Investigation of the Interactions of Argon Particles in a Closed Container

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Abstract

The kinematics of Argon particles in a closed container was investigated using the Lennard-Jones Potential between the particles.The kinematics were successfully mapped, and the results indicate that the particles stay within the boundaries of the container as time progresses.

1 Introduction

Unlike in liquids and solids, gas particles are able to move freely throughout the entire volume the container the gas occupies. In a closed container, particles collide with the walls of the container and other particles in the container.We are interested in the motion of these particles in the container known as the kinematics of the particles. Determining the kinematics of particles in a closed container is important in predicting how the particles will behave in the future. It is important to note that when we say a closed container we are referring to a container in which the particles can't escape and the volume is fixed (the walls of the container do not expand or contract). Considering these assumptions, we can further assume that all interactions between the particles and the walls of the container as well as with the other particles are perfectly elastic. Perfectly elastic interactions occur between two particles in which the total kinetic energy of the particles is unchanged. Therefore, when two particles collide, the kinetic energy of the two particles are transferred in a way such that the sum of kinetic energy of the first particle and second particle after the collision is the same as the sum of the kinetic energy of particles one and two before the collision. If the interactions between the two particles are not elastic (inelastic), then the collision of two particles would result in a loss in the overall kinetic energy of the two particles (in the form of heat or some other form of energy).

To describe the interactions of the particles in the system, we use the Lennard-Jones potential (L-J potential). The L-J potential describes two forms of interactions that neutral particles experience when in a closed system. When particles come into close proximity with one another, the electron orbitals of both particles overlap which causes a repulsive force between the particles. The repulsive force is the stronger of the two interactions and is represented by the term raised to the twelfth power in the L-J potential formula. In addition to repulsive forces between particles, there exists long range attractive forces between other particles represented by the term in the equation raised to the sixth power. These long range attractive forces are known as van der Waals forces and result from the temporary dipole moments that occur in molecules or atoms. The repulsive and attractive forces oppose each other; therefore, the attractive forces are substracted from the repulsive forces. The closer two particles are to each other in the system, the stronger the repulsive and attractive forces are between the particles; therefore, the distance between two particles in a system is important to determine the potential between the two particles.

In this paper, we consider a system of four argon particles in a closed container. Since we are considering a theoretical system, we first establish the initial conditions of the argon particles: therefore, in Section 1 we establish the initial conditions of our system to be used in the future derivations. In Section 2, we investigate the Lennard-Jones potential formula, and use the formula to derive the force between the particles. In Section 3, we use the force derived in Section 2 to determine the

accelerations for the particles in the x, y, and z directions. After we determine the accelerations, we use the new accelerations to determine the new velocities in the x, y, and z directions for the particles. Lastly, in Section 4 we determine the new positions of the particles and graph the new locations as the particle moves throughout the closed container.

2 Section 1:

To determine the initial positions of the the particles, we use a random number generator, which provides an initial x, y, and z position for each particle. In the theoretical system we have established, the random number generator provided the initial postions of the particles in the matrix labeled p shown below. In addition to using a random number generator, we used a random sign generator that rnadomly assigned the x, y, and z positions of each particle either a positive or negative sign.

$$p = \left| \begin{array}{cccccc} & Particle1 & Particle2 & Particle3 & Particle4 \\ x & 1.647 \cdot 10^{-9} & -2.623 \cdot 10^{-10} & -2.232 \cdot 10^{-9} & 8.478 \cdot 10^{-10} \\ y & 2.099 \cdot 10^{-9} & -1.344 \cdot 10^{-9} & 1.494 \cdot 10^{-9} & -2.25 \cdot 10^{-9} \\ z & -1.874 \cdot 10^{-10} & 3.734 \cdot 10^{-9} & 8.258 \cdot 10^{-10} & 6.744 \cdot 10^{-9} \end{array} \right| .$$

In a physical system in which gas particles are in a closed container, the particles are constantly moving throughout the volume; therefore, the particles must have an initial velocity. To determine the initial velocities of the particles, we will examine the Maxwell-Boltzmann distribution of velocities for Argon particles:

$$P(v) = 4 \cdot \pi \cdot (m/(2 \cdot \pi \cdot k \cdot T))^{3/2} \cdot v^2 \cdot e^{(-m \cdot v^2)/(2 \cdot k \cdot T)}$$

where k is Boltzman's constant, T is the temperature in Kelvin, and m is the mass of the particle. For our system, $T = 300K$ and $m = 6.634 \cdot 10^{-26}$.

In our system, we wanted to make the system as random as possible, so we used a random number generator to determine the velocities for each of our particles. In order to do so, the generator assigned half of our particles a velocity above the maximum possible velocity and and the other half a velocity below the maximum possible velocity. To determine the maximum possible velocity of the particles in the system, we took the first derivative of the probability function (Maxwell-Boltzmann Distribution) and set the derivative equal to zero as shown:

$$8 \cdot \pi \cdot v \cdot exp(-m \cdot v^2)/(2 \cdot T \cdot k) \cdot m/(2 \cdot \pi \cdot T \cdot k)^{3/2} -$$

$$-(4 \cdot \pi \cdot m \cdot v^3 \cdot exp[(-m \cdot v^2)/(2 \cdot T \cdot k)] \cdot m/(2 \cdot \pi \cdot T \cdot k)^{3/2})/(T \cdot k) = 0$$

The solution to the above equation is known to be $v = \sqrt{(2 \cdot k \cdot T)/m} = 353.415 m/s$. Again, a random sign generator was used to assign the velocities negative and positive directions. The velocities for each particle are described as velocities in the x, y, and z direction for each particle. The resulting velocities of the particles are shown in the matrix v shown below. The velocities are displayed in meters/second.

$$v = \left| \begin{array}{cccccc} & Particle1 & Particle2 & Particle3 & Particle4 \\ x & 298.179 & -249.123 & 228.16 & -277.216 \\ y & -521.601 & 270.458 & -264.103 & 515.245 \\ z & -20.388 & 701.087 & -2.454 & -678.245 \end{array} \right| .$$

3 Section 2:

Once we have established the initial positions and velocities of the particles in our system, we consider the Lennard-Jones Potential formula to derive the interparticle forces. We know that the total force in a particular direction (x, y, or z) experienced by the particle is the sum of all the forces experienced by that particle in each direction. For example, Particle 1 (P1) experiences force in the x-direction as a result of the potential between P1 and Particles 2-4. The same goes for the y and z directions. Therefore, we must use the Lennard-Jones potential (L-J) formula to determine the potential between all of the particles in the system. The L-J potential (shown below) contains two different terms that represent two different forces present between the particles. In the formula, R represents the distance between the particles in consideration; therefore, the closer the proximity of the particles, the stronger the forces. The first term, $4\epsilon(\frac{\sigma}{R})^{12}$, represents the repulsive force that results from the electron clouds of the particles coming into close proximity. The second term, $4\epsilon(\frac{\sigma}{R})^{6}$, represents the attractive forces present between the particles that result from the temporary dipole moments of the particles. As indicated by the opposite signs of the terms, the repulsive and attractive forces oppose each other with the repulsive forces between the stronger of the two forces. To determine the force between the particles, we use the formula $\vec{F} = -\vec{\bigtriangledown} V$ Anoter well known formula for force is $\vec{F} = m \cdot \vec{a}$. We can then derive the initial accelerations of our particles by rearranging the formulas to give:

$$a_x = -\frac{1}{m}\frac{\partial V}{\partial x} \quad a_y = -\frac{1}{m}\frac{\partial V}{\partial y} \quad a_z = -\frac{1}{m}\frac{\partial V}{\partial z}$$

Using the initial positions and velocities determined earlier, we obtain our initial accelerations for the particles shown in a.

$$a = \left| \begin{array}{cccccc} & Particle1 & Particle2 & Particle3 & Particle4 \\ x & -2.674x10^{7} & 5.182x10^{10} & 1.141x10^{8} & -5.19x10^{10} \\ y & -3.068x10^{7} & -4.221x10^{10} & -1.391x10^{8} & 4.238x10^{10} \\ z & 2.798x10^{7} & 1.408x10^{10} & -3.114x10^{7} & -1.408x10^{10} \end{array} \right| .$$

4 The Runge-Kutta

The purpose of this study is to determine the positions of the four particles in the system as time progresses. Since we do not have an explicit position function, we must use a differential equation method (shown below) for predicting the position of the particles. In addition, we do not have a velocity function defined for our system. By considering the acceleration derived from the L-J potential formula and the formula $\frac{dv}{dt} = a$ as well as $\frac{ds}{dt} = v$ (where s is position of the particle), we can see that we have to establish a Runge-Kutta to estimate the new velocity based on the aceleration given by the L-J potential which will be used to determine the position. Runge Kutta methods are used to provide approximate numerical solutions to initial value problems. In this problem, a fourth order Runge-Kutta (general formula shown below) is implemented to first predict the new velocities of the particles, then predict the new positions of the particles from the newly calculated velocities. Once we have the new positions, we use these positions to determine the new potential between the particles, which in turn gives a new force experienced by the particles. The new force is used to determine the new accelerations, new velocities, and the new positions of the particles. The Runge-Kutta continues this process for the allotted time interval given. The duration of this problem is 400 pico seconds with 100 implementations (steps in time) of the Runge-Kutta. We then graph the results of the Runge-Kutta to show the new velocities and positions (Figure 1).

General Formula of Fourth Order Runge-Kutta:
h=the step size for the Runge-Kutta ($4 \cdot 10^{-15}$s)

$$\dot{s}_{n+1} = \dot{s}_n + \frac{h}{6} \cdot (k_1 + 2k_2 + 2k_3 + k_4)$$

$$s = g(t, s), s(t_0) = s_0$$

$k_1 = g(t_n, s_n)$
$k_2 = g(t + \frac{h}{2}, s + \frac{h}{2}k_1)$
$k_3 = g(t + \frac{h}{2}, s + \frac{h}{2}k_2)$
$k_4 = g(t + h, s + hk_3)$

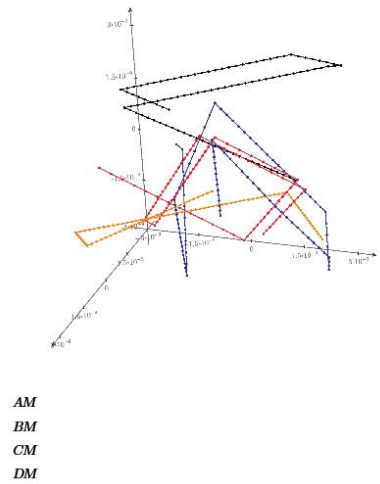

Figure 1: Mapping of the Positions of the Particles in the Container over 400 pico seconds

5 Conclusion

In conclusion, we have been able to successfully graphed the kinematics of four particles of Argon in a closed container. Additionally, our calculations indicate that the particles will remain in the container as time progresses. For future research, we would like to expand our system to a larger container with more particles. We would also like to consider a system in which the walls of the container can expand and contract.

6 Acknowledgements

I would like to thank Dr. McGill for his guidance and assistance with solving this problem. I would like to greatly thank Dr. Yue for her extensive help with interpreting the results and her guidance with writing this report.