Intermediate Scientific Computing : Final Assessment

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Title : Report on the investigation of behaviours of Argon gas particles in N-body system

Abstract

This investigation is to study the behaviour of the system of particles, specifically the Argon gas. In approaching this matter, the investigation will focus on designing an N-body simulation using Python and applying the Lennard-Jones potential as the baseline model of the Argon gas particles.

Introduction

The procedures of this investigation are separated into three main tasks. The investigation starts off with the setting of functions to incrementally update the states of each gas particle to replicates the motion of an Argon gas particle. The second task is to design an enclosed container for the N-body simulation of the gas particle. The final task is where the investigation focuses on the trend of behaviours of the Argon gas model with the changing of variables. To be precise, the behaviours in discussion constitute the trend of pressure exerted by the Argon gas model in the enclosed container when variables such as the volume of the container are controlled. In studying this behaviours, the investigation will focus on simulation of the motions of chosen number of Argon gas particles in an enclosed container for a specific chosen period of time. Be reminded that in running the simulations the investigation only centred on the overall behaviours of Argon gas particle in an enclosed container, so the choice for the scales of the initial conditions such as the position and velocity of the particles are not in major concerns. Hence, for the sake of simplicity the units for the initial conditions are set in standard units, eg. m and ms^{-1}.

Part 1

Throughout this investigation, the Argon gas particle is individually categorised into a class named Body that contains three main attributes which are the vector of position, velocity and acceleration in three dimensional space. All of these attributes are crucial to study the behaviour of the gas particles in tested simulation by updating these three attributes. In this investigation, we will use the Lennard-Jones potential as the baseline to model the Argon gas particles.

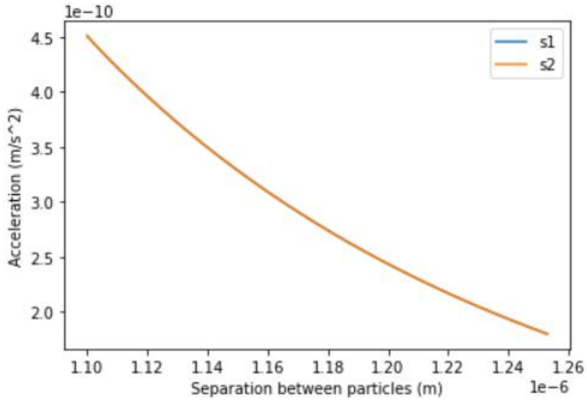
$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

And by deriving this formula, one can obtain the vector for the directional force which will be used to update the position and velocity of the Argon gas particles using a numerical integration method.

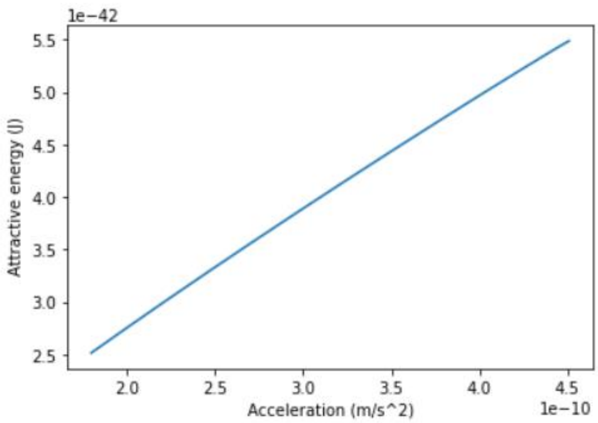
$$F = -\frac{dV}{dr} = \frac{24\epsilon}{r}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$F_{x_{ij}} = \frac{24\epsilon}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right](x_i - x_j)$$

By running a test simulation of the Argon gas particle model by updating its position and velocity for a total of 20 increments, it is observe that the acceleration of the Argon gas particles drop as the separation between particles increases (Be reminded that in this model we assumed there is no external force on each particle or the initial accelerations equal zero).



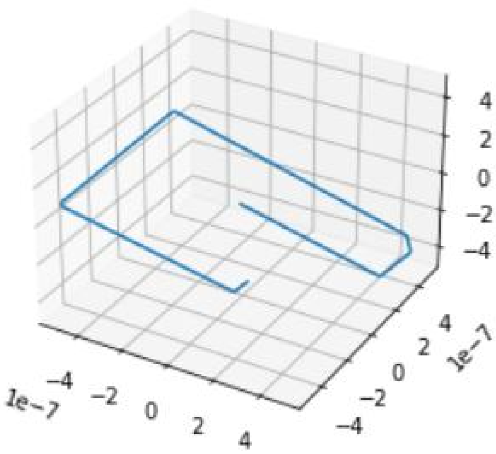
Observe that the magnitude of acceleration of both particles are equal to each other throughout the simulations of 20 increments. This is due to how the acceleration acted on both particles are due to the repulsion and attraction from both particles without any other external factors. Besides, the acceleration of both particles reduces as the separation between the particles increases. This follows the Lennard-Jones potential where the separation between particles is the denominator or reducing factor of the force. In addition to that, the attractive energy that acted upon each of the particles the result is proportional to the magnitude of the accelerations for both particles.



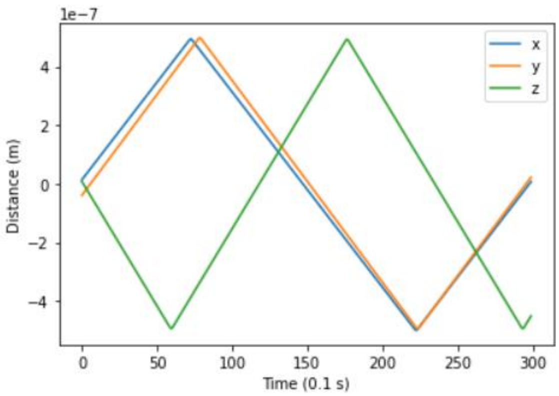
This result shows that the N-body system follows the correct nature for the particles motion at the system obeys the Lennard-Jones potential.

Part 2

In completing the N-body system of Argon particles, one should be able to constrict the movement of all the particles in a specific enclosed container. To design this restriction to the model, a class named N is created to store N number of instances of class Body and also the length of the closed container which will restrict the movements of all of the particles represented by the instances of class Body. To further confirm the working of this N-body system inside an enclosed container, a simulation is run by updating the velocity and position of one Argon particle for 300 increments of time step 0.1s. Below is the visualised three dimensional route taken by the Argon particle throughout the simulation.



To study at which increments does the particle collides with the vertical or side walls, the trajectory of the particle is separated into three axes of x, y and z. Below is the visualised directional trajectory of the particle during the simulation over the 300 increments.



Part 3

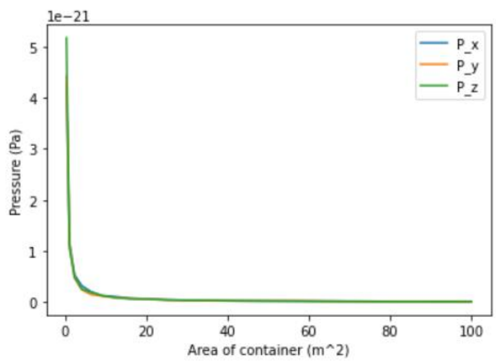
Since this investigation focuses on the pressure of the Argon gas in an enclosed container, it is worth noting upon the parameters or variables that are chosen to be controlled upon. The parameters in discussion are the cross sectional area of the enclosed container and the temperature of the Argon gas particles.

(a)

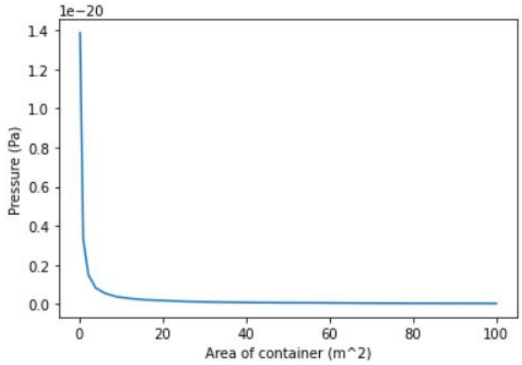
This investigation initially suspected the influences of these two parameters on the pressure of the gas due to the definition of pressure,

$$P_x = \frac{1}{A\Delta t}\sum m_i v_x, i$$

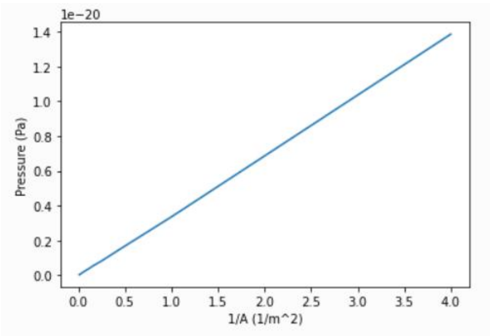
Where A is defined to be the plane where the direction of pressure is acted upon. In supporting this claim, the investigation is done by running a test simulation of a total of 40 bodies of particles with each having the mass of one Argon particle (6.64×10^{-23} g) with randomly generated initial position in the enclosed container and initial velocity ranging around $0.5ms^{-1}$ (in standard units). This setting of simulation is repeated for different lengths of the enclosed container ranging from 1m to 21m and the magnitude of the average pressure is recorded after 100 increments of time steps of size 0.1s. From these simulations, the results are recorded as follows



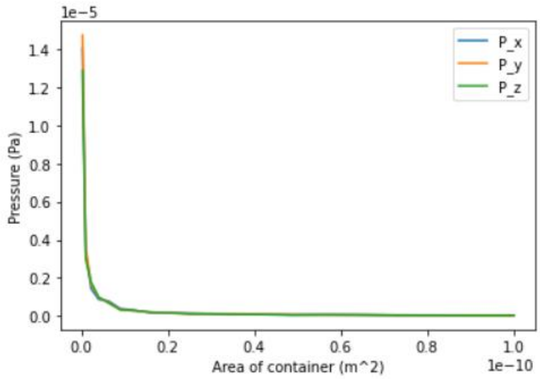
From the obtained results, it is clear that the increase of volume of the enclosed container causes the pressure in every direction to reduce. In which the trend of the three curves is suspected to follow the reciprocal function of pressure in term of the cross sectional area of container.

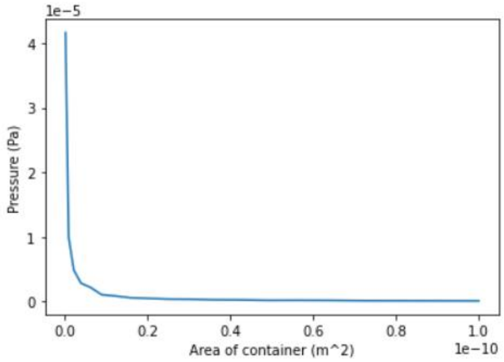


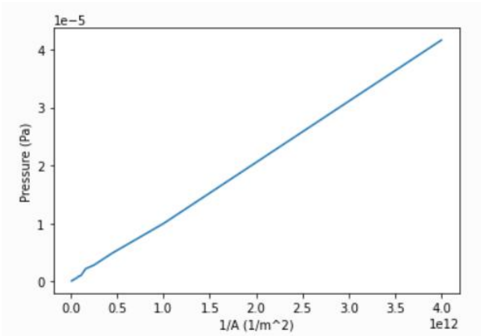
In addition, the curve also behaves as expected for the total pressure in every axis of direction since it represents the approximate reciprocal trend of pressure in terms of the area of the container. The approximate trend of the pressure due to the area of the container is then supported by the plotting curve of pressure against the inverse value of the tested cross sectional area of the container.



From the above diagram, one can see how the trend of pressure approximately grows proportionally with the inverse value of the cross sectional area of the container. Hence, this behaviour follows the initial idea that pressure exerted by gas particles is inversely proportional to the area of an enclosed container. However in close proximity of initial Argon gas particles position ranging around 50nm, the trend for the pressure in the N-body system can vary depending on the input time step. To obtain similar results as in previous simulations, we repeat the procedures of simulating a total of 40 bodies of particles with each having the mass of one Argon particle (6.64×10^{-23} g). But in this case, we randomly generate initial velocity ranging around 5.0×10^{-8} ms^{-1} with initial randomly generated initial position inside the enclosed container. In addition, the choices for the lengths of the enclosed container now ranging from 1.0 x 10 $^{-6}$ m to 21.0 x 10 $^{-6}$ m and the magnitude of the average pressure is recorded after 100 increments of time steps of size 1.0 x 10 $^{-11}$ s. From these simulations, the results are recorded as follows







From the results above, one can observed that the settings for the simulations result in the same pattern of behaviours as the previous simulations had suspected. However, be reminded that the value for the pressure recorded throughout the simulation has significantly increases. Hence, supported the inference that decrease in cross sectional area of the enclosed container causes increase in pressure of the N-body system.

(b)

Next, the investigation will focus on the influence of temperature towards the magnitude of pressure of the Argon gas. In which to study this behaviour and manipulate the temperature of the system, one should refer to the relation between overall speed of particles and temperature from the formula of total kinetic energy.

$$E = \sum_{i}^{N} \frac{1}{2} m_i v_i^2 = \frac{3}{2} N k_B T$$

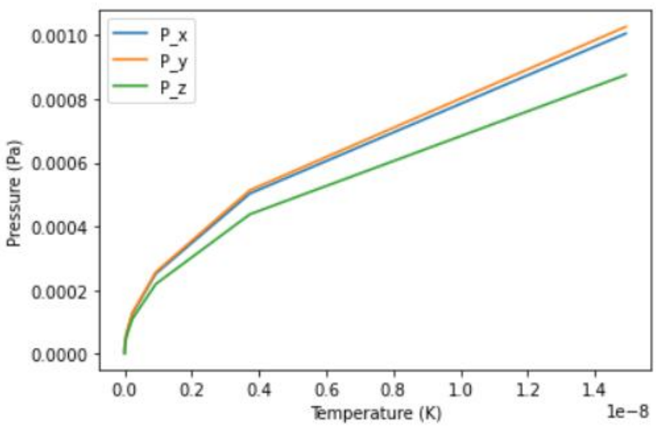
Referring to the above equation, one can define the magnitude of temperature in terms of the expression of total kinetic energy by rearranging the formula.

$$T = \frac{2}{3Nk_B}\sum_{i}^{N}\frac{1}{2}m_i v_i^2$$

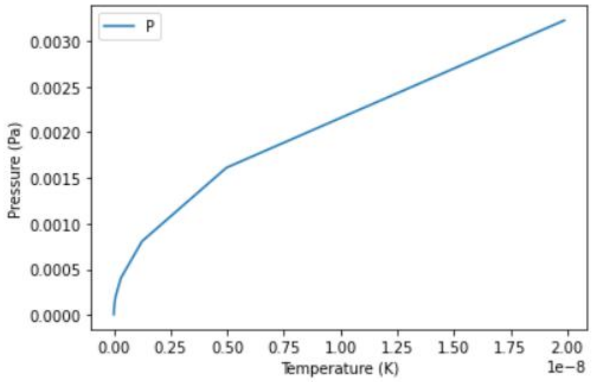
Applying this formula, one can possibly control the temperature of the system by altering the initial speed of the Argon gas particles in the N-body simulation. To manipulate the speed of the gas particles in the N-body system, one can make changes to the initial velocity of the gas particles since speed can be derived from the magnitude of velocity components of an object.

$$v = \sqrt{x^2 + y^2 + z^2}$$

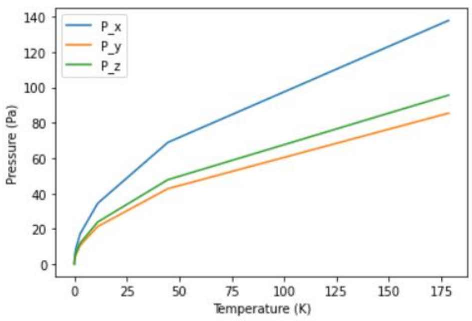
By the same system conditions as before, the investigation is run through by a test simulation of a total of 40 bodies of particles with each having the mass of one Argon particle (6.64 x 10^{-23} g). However, in contrast to the change in the length of the enclosed container as in the previous investigation, we now fixed the length of the container to 1.0 x 10^{-7} m and randomly generate the initial positions of the particles within this container. To modify the temperature of the N-body system, we change the initial velocity for each Argon gas particles by doubling the subsequent initial velocity in each simulations. Hence, for every subsequent simulation the magnitude of initial velocity of all Argon gas particles will be twice the magnitude of initial velocity of the Argon gas particles in the previous simulation starting with initial velocity ranging around 5.0 x 10^{-8} ms^{-1} for the first simulation. From 10 simulations with increasing magnitude of initial velocities for the Argon gas particles, the results for the magnitude of directional pressure against temperature are obtained as follows

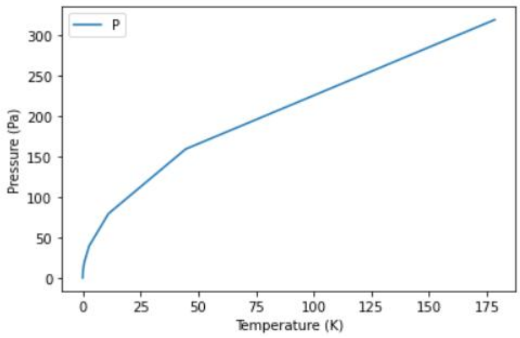


From the obtained results, it is clear that increasing in temperature causes the pressure in every direction to increase. In which the trend of the three pressure curves can be said to be proportionally grows with the increasing temperature.



In addition, the curve also behaves as expected for the total pressure in every axis of direction since it represents the approximate proportional trend between pressure and temperature. However, be noted that the slope of the curve tends to be less and less steeper as the temperature increases. Same as before, we can rescale some of the specifications and initial conditions for the simulations to obtain much better results. In which, by increasing the initial velocity of all the gas particles for the setting of the first simulation, we can investigate the behaviours of the N-body system at higher temperature. For instance, when the initial velocity of all the particles are set to be around 0.005ms^{-1} the results obtained are as follow,





One can observed that the settings for the simulations result in the same pattern of behaviours as the previous simulations had suspected. However, be reminded that the value for the pressure recorded throughout the simulation has significantly increases. Hence, supporting the inference that increase in temperature of the enclosed container causes increase in pressure of the N-body system.

Conclusion

Based on the observation from the simulation, one can find that the trends for pressure of gas roughly follows the Ideal Gas Law which is of the form,

$$P = \frac{nRT}{V}$$

Where P is pressure exerted by the gas particles, T is temperature of the system and V is the volume of the enclosed container. From this expression, one can observe how it is expected for the pressure to increase when the temperature of the system increases whereas the pressure is expected to reduce as the volume of the enclosed container increases. Although by the simulations in this investigation, the curves do not fully represent the trend as in the Ideal Gas Law there are still some baseline to how the overall behaviours of the gas particles in the N-body system should be when we controlled some variables. This may be due to the restriction of the model for ideal gas where there should be no repulsion or attraction between gas particles in the system. However, this N-body system wanted to include the factor of Lennard-Jones potential that influenced the motion of the gas particles in the system. Hence, resulting in some changes in the trend for the pressure of gas especially when the separations between particles are smaller. This is due to the limited range of attraction and repulsion of particles which reduces as the separation between particles increases. Also when the temperature of the system increases, the slope for the increasing pressure is greater at the lower temperature compared to higher temperature. This may be due to how the manipulation of temperature is done in this investigation. In the investigation for the relationship between pressure of gas and temperature is done by increasing the initial velocity for simplicity, we cannot obtain the expected trend as in the Ideal Gas Law. This is because the computation for pressure in the simulation uses the magnitude for directional velocity instead of the square value for the magnitude of velocity as in the expression of temperature in terms of the total kinetic energy. Thus, although this simulation suffers some complications to obtain the exact mathematical trends as in Ideal Gas Law, the approximate trends for the system shows that the gas particles still behave as expected if one can specifically choose the suitable specifications (e.g time step and initial velocity) to initiate the N-body simulations.