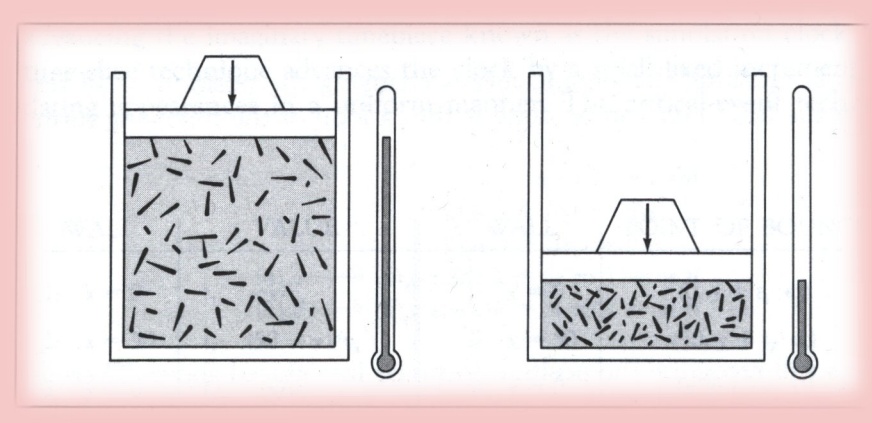
TO TREAD UPON THE AIR

Introduction

This project explores a very simple classical model of a gas, and looks at the effects of fluctuations when only a small number of molecules are present. It uses the molecular dynamics method, in which the motion of molecules is treated using classical mechanics. Although a 'stripped-down' molecular dynamics method is used here, the method in general provides a very powerful tool for exploring the properties of matter in the gas, liquid and solid phases and the phase transitions between them.

A simplified model

We consider a two-dimensional gas of point-like atoms, which do not interact with one another. The atoms are held in a container which has a solid, fixed, base and sides, but the top of the container is a piston which is free to move up and down. The atoms move in the container with a speed which is characteristic of their temperature. When they reach the confining surfaces, they bounce off elastically. The sides and bottom do not react to the corresponding mechanical impulse, but the piston at the top does – its motion is governed by the impacts of the molecules and by the acceleration due to gravity. We expect that increasing the molecular speed (increasing the temperature) will cause the gas to expand.



Molecular dynamics calculations usually operate in one of two modes. In the time-slice mode, the forces and hence the accelerations of the molecules are evaluated at some time t, and used to predict the positions and velocities at some later time $t + \delta t$. This is the only practical approach when the molecules interact with each other. In our model, the moelecules move in straight lines at constant speeds until they collide with the confining surfaces. In that case an event-driven scheme is more efficient. We start with the positions and velocities of all the molecules. For each molecule i, we calculate the time it will take to hit a boundary, Δt_i. We find the minimum of these times, $\Delta t_{\min}$, then calculate the new positions of all the molecules after that interval. All the molecular velocities will remain the same, except for the one that hits the boundary: it will have the component of its velocity normal to the boundary reversed. Finally, if the boundary impacted was the piston, we modify the speed of the piston appropriately (we also need to keep track of the position of the piston when calculating impact times).

The project

Imagine a box of width w, height h (the position of the piston). The first task is to set up the equations for determining the intersection times with the four boundaries of a molecule that starts at (x, y) inside the box and moves with velocity (u, v). Remember later, when you solve these equations, that only positive values of the time are of interest. Assume that the molecules are not influenced by gravity (though a possible extension is to include loss of energy when atoms hit the boundaries, and to look at the sedimentation of particles).

Then write a computer program for the model. Mathematica will be suitable, but use any language you like. It obviously makes sense to start with a fairly small number of molecules, but write the program so that it is easy to vary this. A parameter that you should experiment with is the ratio of the mass of the piston to the mass of the molecules. The mass of the piston accelerating under gravity, of course, represents the pressure being applied to the gas.

To start the model, pick a speed s for the molecules (this will be related to the temperature T by $\frac{1}{2}ms^2 = k_{\mathrm{B}}T$, where m is the mass of a molecule and k_{B} is Boltzmann's constant. Do not get too tied up with units, though - take most of the constants to be unity. Then for each molecule allocate an x speed u between $-s$ and s, and a y speed $v = \pm\sqrt{s^2 - u^2}$, picking the positive and negative signs with equal probability. You could refine the model by using a distribution of velocities, such as Maxwell-Boltzmann.

The variation of the height h of the piston represents the gas volume. For a classical gas (in which the number of gas molecules is enormous) the volume is a well-defined quantity for any temperature (molecular speed) and pressure – with a small number of molecules the volume will fluctuate because of the discrete impacts of the molecules on the piston. You should investigate both how the average piston height varies with 'temperature' and how the fluctuations vary with the number of molecules.

Your results will include graphs illustrating the fluctuations, but you might also want to include 'snapshots' of the spatial distribution of the molecules.

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