Computer Simulation

of a two-dimensional ideal gas

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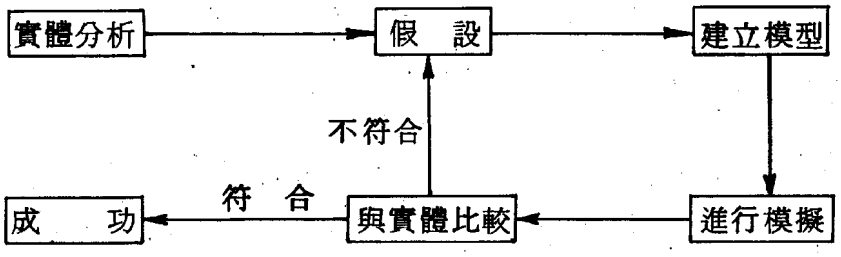
由於電腦性能的不斷提高，使得電腦可應用的範圍亦日漸擴大。其中電腦模擬即最近興起的一種應用，且用途愈來愈廣泛。

電腦模擬大致可區分爲二類：㈠對既有狀況進行分析，並作一些假設，建立模型，輸入電腦中進行模擬，再由得到的結果與實際狀況比較，對不符合實際狀況之處進行分析和檢討，然後對先前的假設進行修改，或捨棄不用另定新假設。其流程圖如下：



㈡利用對實體模擬得到的結果，幫助人們去進行一些其他方面的應用，如對機翼與氣流關係的模擬，來進行輔助機翼的設計，此即目前電腦輔助設計中，最進步的一種模擬。

當然任何一種情況的發展及流行必定有其背景及好處，電腦模擬的背景在於電腦速度愈來愈快，且此種趨勢仍會持續好一陣子，以前一些需要十分複雜運算的工作不得不經由實際試驗才可得知，但目前皆可經由電腦而辦到，且亦由於速度的不斷提昇，相信將會有更多的應用出現；電腦模擬的好處由前面背景部分所提，即可知其爲省時、省力、省錢，因爲不論在㈠或㈡的情形，每作一次眞實的試驗均須花費大量的人力、物力、財力，且又不一定達到預期效果，甚至同樣的試驗作了數次才有一結果，但又不一定符合要求，而電腦模擬則在大致上符合要求了，才去進行實體試驗，在各方面均節省許多。但電腦模擬只是紙上談兵，它永遠也不能完全代替實驗。

此次，我們二人所做的實驗是屬於㈠利用對二維空間氣體行爲的模擬証明理想氣體是屬於Maxwell-Boltzmann 分佈。

0. Introduction

"Simulation is the process of designing a model of a real system and conducting experiments with this model for the purpose either of understanding the behavior of the system or of evaluating various strategies for the operation of the system."[1]

A computer simulation of a two-dimensional ideal gas has been studied in order to observe the time development of the speed distribution function.

1. Purpose

To demonstrate the evolution of the two-dimensional Maxwell-Boltzmann Distribution by simple collisions.

2. Method

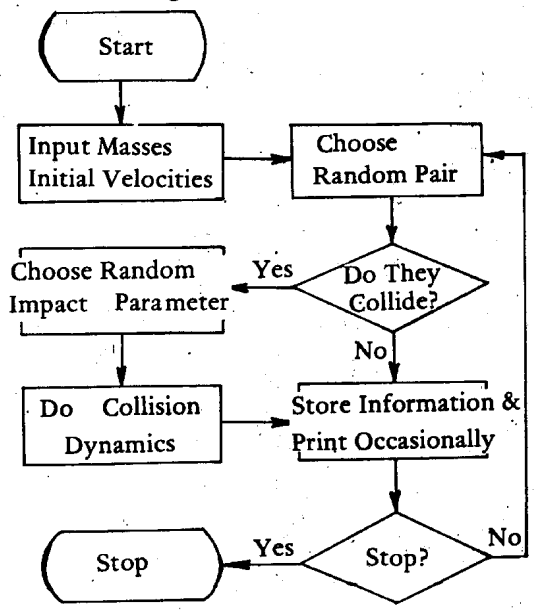
We study a gas of molecules of the order of 10^2 in a given region of space with the following assumptions

(1) all of the molecules are hard circles of equal size,

(2) all collisions are elastic and forces between molecules act only along the line of centers,

(3) the distribution of velocities is identical in all regions of space.

The simulation is then designed according to the following flow chart:



3. Principles

An initial distribution is assumed for the molecular speeds. The computer program chooses at random a pair of molecules that may collide.

Because of assumtion (1), the relative probability of a collision between a pair of molecules having a certain relative velocity is proportional to their relative speed. [2]

The collision is studied assuming an impact parameter a random number in the interval (0.2A). A is the radius of the molecules. This is due to assumption (3) [3].

New velocities are calculated, in the laboratory system, by using an "interaction matrix" that relates v_1' and v_2' (velocities after collision) to v_1 and v_2 (velocities before collision). [4]

Once the new velocities are calculated, they are stored in the new distribution and the calculation is repeated. After N simulated collisions the then distribution gives the speed distribution of 2N molecules that have undergone an average of one collision per molecule. If we assume the whole process as the mechanism of obtaining a distribution at one time and restart the process, we can get the evolution of the speed distribution of the gas.

The interaction matrix

According to assumption (2), the collision in the center of mass frame of reference looks like Fig.1. The circles' velocities undergo mirror reflection with respect to the tangent line common to the circles.

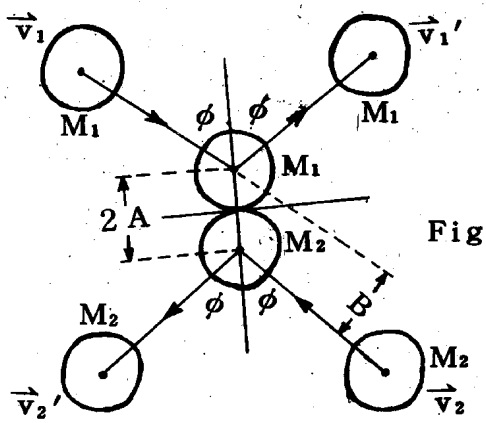


Fig 1

Transforming into the laboratory frame, we find that v_1' and v_2', the velocities after collision, are related to v_1 and v_2 the velocities before the collision, by [5]

$$\begin{pmatrix} v_{1x}' \\ v_{2x}' \\ v_{1y}' \\ v_{2y}' \end{pmatrix} = \begin{pmatrix} m_1 + \alpha m_2 & m_2 \beta \\ m_1 \beta & m_2 + \alpha m_1 \\ m_2 \gamma & -m_2 \gamma \\ -m_1 \gamma & m_1 \gamma \end{pmatrix}$$

$$\begin{matrix} -m_2 \gamma & m_2 \gamma \\ m_1 \gamma & -m_1 \gamma \\ m_1 + \alpha m_2 & m_2 \beta \\ m_1 \beta & m_2 + \alpha m_1 \end{matrix} \begin{pmatrix} v_{1x} \\ v_{2x} \\ v_{1y} \\ v_{2y} \end{pmatrix}$$

A is the radius of the circles, B is the impact parameter, and M_1 and M_2 are the masses of the circles as shown in Fig.1.

The matrix above can be used to calculate the collision dynamics. Whenever two molecules collide, a subroutine base on the matrix is used to calculate the components of the velocities.

There are also subroutines to generate random numbers. We use a random number in choosing a colliding pair; another random number is employed to represent the corresponding impact parameter.

The results of the simulation are presented in the next part.

4. Results

The following program is written in BASIC. However, for the purpose of demonstration in class, we also prepared a disk which contains the same program written in Apple BASIC.

We ran the program on a 16-bit microcomputer Sage. The results are submitted along with this report.

Our program is a flexible one. By changing the corresponding parameters, we can simulate: (1) a gas of more molecules, (2) more than one kind of molecule, (3) more collisions per molecule.

In this paper we consider only one kind of molecule. The number of molecules is 200. The initial velocities are 120 units. (Our program can be modified very easily to different initial velocities for different molecules to see whether the final distribution is Maxwell-Boltzmann.)

From the chart we see that there 6552 actual collisions. This means that there are about 31 collisions per molecule on average.

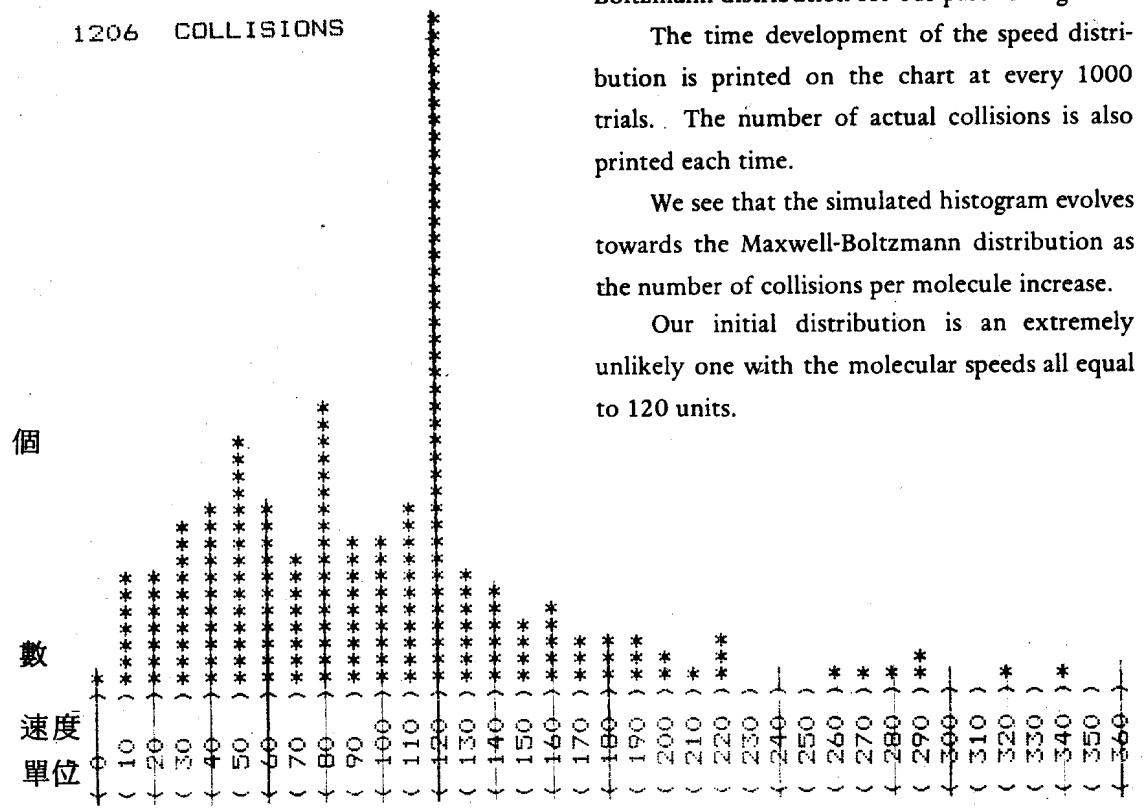
In fact, we have made 28000 trials. However, in this hard circle model, the actual collision is limited by the collision probability which in turn depend on the relative velocities of the interacting molecules.

It is easily observed that about 6 collisions per molecule is enough to establish the Maxwell-Boltzmann distribution for our particular gas.

The time development of the speed distribution is printed on the chart at every 1000 trials. The number of actual collisions is also printed each time.

We see that the simulated histogram evolves towards the Maxwell-Boltzmann distribution as the number of collisions per molecule increase.

Our initial distribution is an extremely unlikely one with the molecular speeds all equal to 120 units.



5. Discussion

If more computer time is allowed, it is possible to modify the program to test more initial conditions. This task is worth trying because theory has shown that the Maxwell-Boltzmann is the most probable one in Nature. This implies that irrespective of initial conditions we can obtain the Maxwell-Boltzmann distribution as the equilibrium distribution.

Of course, the "volume" or the "energy" of our gas should also be discussed. This corresponds to how often we choose two molecules to collide. This is controlled by the random number and the way we use it.

Anyway, we see that the simulation is illustrative in the physical meaning of the Maxwell-Boltzmann distribution.

Finally, the above process can be extended to study the behavior of nonideal gas.

Appendix

1. Robert Shannon, Systems Simulation: The Art & Science
2. This is an approximation which we can verify by our experiment. The theoretical treatment is given by M.Eger and M.Kress, Am. J. Phys. 59, 120(1982).
3. Since the velocity distribution at all points in space is assumed to be the same, all impact parameters are equally likely in the collision of a given pair of molecular velocities.
4. The program simulates the passage of time by calling on a random number generator to choose at random a pair of particles which may collide. They do not collide with certainty since the relative probability of a given pair colliding is proportional to their relative speed. Thus their relative speed is calculated and compared to a standard speed which is chosen to be five times as large as the initial speed. Their ratio P is calculated and compared to a random number R in the interval (0,1). If $P > R$, the pair is permitted to collide with an impact parameter: a random n number in (0,2A). J. Novak and A.B. Bortz, Am. J. Phys. 38,1402(1970).
5. The details for getting the interaction matrix:

   The basic idea is to view the collision in the center of mass system. The calculation here is done by means of matrix transformation.

$$v'_{Lab} - v_{Lab} = NSM \; v_{Lab}$$

where v_{Lab} is the vector $\begin{pmatrix} v_{1x} \\ v_{2x} \\ v_{1y} \\ v_{2y} \end{pmatrix}$, representing the velocity components in the lab. mystem before collision.

$$v'_{Lab} = \begin{pmatrix} v_{1x}' \\ v_{2x}' \\ v_{1y}' \\ v_{2y}' \end{pmatrix}$$

is the velocity "four vector" after collision. M is the matrix that transforms v_{Lab} into the center of mass system, i.e. $v_{CM} = M \; v_{Lab}$

S is the matrix of collision in the CM system. The collision is in effect, a rotation of all the velocity componeats in the CM system.

N is the matrix that transforms a "vector" in the CM system back to the lab. system, i.e.

$$v_{Lab} = N \; v_{CM}$$

To obtain M, consider the position of the center of mass of two bodies in the lab,

$$\vec{R} = \frac{M_1 \vec{r}_1 + M_2 \vec{r}_2}{M_1 + M_2}$$ if we write

$$m_1 = \frac{M_1}{M_1 + M_2} \text{ and } m_2 = \frac{M_2}{M_1 + M_2}$$

we have $\vec{R} = m_1 \vec{r}_1 + m_2 \vec{r}_2$ in the

lab. system. Now, the position of M1 as seen in the CM system is

$$\vec{\bar{r}}_1 = \vec{r}_1 - R = \vec{r}_1 - (m_1\vec{r}_1 + m_2\vec{r}_2)$$

$$= m_2(\vec{r}_2 - \vec{r}_1) \quad \because 1 - m_1 = m_2$$

similarly, $\vec{\bar{r}}_2 = m_1(\vec{r}_1 - \vec{r}_2)$, in component form, we have, for examble

$$\bar{x}_1 = m_2 x_1 - m_2 x_2 \quad \text{and in general,}$$

$$M = \begin{pmatrix} m_2 & -m_2 & 0 & 0 \\ -m_1 & m_1 & 0 & 0 \\ 0 & 0 & m_2 & -m_2 \\ 0 & 0 & -m_1 & m_1 \end{pmatrix}$$

to transform position vectors $\vec{r}_1, \vec{r}_2$ we have

$$\begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \bar{y}_1 \\ \bar{y}_2 \end{pmatrix} = \begin{pmatrix} m_2 & -m_2 & 0 & 0 \\ -m_1 & m_1 & 0 & 0 \\ 0 & 0 & m_2 & -m_2 \\ 0 & 0 & -m_1 & m_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ y_1 \\ y_2 \end{pmatrix}$$

the same matrix M transforms all "four vectors" from the lab system to the CM system.

$$\therefore \quad v_{CM} = M\, v_{Lab}$$

To obtain N, consider adding $\vec{R}$ to $\vec{\bar{r}}_1$ and $\vec{\bar{r}}_2$ in the CM system, physically this takes us back to the lab system,

$$\vec{r}_1 = \vec{\bar{r}}_1 + (m_1\vec{\bar{r}}_1 + m_2\vec{\bar{r}}_2)$$

$$\vec{r}_2 = \vec{\bar{r}}_2 + (m_1\vec{\bar{r}}_1 + m_2\vec{\bar{r}}_2)$$

in component form, we have, for example

$$x_1 = (m_2 + 2m_1)\,x_1 + m_2 x_2$$

in general, we have

$$\begin{pmatrix} x_1 \\ x_2 \\ y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} m_2 + 2m_1 & m_2 & 0 & 0 \\ m_1 & m_1 + 2m_2 & 0 & 0 \\ 0 & 0 & m_2 + 2m_1 & m_2 \\ 0 & 0 & m_1 & m_1 + 2m_2 \end{pmatrix} \begin{pmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \bar{y}_1 \\ \bar{y}_2 \end{pmatrix}$$

$$\therefore N = \begin{pmatrix} m_2 + 2m_1 & m_2 & 0 & 0 \\ m_1 & m_1 + 2m_2 & 0 & 0 \\ 0 & 0 & m_2 + 2m_1 & m_2 \\ 0 & 0 & m_1 & m_1 + 2m_2 \end{pmatrix}$$

the matrix N, as before, transform the velocity components.

To obtain S, the collision matrix in the center of mass system, let's look at the picture there,

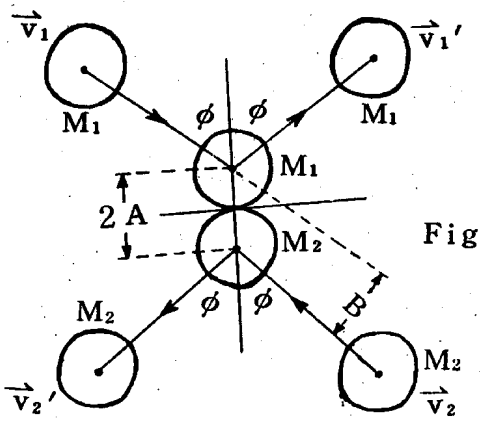


Fig 1

We note that the collision merely rotates the velocities. We take the view that the axes are fixed in the rotation, only the vectors themselves are affected. For one point-transformation,

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} -\cos 2\phi & -\sin 2\phi \\ \sin 2\phi & -\cos 2\phi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\sin\phi = \frac{B}{2A}$$

$$\sin 2\phi = 2\sin\phi\cos\phi$$

$$= 2\left(\frac{B}{2A}\right)\left(\frac{\sqrt{4A^2 - B^2}}{2A}\right) \equiv \gamma$$

$$\cos 2\phi = 1 - 2\sin^2\phi = 1 - \frac{B^2}{2A^2}$$

$\equiv \beta$, and let $\beta = 1 - \alpha$

in the figure, we have

$$\begin{pmatrix} v_{1x}' \\ v_{1y}' \end{pmatrix} = \begin{pmatrix} -\beta & -\gamma \\ \gamma & -\beta \end{pmatrix} \begin{pmatrix} v_{1x} \\ v_{1y} \end{pmatrix}$$

and $$\begin{pmatrix} v_{2x}' \\ v_{2y}' \end{pmatrix} = \begin{pmatrix} -\beta & -\gamma \\ \gamma & -\beta \end{pmatrix} \begin{pmatrix} v_{2x} \\ v_{2y} \end{pmatrix}$$

$$\therefore \begin{pmatrix} v_{1x}' \\ v_{2x}' \\ v_{1y}' \\ v_{2y}' \end{pmatrix} = \begin{pmatrix} -\beta & 0 & -\gamma & 0 \\ 0 & -\beta & 0 & -\gamma \\ \gamma & 0 & -\beta & 0 \\ 0 & \gamma & 0 & -\beta \end{pmatrix} \begin{pmatrix} v_{1x} \\ v_{2x} \\ v_{1y} \\ v_{2y} \end{pmatrix}$$

$$\therefore \quad S = \begin{pmatrix} -\beta & 0 & -\gamma & 0 \\ 0 & -\beta & 0 & -\gamma \\ \gamma & 0 & -\beta & 0 \\ 0 & \gamma & 0 & -\beta \end{pmatrix}$$

$$v'_{Lab} - v_{Lab} = NSM \; v_{Lab}$$

physically this means that the differences in the velocity components is due to the collision, which is represented by the product NSM.

(don't forget that we've been working in CM system and have to transform everything back into the lab system)

$$SM = \begin{pmatrix} -\beta m_2 & \beta m_2 & -\gamma m_2 & \gamma m_2 \\ \beta m_1 & -\beta m_1 & \gamma m_1 & -\gamma m_1 \\ \gamma m_2 & -\gamma m_2 & -\beta m_2 & \beta m_2 \\ -\gamma m_1 & \gamma m_2 & \beta m_2 & -\beta m_1 \end{pmatrix} = S'$$

the final matrix is $I_4 + NS'$ where

$$I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$