NVE Molecular Dynamic Simulation of an Argon system

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Introduction

For this project an NVE molecular dynamics simulation was carried out for a fixed volume cubic box with periodic boundary conditions containing N = 256 spherical particles. The particles acted via a Lennard-Jones potential as follows:

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{12}\right]$$

Where r is the separation distance between two atoms, ε is the depth of the potential well, and σ is the location where the potential due to particle separation is zero. Values suitable for Argon (σ=0.3405 nm, ε/kb = 119.8 K, and m = 6.63382×10^{-26}kg) were chosen and a simple Verlet algorithm with a cutoff distance of r = 2.5 σ was used to carry out the NVE molecular dynamics simulation. In reduced units, a density of 0.636 atoms per length and a total energy E* = 101.79 was used.

Methods

For all calculations reduced units were used such that m = 1, ε =1, and σ =1.

To create the cubic box, atoms where placed in a face-centered cubic lattice pattern based off a molecule density of 0.636. Initial velocities were then chosen for each atom by randomly sampling from a Gaussian distribution and then scaled in such a way that the potential energy of the lattice plus the total kinetic energy was equal to the total energy E = 101.79 used for this project.

After the initial positions and velocities were calculated a simple Verlet algorithm was carried out for 1000 time steps with a time step size of dt = 0.01s. The Verlet algorithm is as follows:

$$x_{n+1} = 2x_n - x_{n-1} + A * dt^2$$

Here $x_n$is the current position, x_{n-1} is the position one time step before the current and A is the acceleration. In order to use this algorithm two positions are required and therefore the first time step after the initialized positions was determined via the Euler method:

$$x_{n+1} = x_n + \Delta t * \frac{dx}{dt}$$

Velocities were calculated for each particle after each Verlet step using the formula:

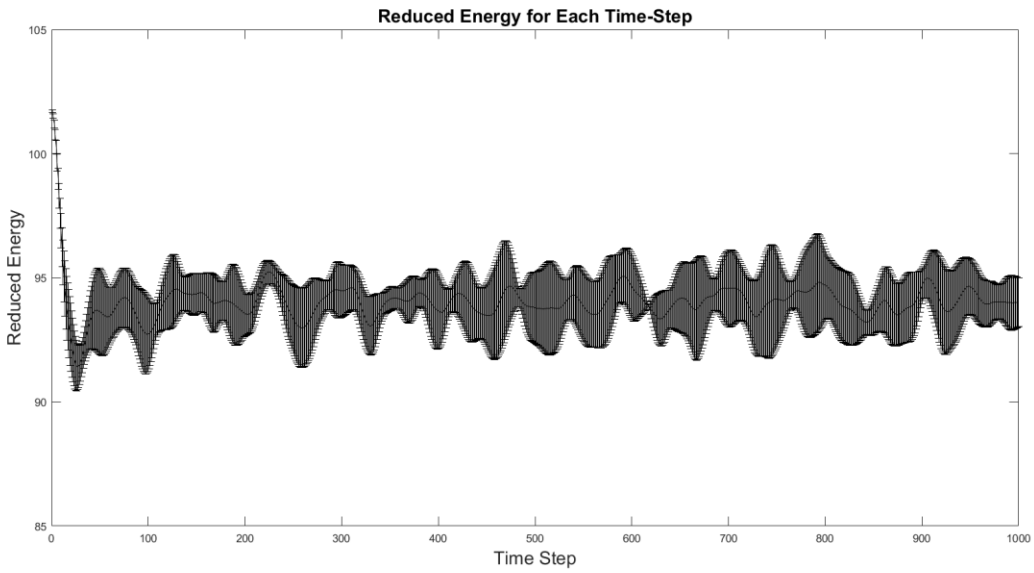
$$v = \frac{x_{n+1} - x_{x-1}}{2 * dt}$$

The accelerations for each particle were determined by calculating the gradient of the Lennard-Jones potential using a cutoff distance of 2.5σ. Careful consideration of the periodic boundary conditions meant that the minimum-image convention was upheld during calculations of the accelerations. The

maximum and minimum values of the initialized velocities lie between -1.0 and 1.0 and so the time step 0.01 was chosen as sufficiently small enough so that the errors in Verlet algorithm (as well as the initial Euler method step) would not be too great. This time step also prevents atoms moving too close together or overlapping which would cause the potential calculations to blow up toward infinity.

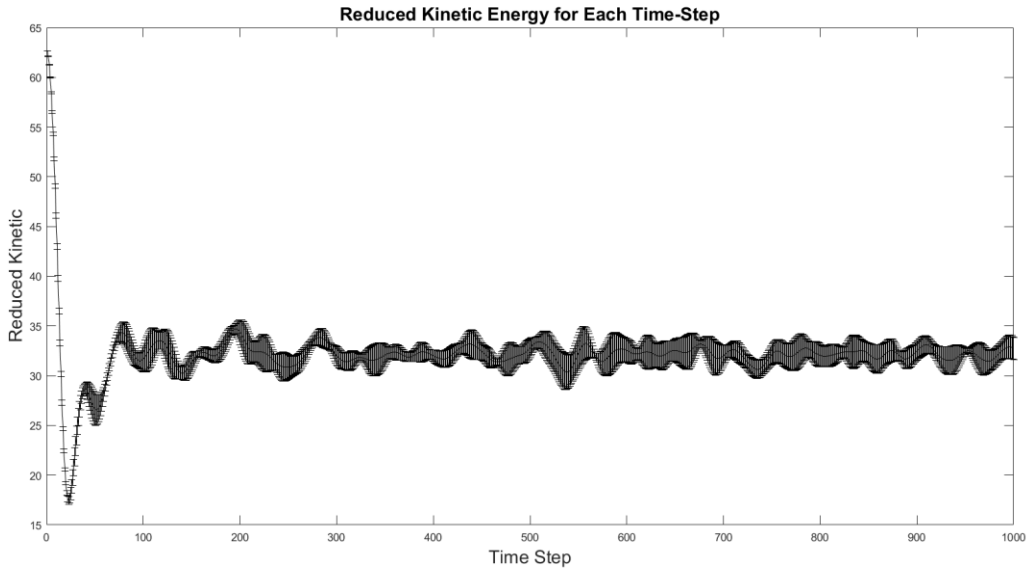
Results and Discussion

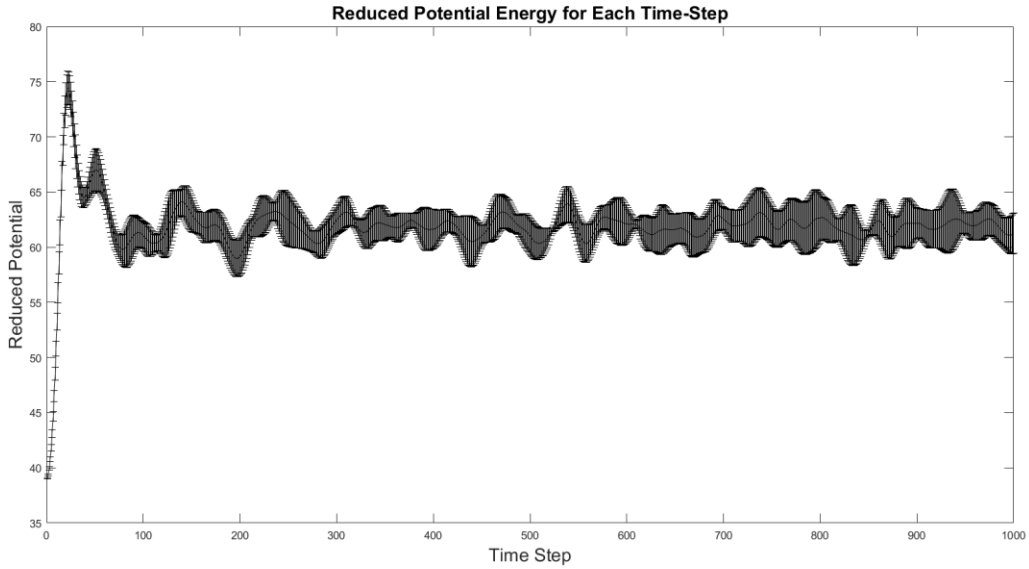
For each plot in the results section a total of five separate trials were run to calculate reduced potential energy, reduced kinetic energy, and total reduced energy. The mean of the five trials was found and error bars representing one standard deviation from this mean were also plotted. The close proximity of the error bars in these plots seem to form one thick solid line but in the center of each a darker line can be seen which represents the mean value.



From the **Reduced Energy for Each Time-Step** plot it can be seen that the total energy initially starts at 101.79 but initially quickly drops to around 90. Around the 50th time-step a kind of equilibrium can be seen where the total energy oscillates around 92 to 97. This initial drop suggests that the separation distances between each atom need to be more carefully considered when calculating potentials. This should be done by utilizing a Verlet List which was unfortunately omitted in this project due to time constraints. However, after this initial drop in total energy it can be seen that overall the energy is being conserved in the algorithm, suggesting that overall the energy is conserved and the true value of the total energy could be calculated provided a more appropriate nearest neighbor calculation in the Lennard Jones potential.

The **Reduced Kinetic Energy for Each Time-Step** plot shows a very steep decrease from an initial value of 62.84 to around 17.00, while the **Reduced Potential Energy for Each Time-Step** plot shows just the opposite trend of steeply increasing from 38.96 to around 75.00. After around 100 time steps both the kinetic and potential energies level off suggesting that initially the system was not in equilibrium and thus needed to relax into equilibrium. Once the system has reached equilibrium we see that kinetic and potential energies deviate slightly, trading off energies as the particles move around. After about 100 time steps the system seems to be in equilibrium with a mean reduced temperature T* = 0.16.


Reduced Kinetic Energy for Each Time-Step
Reduced Kinetic
Time Step
65
60
55
50
45
40
35
30
25
20
15
0
100
200
300
400
500
600
700
800
900
1000


Reduced Potential Energy for Each Time-Step
Reduced Potential
Time Step
80
75
70
65
60
55
50
45
40
35
0
100
200
300
400
500
600
700
800
900
1000