Checkpoint1

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Abstract

In this project, we plan to establish a system incorporating various types of ideal gas particles, potentially featuring two distinct kinds, such as Nitrogen and Oxygen. The goal is to simulate a fluid representation that mirrors the smooth behavior characteristic of gases, as to observe the intricate movements of gas molecules and, importantly, to assess whether the ideal gas law remains applicable when considering some other factors. Additionally, we will introduce several other operations into the system extending beyond the ideal gas model. These operations will involve adjusting the total volume, inserting and extracting particles strategically, and introducing external factors such as a heat source. We intend to use an agent-based model to simulate particles individually, while using numerical methods and high-performance libraries to optimize the performance of the simulation.

Ideal Gas System

The ideal gas law describes the relationship between pressure p , volume V, and temperature T for a number N of particles in a gas as follows

$$pV = NkT$$

Where k is the Boltzmann constant. The ideal gas law simplifies real gas particle dynamics, making it ideal for simple simulations. It is used to understand the behavior of gases in many scientific and engineering fields, including those utilizing thermodynamics and fluid dynamics.

According to Kinetic Molecular Theory, the relationship between the average kinetic energy of a system of ideal gas and the root mean square velocity of the particles can be written as

$$KE_{avg} = \frac{1}{2} m v_{rms}^2$$

The relationship between average kinetic energy and the temperature can be written as

$$KE_{avg} = \frac{3}{2} kT$$

Hence, we can get

$$v_{rms} = \sqrt{\frac{3kT}{m}}$$

This formula can be used to calculate the temperature by the measurement of velocity. There are many existing software packages for simulating an ideal gas. These simulations focus on validating and demonstrating physical laws for educational purposes. We will introduce them respectively in the following section.

We noticed that these simulators usually model individual gas particles as solid spheres with perfectly elastic collision [4-8]. However, using solid spheres to represent gas particles does not seem realistic, as gas is a kind of smooth fluid instead of discrete spheres. We would like to improve the visualization so that the gas particles will look more like gas in the real world. The following section introduces some of the possible methods to achieve this.

Conceptual Model

In this section, setting of parameters and the related numerical calculations will be described. As we set our model to be ideal gas, it would follow the ideal gas law formula:

$$pV = NkT$$

The unit for p as Pa , V as m^3, T as K , N as the number of particles. This helps us get the unit for ideal gas constant k as J/K ,since $Pa \cdot m^3$ can be considered as $Pa \cdot m^2 \cdot m$, from $F = P \cdot A$, we can get the unit for F is Newton N . Then we can use the formula for work as $W = Fs$ to get the unit of W as J .

In the ideal state as $p = 1.013 \cdot 10^5 Pa$, $T = 273.15K$, the volume of $1\ mol$ ideal gas is $22.4L$. This gives us the ideal gas constant $k = 1.38 \times 10^{-23}\ J/K$.

In our system, we might consider several scenarios:

Scenario 1: Adjust the number of the particles
Assume the system volume and the temperature does not change, by the ideal gas formula, if we have more particles in the system would cause higher pressure, vice versa.

Scenario 2: Adjust the volume of the system
If we add a piston to the system to help adjust the volume, assume the number of particles inside the system and the temperature does not change. The smaller the system, the higher the pressure, vice versa.

Scenario 3: Adjust the temperature
We will add a heater for the system. Assume the number of particles and the volume of the system stays the same, if we have a higher temperature, we will get a higher pressure, vice versa.

Our model is an agent-based model, which means that all particles are considered individually. We will set a target temperature for the system. Because the temperature is related to the V_{rms} , and the V_{rms} of all particles are random distribution, which are 10% variance. After having these values of V_{rms}, they would be used to calculate the real temperature again.

In addition, we suppose that all particles are confined in the box and assume that collisions between particles and walls of the box are perfectly elastic collisions. We want to acquire the total pressure on the box.

To acquire the pressure, we need to find the impulse first. The mathematical expression for impulse is usually written as:

$$J = F \cdot \Delta t = m \cdot \Delta v$$

Where J represents the impulse, m is the mass of the object, and Δv is the change in velocity.

Once we have all the impulses of particles, the pressure can be acquired by summing up all impulses and being divided by the period of time and the area of the box. The mathematical expression for the pressure is written as:

$$P = \frac{\sum_{i=0}^{N-1} J_i}{A \cdot \Delta t}$$

Where J_i represents the impulse of one particle, N is the number of particles, A is total surface area of the box, and Δt is the change of time in a period.

Platform

We will use Python 3.9 as our coding languages, using the Taichi and Numpy libraries for the mathematical calculations for performance purposes.

Literature Review

A plethora of ideal gas law simulators utilizing simplified particle models, such as the perfectly elastic sphere particle model, are readily available on platforms like GitHub[4-8]. These simulators extend beyond basic ideal gas law modeling, serving various purposes such as validating the Maxwell-Boltzmann distribution[4], performing 3D simulations[5], exploring a simplified version of particle fusion[6], conducting calculations for incident and reflected shock waves in a shock tube[7], and establishing connections between the ideal gas law and specific heat capacity[8]. Additionally, online Graphical User Interfaces (GUIs) of ideal gas law simulators, exemplified by the University of Colorado's online tool[1], provide accessible demonstrations of ideal gas behavior.

Addressing the visual representation of gas particles, there is a collective effort to move beyond the simplistic model of solid spheres with perfectly elastic collisions [4-8]. To impart a more realistic appearance resembling continuous gas, an assumption inherent in ideal gas theory is employed — particles themselves have no volume. This involves representing gas particles using numerous small points, creating the illusion of a continuous gas medium. Furthermore, the incorporation of fluid models, such as Smoothed Particle Hydrodynamics (SPH) [9-11], is explored to enhance the visual fidelity of gas simulations.

In this simulation, we seek to cover scenarios that the above-mentioned ideal gas simulators may overlook. For instance, introducing colored gas particles into the system prompts inquiries into their diffusion patterns within the container. Opening a drain at the bottom raises questions about the evacuation dynamics of gas particles. Furthermore, introducing a heat source beneath the container offers an opportunity to observe how particles respond, potentially unveiling thermal convection movements. These diverse scenarios not only enrich the simulations but also expand the applicability of ideal gas models to real-world situations, fostering a more comprehensive understanding of gas behavior.

Reference

[1] The ideal gas diffusion simulator developed by the University of Colorado. https://phet.colorado.edu/en/simulations/gas-properties

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[4] Simulation of an Ideal Gas to Verify Maxwell-Boltzmann distribution. https://github.com/rafael-fuente/Ideal-Gas-Simulation-To-Verify-Maxwell-Boltzmann-distribution.git

[5] Ideal gas simulation in a 3D system. https://github.com/labay11/ideal-gas-simulation.git

[6] Skiverse: A SKI universe. https://github.com/mountain/skiverse.git

[7] Python Real Gas FROzen SHock (RGFROSH) https://github.com/VasuLab/RGFROSH.git

[8] Thermodynamic Cycles. https://github.com/geokosto/Thermodynamic-Cycles.git

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[11] Ren, B., Yan, X., Yang, T. *et al.* Fast SPH simulation for gaseous fluids. *Vis Comput* **32**, 523–534 (2016). https://doi.org/10.1007/s00371-015-1086-y

Progress

We have established our coding environment on GitHub and effectively employed Numpy and Taichi to simulate the motion of 81 gas particles in a confined space. Taichi, known for its robust physics simulation capabilities, offers excellent visualization for physics-based animations. Meanwhile, Numpy's proficiency in array operations supports efficient calculations. By leveraging Numpy for computations and Taichi for visualization, we ensure our program can achieve real-time simulations. In the upcoming days, we'll integrate additional devices like gas sources, gas drains, a piston, and a heater to manipulate the ideal gas system's parameters (P, V, N, T), observing the resulting changes.

Division of Labor

Name	Tasks
James Yu	Project overview, Literature Review, Physics equations, Coding environment (Github) setup
Chun-Fu Kuo	Conceptual Model, Piston (adjust volume)
Ping-Chuan Lin	Conceptual Model, Heater (adjust temperature)
Felicity Nielson	Literature Review, Gas sources
Ziming Liu	Gas collisions between particles
Andy Yu	Abstract Writing, Gas collision with box sides (basis for heater)

Git Repository

https://github.gatech.edu/jyu678/CSE6730_Gas_Simulation.git