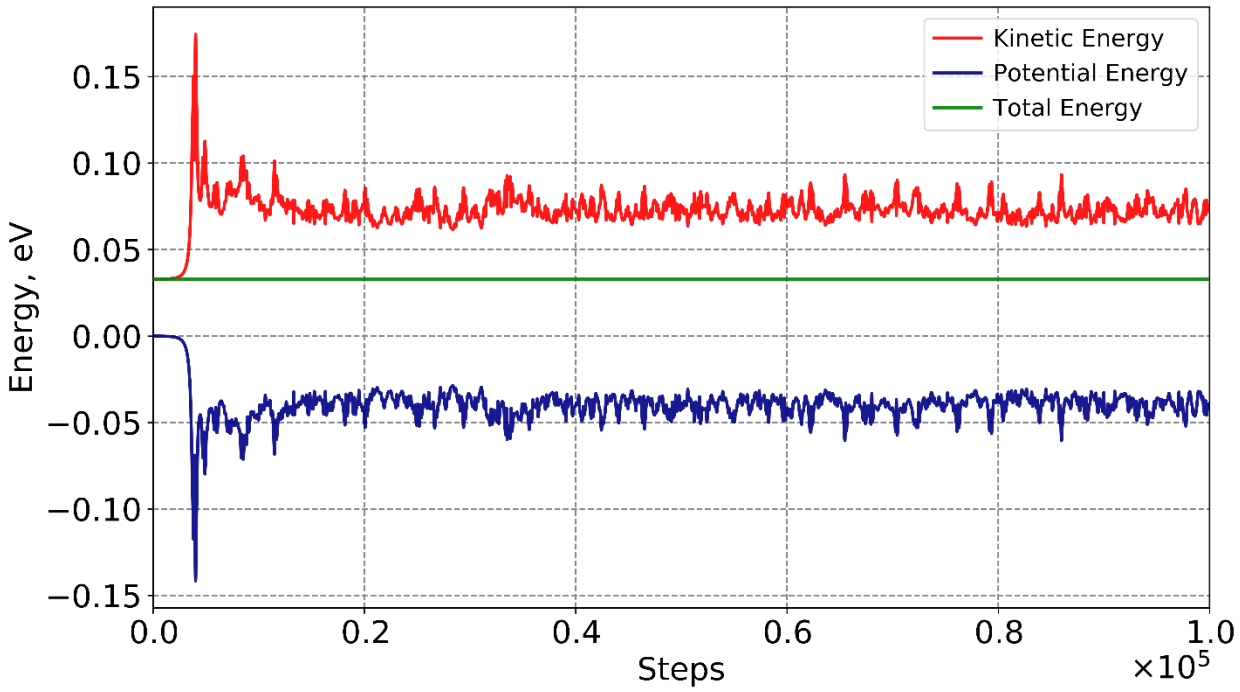

Figure 10 – Kinetic, potential and the total energy of the system of eight colliding argon atoms

After the collision, an atomic cluster of five argon atom is formed due to relatively low initial kinetic energy. The formation of the cluster and subsequent residual motion of the atoms in the cluster create the fluctuations in both potential and kinetic energy, but the total energy stays the same.

Conclusion

The present code can be used to compute the potential energy of the system of N particles, interacting via Lennard-Jones potential and the force, acting on each particle in the system, as well as to integrate the equations of the particles' motion with minimal errors. Therefore, it will be used for the subsequent project development.