Ideal Gas Simulation Lab (Make your own lab)

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**Introduction:** For an ideal gas, we know that $pV = nRT$. An ideal gas has four assumptions:

1. There is a very large number of molecules of the gas in a given volume V.
2. Each molecule is a point particle that is significantly smaller than the distances in V.
3. The molecules are in constant motion and collide with the wall completely elasticity.
4. The walls are rigid and cannot be moved.

In real life, we need instruments to measure pressure. Some instruments use different properties of pressure to calculate the pressure compared to a reference pressure (usually atmospheric pressure). However, through a simulation, we can measure pressure using its definition, $p = \frac{F}{A}$. Using an ideal gas simulation, this experiment aims to a) verify the ideal gas equation, b) verify that the ideal gas equation is independent of the molecule's mass.

**Hypothesis:** For an ideal gas, $pV = nRT$ will be true. If it is true, regardless of the molecules' mass, if the above quantities are constant, the pressure should be the same.

**Materials + Methods:**

For this experiment, I added a 5th assumption to our ideal gas model:

5. Particles cannot collide with each other.

This assumption was added to reduce the amount of calculations that was needed for the simulation. It would be possible to make particles collide with each other but that would sacrifice framerate quite a bit.

Using UnrealEngine 4, I created a molecule object and a box object. The box object cannot be moved in anyway. The molecules only collide with the walls of the box and the collision is set to always be completely elastic.

The program works in the following steps:

1. The user inputs the molecules' mass in kg, the absolute temperature of the system, the length of the box in meters, and the number of molecules.
2. Using the equation $v_{rms} = \sqrt{\frac{3kT}{m}}$, the $v_{rms}$ of the molecules are calculated.
3. The user input number of molecule objects are created with their speed set to $v_{rms}$
4. Upon creation, each molecule object gets a random unit vector in three-dimensional space.
5. This unit vector is multiplied with the initial speed to set the initial velocity of the molecule.
6. Whenever a molecule collides with the walls of the box, the force applied by the molecule is calculated. The force applied by the molecule is calculated using the equation $F = \frac{dp}{dt}$. After the collision, the wall object retrieves the velocity of the molecule right after the collision. The only component of the momentum that changes is the component that is perpendicular to the wall. As such, the velocity is divided into x,y,z-components and the perpendicular component is used

for the equation $dp = -2 * m * v_{perpendicular}$. Using $F = \frac{dp}{dt}$, we find the force applied on the molecule by the wall. The force applied on the wall by the molecule is same in magnitude and goes in the opposite direction.

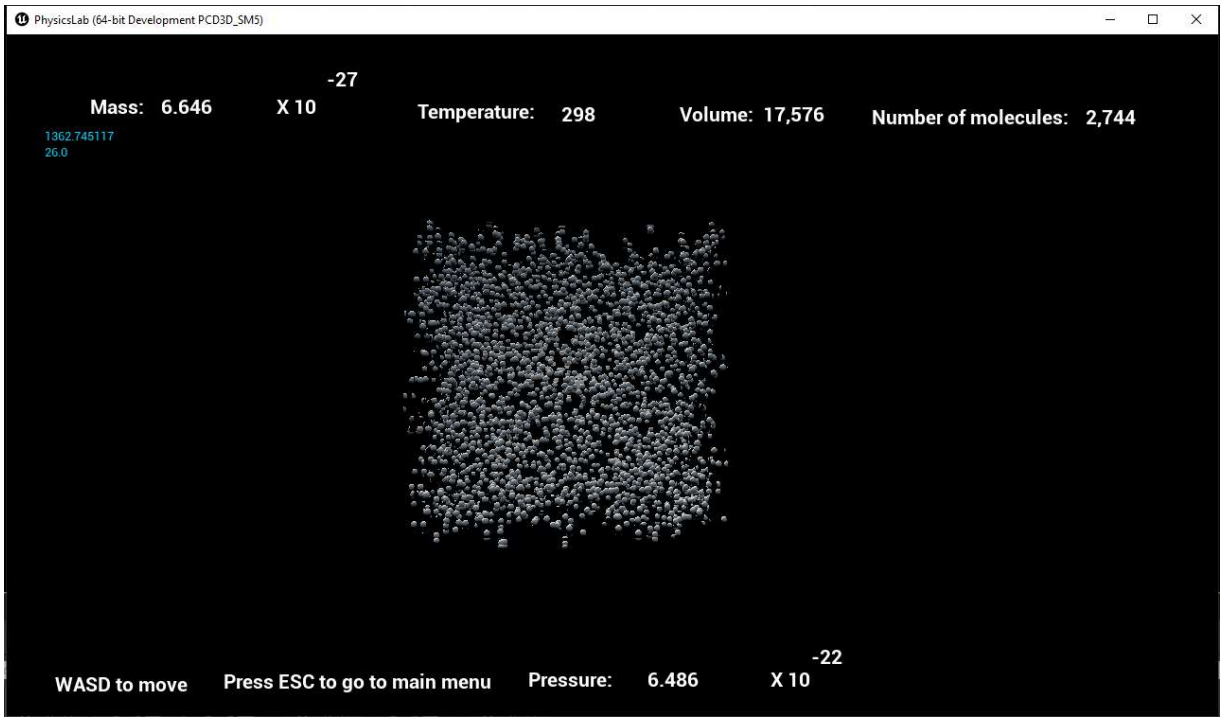
7. The calculated force is added on to a variable, (Total Force).
8. After a certain amount of time, (Total Force) is divided by the surface area of the inside of the box and then divided by the time elapsed, giving us the pressure at that moment.
9. Each time the pressure is calculated, the value is added to an array of pressures and the average value of this array is displayed on the screen.

**Results:**

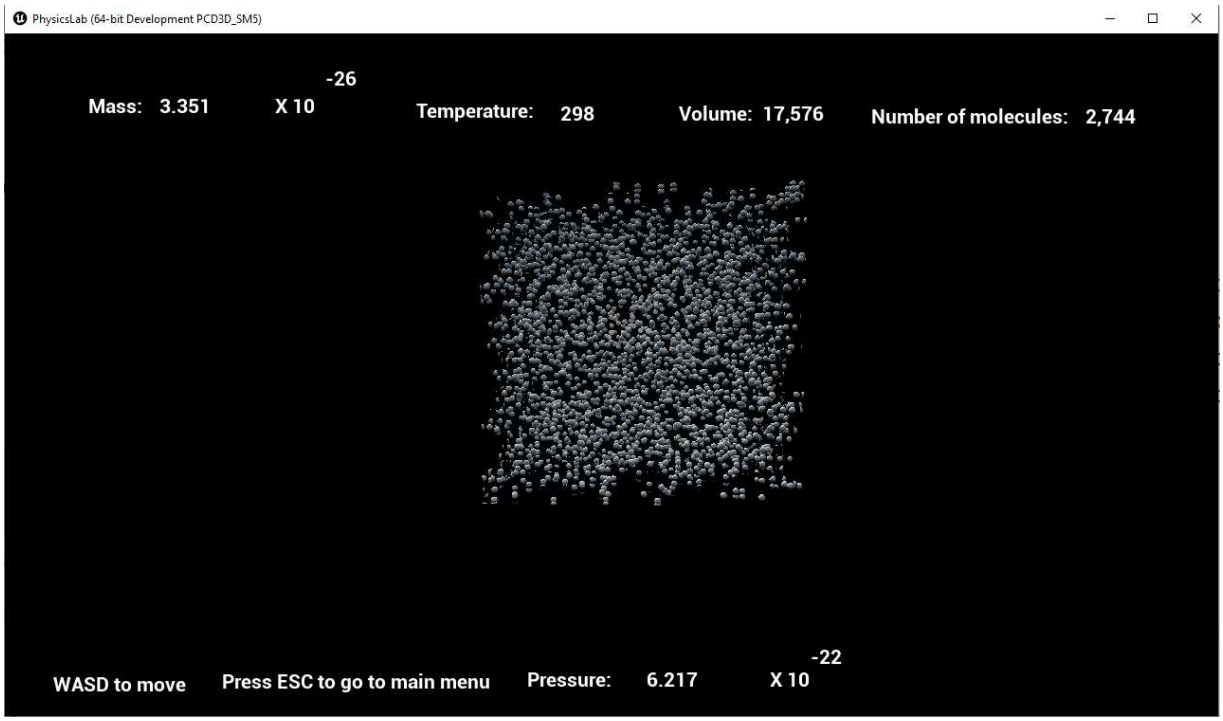
Mass of Helium = $6.646 \times 10^{-27}$ kg

Mass of Neon = $3.351 \times 10^{-26}$ kg

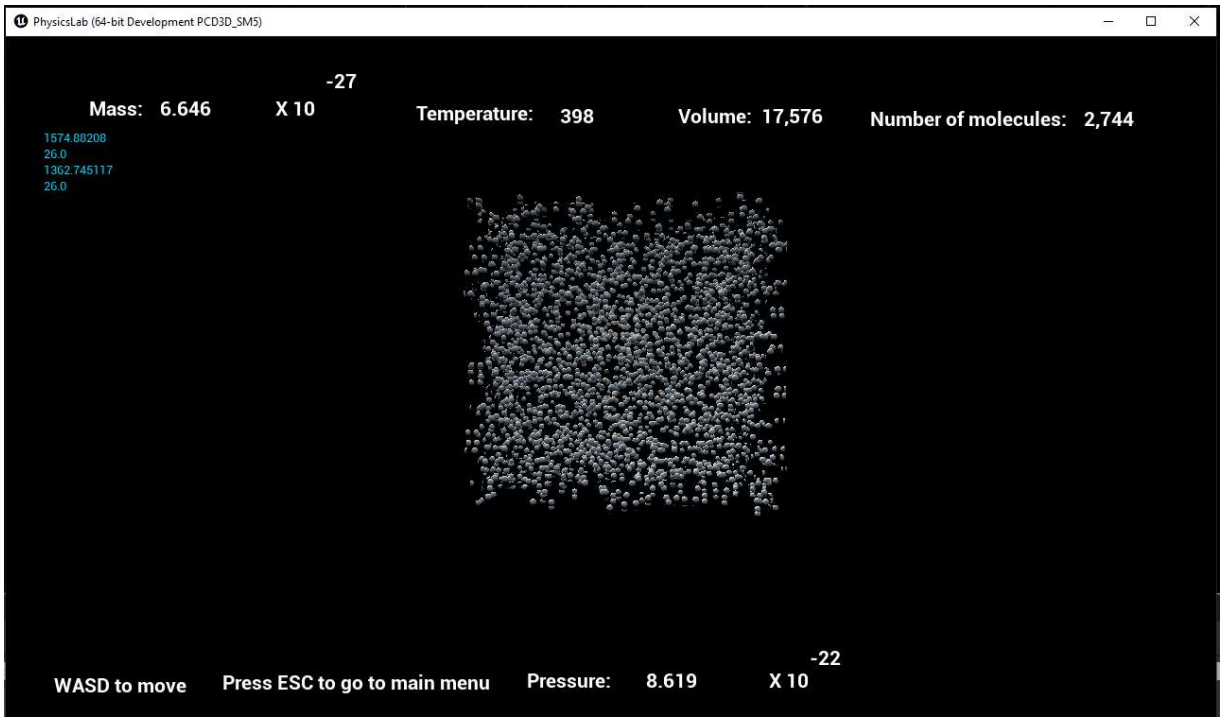
Helium with default parameters (T = 298K, V = 17576 $m^3$, num_molecules = 2744)



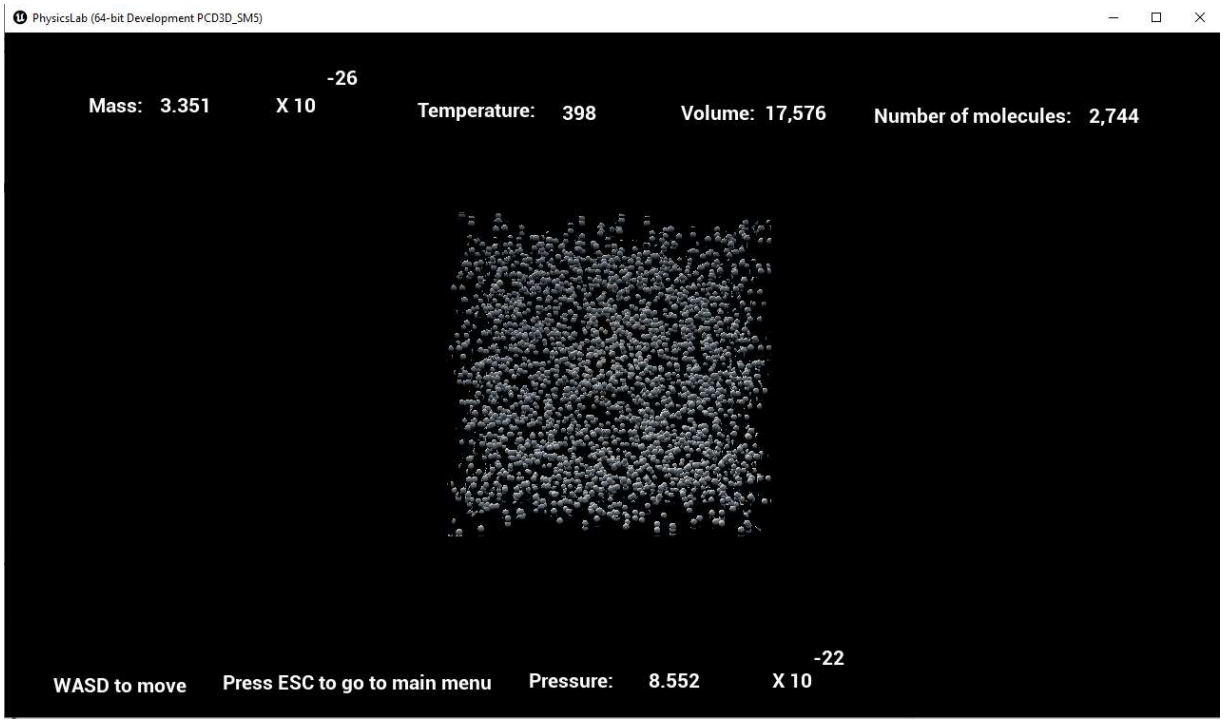

Neon with default parameters (T = 298K, V = 17576$m^3$, num_molecules = 2744)



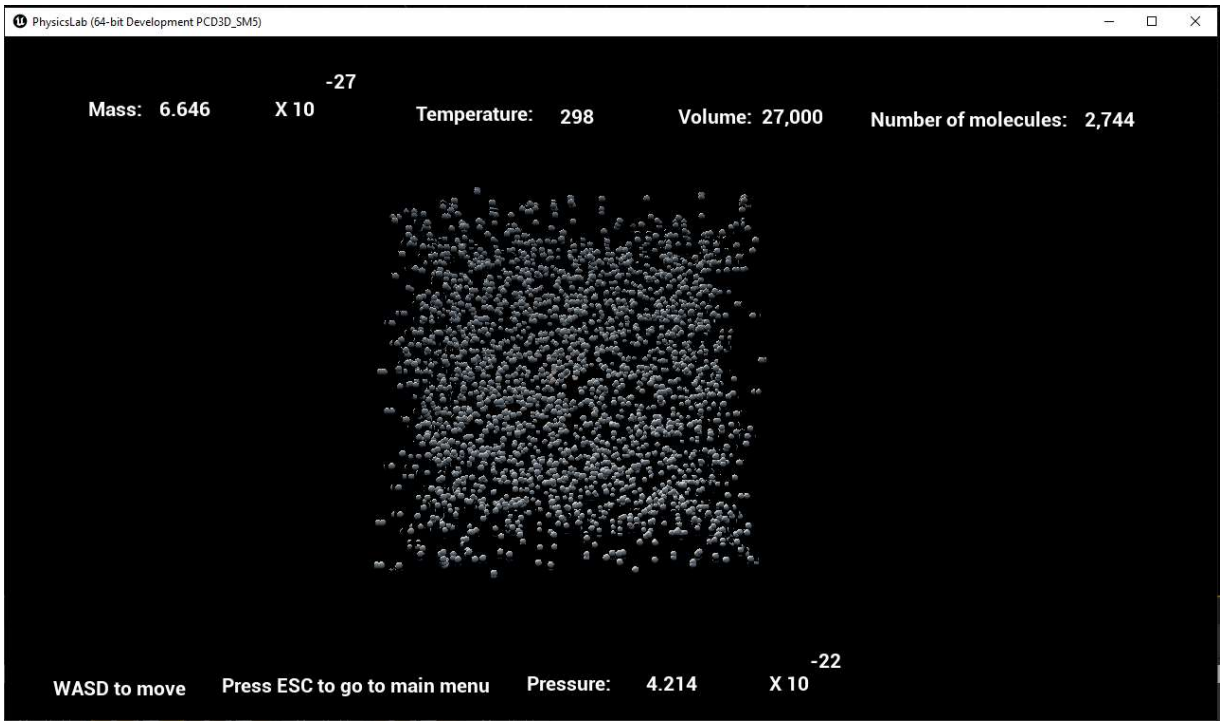
Helium with increased temperature (T = 398K, V = 17576$m^3$, num_molecules = 2744)



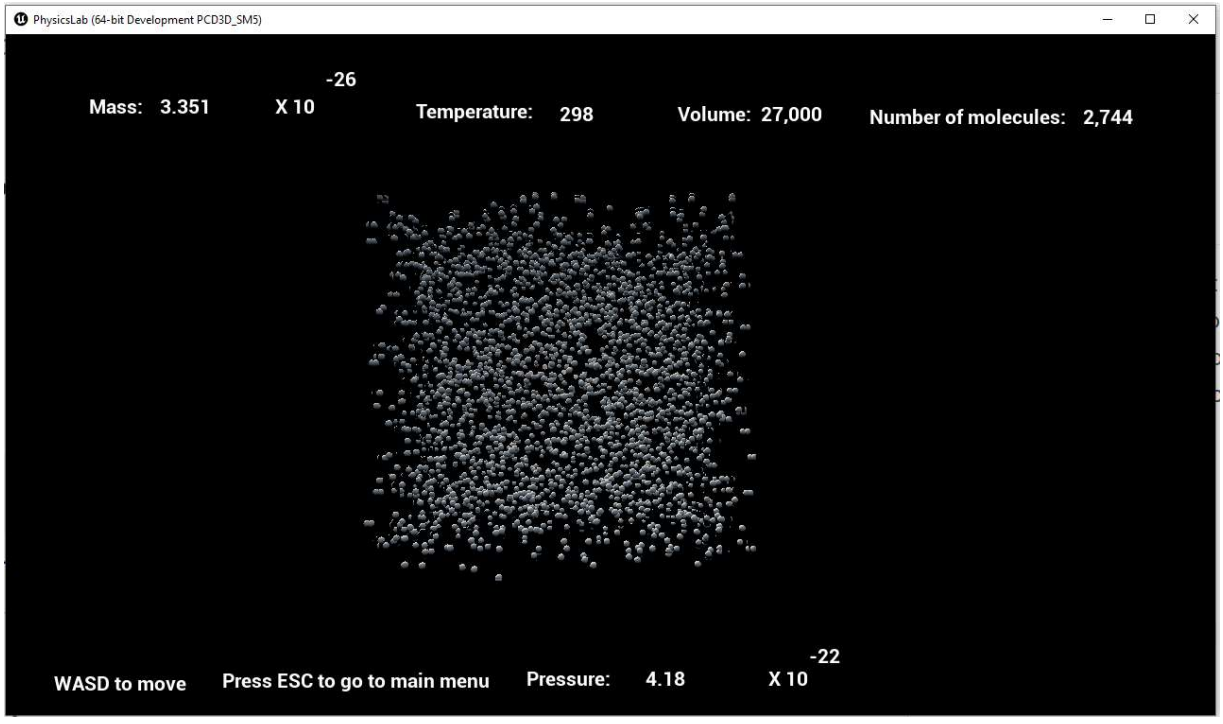

Neon with increased temperature (T = 398K, V = 17576$m^3$, num_molecules = 2744)



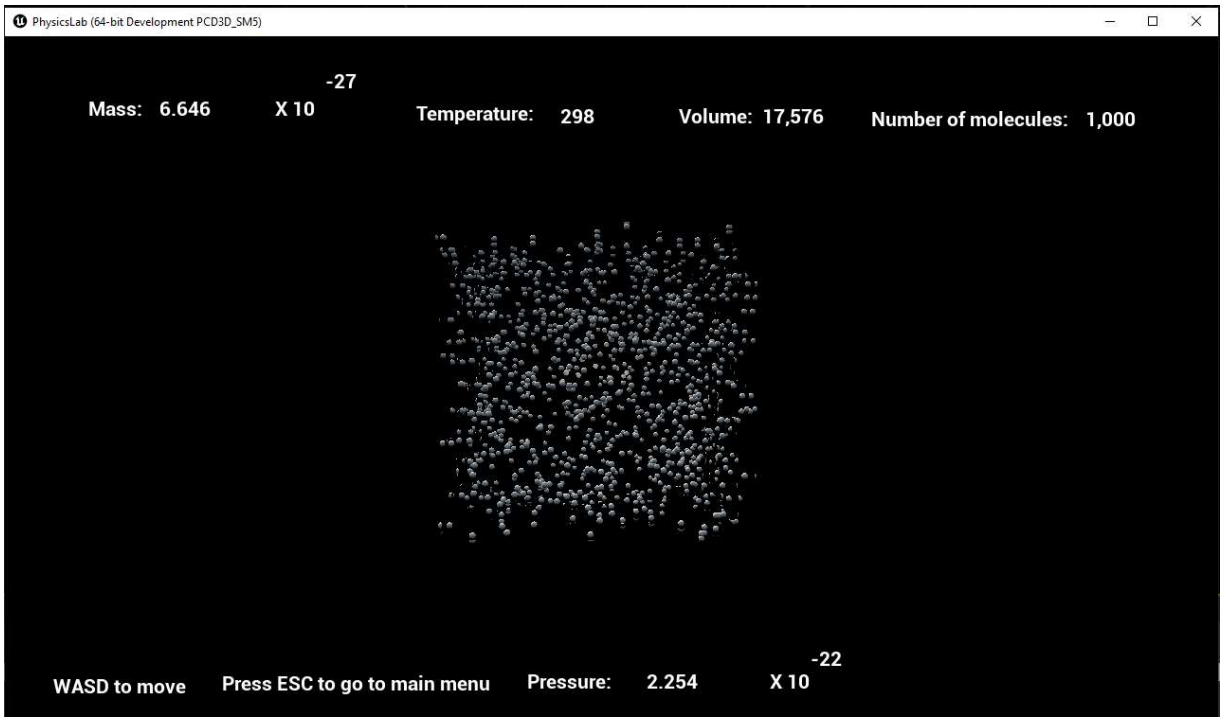
Helium with increased volume(T = 298K, V = 27000$m^3$, num_molecules = 2744)



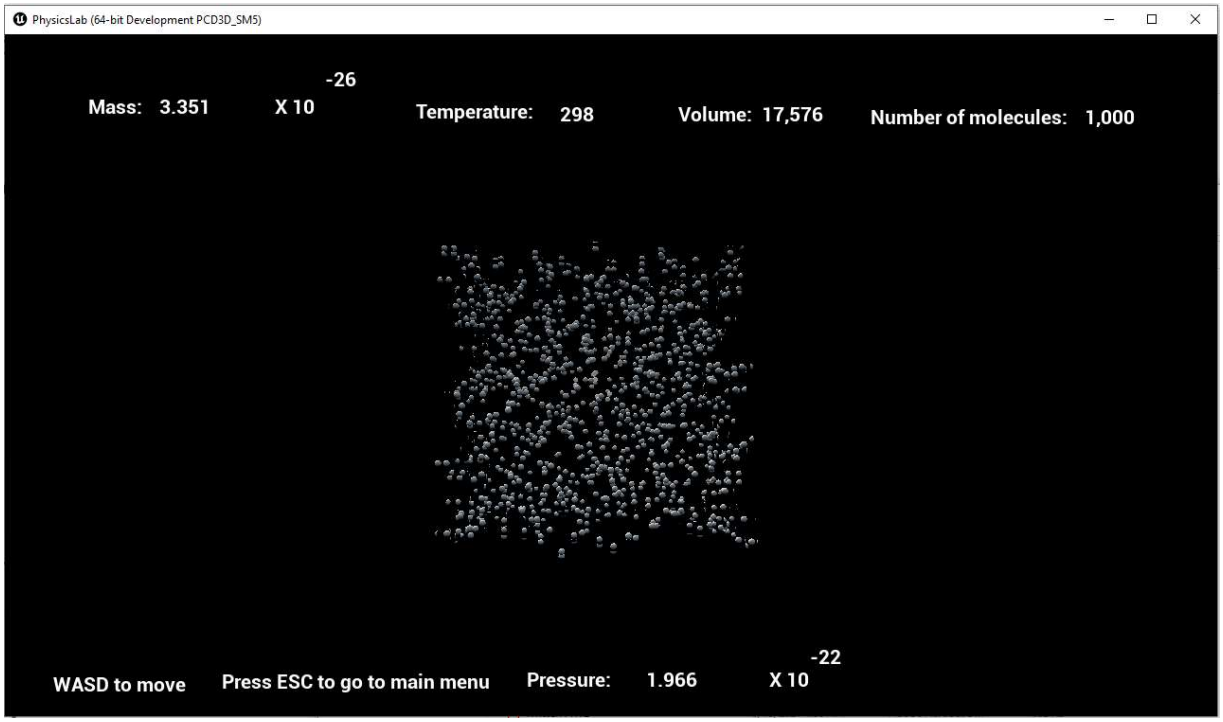

Neon with increased volume(T = 298K, V = 27000$m^3$, num_molecules = 2744)



Helium with decreased number of molecules(T = 298K, V = 17576$m^3$, num_molecules = 1000)




Neon with decreased number of molecules(T = 298K, V = 17576$m^3$, num_molecules = 1000)



**Analysis of data: (all values except the error is in Pascal or Pa)**

| | Standard | T = 398 | V = 27000 | Num_molecule = 1000 |
|---|---|---|---|---|
| Helium | $6.486 \times 10^{-22}$ | $8.619 \times 10^{-22}$ | $4.214 \times 10^{-22}$ | $2.254 \times 10^{-22}$ |
| Neon | $6.217 \times 10^{-22}$ | $8.552 \times 10^{-22}$ | $4.18 \times 10^{-22}$ | $1.966 \times 10^{-22}$ |
| Expected Value | $6.424 \times 10^{-22}$ | $8.579 \times 10^{-22}$ | $4.181 \times 10^{-22}$ | $2.341 \times 10^{-22}$ |
| Error(Helium) | -0.972% | -0.465% | -0.777% | -3.714% |
| Error(Neon) | 3.245% | 0.316% | 0.036% | 16.0169% |

**Discussion:**

As seen by error percentage, the simulation is fairly accurate except for the simulation of Neon with 1000 molecules. For any given set of parameters, the simulation of Helium and Neon produce similar pressures. As such, it seems clear that the pressure is independent of the molecule's mass and that pressure can only be changed by changing parameters T, V and Num_molecules.

In the rest of this section, I will attempt to explain some of the oddities that can be seen in the data.

First, the error percentages for Helium are always negative while they are always positive for Neon. This can likely be explained by the frame rate dependence of the program. I ran the simulation with extreme values such as num_molecule = 100000. Obviously, with the increase in the number of calculations needed, the frame rate heavily suffered. In some cases, the simulation simply did not run. However, for those cases where the simulation ran with lowered framerates, the pressure was always very different from the expected value. As such, it was clear that the pressure calculation algorithm I used was dependent on framerate. Specifically, I believe this is because of the discrepancy between 1 second in the simulation and 1 second in real life. It seems that there is a difference between these measures of time and that this difference is caused by the frame rate. To explain the error percentages of Helium and Neon, I think this explanation is quite accurate. Helium molecules have a much lower mass and thus will have a higher velocity than Neon molecules. Unfortunately for the simulation, increased velocity means an increase in needed calculations, as such, the framerate of the Helium simulations were lower than that of the Neon simulations. As such, the simulation seems to be framerate dependent.

Second, the error percentage is especially high for the simulation of Neon with 1000 molecules. I believe this is because of the low amount of molecules and the relatively low speed of the molecules. These two factors combined means that there are simply a lot less instances of collision between the walls and the molecules. With a lower total number of collisions, the average number of collisions for a given amount of time varies quite a bit. In addition to this, it may be that the framerate is too low at this point. Another explanation may be that 1000 molecules does not meet our criteria of a "very large number of molecules" in our assumption #1.

**Conclusion:** $pV = nRT$ holds true for an ideal gas. In addition, it holds true that pressure is the same, if the quantities V, n, R, T are the same, regardless of the mass of the molecule.

Here is a link to download the simulation:
https://drive.google.com/file/d/1QI-RsnSnPTo1CdBvDM3A7-wv4cApDqbg/view?usp=sharing

Be aware that the simulation is framerate dependent.