Diffusion of a 2D gas

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Summary

A 2D rectangle-shaped container is 2*L* long and *L* high. It is divided into two equal square chambers D1 and D2, with a diaphragm TU. In the middle of the diaphragm, there is a gap of height *h* which is initially closed by a barrier (Figure 1). In the container, there are *N* identical but discrete particles. Each particle has the shape of a disc of radius *r* and mass *m*. The particles interact in pairs (p-p interactions). During each interaction, the momentum and energy of the pair are conserved. The interactions of particles with the walls of the container are elastic collisions.

At time t=0 all particles are in the left compartment D1 and have random positions, and velocities of random magnitudes and directions. The initial velocity distribution of the gas, although it is not identical to the Maxwell-Boltzmann (M-B) distribution, it is very "near" to this and, because of the p-p interactions, it converges extremely fast to it[1,2,3].

Over time, particles are transferred through the gap from D1 to D2 and vice versa, so that the numbers (n_1, n_2) of particles in each chamber are changing. The program counts n_1, n_2 in real time and draws their graphs with time. On the other hand, a mathematical model has been composed, by which the variation of n_1 and n_2 is calculated over time and the corresponding graphs are depicted. The user compares the theoretical graphs with the experimental.

The user can select the values of the length *h* of the gap and the mean energy of the particles. He can also adjust the value of a statistical-phenomenological parameter P_{pass} so that the agreement of the experimental data with the theoretical graphs be the best possible.

To monitor the movement of each particle and its interactions with the rest and with the walls of the container or with the diaphragm, the program is drawing the trajectory of a particular particle in red.

Key concepts and relationships

Random variable - Probability density of a random variable - Probability distribution of a random variable - Uniform distribution - Maxwell-Boltzmann distribution - Markov process - Inertial reference system – Center-of-mass inertial frame - Linear momentum conservation in a p-p interaction - Energy conservation in a p-p interaction

The mathematical model

In the virtual gas, the initial positions of the particles are random. The velocity directions are random and the velocity magnitude of each particle is a random number in an interval $\left[0, v_{in.}\right)$, where $v_{in.}$ is determined by the program according to the selection of the energy level by the user. This state, although not identical to the thermodynamic equilibrium state, it is extremely near to this [1]. Nevertheless, fast enough the velocity distribution of the virtual gas converges to the Maxwell-Boltzmann (M-B) distribution [1,2,3]. Then, the probability of the event: "The velocity magnitude V_j of the j-particle is in the interval $\left[v, v+\Delta v\right)$, $\left(\Delta v \to 0\right)$", for any j=0,1…N-1 is:

$$p\left[v \le V_j < v + \Delta v\right] = \beta m e^{-\beta \frac{mv^2}{2}} v \Delta v \tag{1a}$$

The constant β is a function of the particles' average energy. It can be proved [1] that:

$$\frac{1}{\beta} = \frac{1}{N}\sum_{j=1}^{N}\frac{1}{2}m v_j^{\,2} = \langle E \rangle \tag{1b}$$

On the other hand, the probability of the event: "The angle Θ_j formed by the j-particle's velocity with the Ox axis is in the interval $\left[\theta, \theta + \Delta\theta\right)$" is:

$$p\left(\theta \le \Theta_j < \theta + \Delta\theta\right) = \frac{\Delta\theta}{2\pi} \tag{2}$$

Hence, the probability of the composite event: "The j-particle velocity has a magnitude in the interval $[v, v+\Delta v)$ AND its angle with the Ox axis is in the interval $[\theta, \theta+\Delta\theta)$" is given by the analytic expression:

$$p\left[\left(v \le V_j < v+\Delta v\right) \text{ AND } \left(\theta \le \Theta_j < \theta+\Delta\theta\right)\right] = \frac{\beta m}{2\pi} e^{-\beta\frac{mv^2}{2}} v\Delta v \wedge \Delta\theta \quad (3)$$

Regarding the particle positions in the initial state, it holds that:

$$p\left(x \le X_j < x+\Delta x\right) = \begin{cases} \frac{\Delta x}{L} \text{ if } 0 \le x < L \\ 0 \text{ otherwise} \end{cases} \quad (4a)$$

$$p\left(y \le Y_j < y+\Delta y\right) = \begin{cases} \frac{\Delta y}{L} \text{ if } 0 \le y < L \\ 0 \text{ otherwise} \end{cases} \quad (4b)$$

Calculation of the particles' variation in each chamber over time

Suppose that at time *t* there are $n_1(t)$ particles in D1 and $n_2(t)$ in D2. It is true that:

$$n_1(t) + n_2(t) = N \quad (5a)$$

In the time interval $[t, t+\Delta t)$, $\Delta n_{1\to 2}(t)$ particles pass from D1 to D2 and $\Delta n_{2\to 1}(t)$ from D2 to D1. The variations of $n_1(t)$ and $n_2(t)$ in the same time interval are $\Delta n_1(t)$, $\Delta n_2(t)$. From 5a it is implied that:

$$\Delta n_1(t) + \Delta n_2(t) = 0 \quad (5b)$$

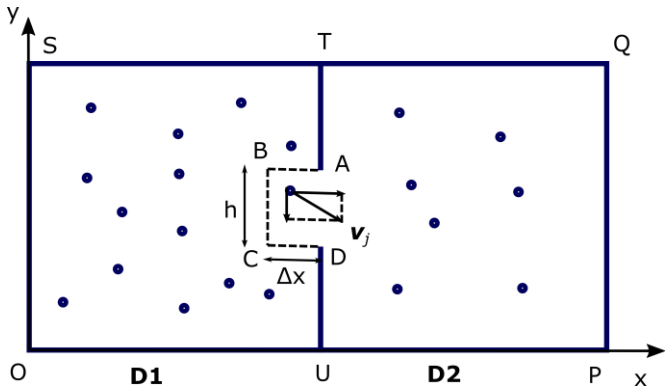

Figure 1

Consider the event $E_{1\to 2}[j; t, \Delta t]$: "The j-particle in the time interval $[t, t+\Delta t)$ passes from D1 to D2".

Event $E_{1\to 2}[j; t, \Delta t]$ is composed of the following independent events:

$E1(t; D1)$: "At time *t* the j-particle is in chamber D1".

$E2[t; (ABCD)]$: "At time *t* the j-particle is in the orthogonal parallelogram (ABCD) with $V_{jx} > 0$ AND it passes through the gap to chamber D2 in the time interval $[t, t+\Delta t)$" (see Figure 1).

Let P_{pass} be the probability for the j-particle to pass through the gap, given that at time *t* it is in (ABCD) with the right x-velocity. P_{pass} depends on many parameters: the length of the gap, the frequency of the p-p interactions, the density of the gas, etc. ***The value of P_{pass} is determined phenomenologically: In the virtual environment of the simulation, the user is being experimented with the values of P_{pass} in the interval $(0,1]$ so that to obtain the best fitting of the experimental with the theoretical graphs***.

Hence, the probability of $E_{1\to 2}[j; t, \Delta t]$ is:

$$p_{1\to 2}[j; t, \Delta t] = \frac{n_1(t)}{N} \cdot P_{pass} \cdot \sum_{\substack{v\in[0,+\infty] \\ \theta\in[0,2\pi]}} \left(p\left[V_{jx} \in [v_x, v_x+\Delta v_x)\right] \cdot p[v_x > 0] \cdot \frac{h \cdot v_x \cdot \Delta t}{L^2} \right) \quad (6)$$

Since:

$\Delta v_x \wedge \Delta v_y = (\Delta v \cos\theta - v\Delta\theta \sin\theta) \wedge (\Delta v \sin\theta + v\Delta\theta \cos\theta) = v\Delta v \wedge \Delta\theta$

From 3 and 6 it is obtained:

$$p_{1\to 2}\left[j;t,\Delta t\right]=\frac{n_1(t)}{N}\cdot P_{pass}\cdot \iint\limits_{C\left[0,v_{\max}\right]}\left(p\left[V_{jx}\in\left[v_x,v_x+\Delta v_x\right)\right]\cdot p\left[v_x>0\right]\cdot\frac{h\cdot v_x\cdot\Delta t}{L^2}\right)=$$

$$=\frac{n_1(t)}{N}\cdot P_{pass}\cdot\int\limits_{v_x=0}^{v_x=+\infty}\int\limits_{v_y=-\infty}^{v_y=+\infty}\frac{\beta m}{2\pi}e^{-\beta\frac{mv^2}{2}}\Delta v_x\wedge\Delta v_y\frac{hv_x\Delta t}{L^2}=\Delta t\frac{n_1(t)}{N}P_{pass}\frac{\beta mh}{2\pi L^2}\int\limits_{v_x=0}^{v_x=+\infty}\int\limits_{v_y=-\infty}^{v_y=+\infty}e^{-\beta\frac{mv^2}{2}}v_x\Delta v_x\wedge\Delta v_y=$$

$$=\Delta t\frac{n_1(t)}{N}P_{pass}\frac{\beta mh}{2\pi L^2}\left(\int\limits_{v_x=0}^{v_x=+\infty}e^{-\beta\frac{mv_x^2}{2}}v_x dv_x\right)\left(\int\limits_{v_y=-\infty}^{v_y=+\infty}e^{-\beta\frac{mv_y^2}{2}}dv_x\right)=$$

$$=\Delta t\frac{n_1(t)}{N}P_{pass}\frac{\beta mh}{2\pi L^2}\frac{1}{\beta m}\sqrt{\frac{2\pi}{\beta m}}=\Delta t\frac{n_1(t)}{N}P_{pass}\frac{h}{L^2}\left(2\pi m\beta\right)^{-1/2}$$

The total number of particles passing through the gap, from D1 to D2, over the time interval $\left[t,t+\Delta t\right)$ is:

$$\Delta n_{1\to 2}(t)=\sum_{j=1}^{N}p_{1\to 2}\left[j;t,\Delta t\right]=\Delta t\, n_1(t)P_{pass}\frac{h}{L^2}\left(2\pi m\beta\right)^{-1/2}$$

Similarly: the total number of particles passing through the gap, from D2 to D1, over the time interval $\left[t,t+\Delta t\right)$ is:

$$\Delta n_{2\to 1}(t)=\sum_{j=1}^{N}p_{2\to 1}\left[j;t,\Delta t\right]=\Delta t\, n_2(t)P_{pass}\frac{h}{L^2}\left(2\pi m\beta\right)^{-1/2}$$

It is concluded that the variation of the particles' number n_1 over $\left[t,t+\Delta t\right)$ is:

$$\Delta n_1(t)=-\Delta n_{1\to 2}(t)+\Delta n_{2\to 1}(t)=-\Delta t\frac{h}{L^2}P_{pass}\left(2\pi m\beta\right)^{-1/2}\left(n_1(t)-n_2(t)\right)\qquad(8a)$$

The variation of the particles' number n_2 over the same time interval is:

$$\Delta n_2(t)=\Delta n_{1\to 2}(t)-\Delta n_{2\to 1}(t)=\Delta t\frac{h}{L^2}P_{pass}\left(2\pi m\beta\right)^{-1/2}\left(n_1(t)-n_2(t)\right)\qquad(8b)$$

8a and b are first-order differential equations. The initial conditions that uniquely define their solutions in the context of the simulation are:

$$n_1(0)=N,\ n_2(0)=0\qquad(8c)$$

By solving equations 8a and 8b, it is found that:

$$n_1=\frac{N}{2}\left(1+e^{-\lambda t}\right),\ n_2=\frac{N}{2}\left(1-e^{-\lambda t}\right)\qquad(9a)$$

$$\lambda=P_{pass}\frac{2h}{L^2}\left(2\pi m\beta\right)^{-1/2}=P_{pass}\frac{2h}{L^2}\sqrt{\frac{\langle E\rangle}{2\pi m}}\qquad(9b)$$

The system approaches the equilibrium state asymptotically:

$$\lim_{t\to+\infty}\left(n_1\right)=\lim_{t\to+\infty}\left(n_2\right)=\frac{N}{2}$$

The time constant is:

$$\tau=\frac{1}{\lambda}=\frac{L^2}{hP_{pass}}\sqrt{\frac{\pi m}{2\langle E\rangle}}\qquad(10)$$

Remark: The particles of the virtual gas are discs of a radius of *r*. Therefore, a particle will pass through the gap, if at time *t* the y-position of its center is in the interval: $\left(\frac{L-h}{2}+r,\frac{L+h}{2}-r\right)$

Hence, the actual length of the gap is *h-2r*. Relation 10 is modified to the following:

$$\tau=\frac{1}{\lambda}=\frac{L^2}{P_{pass}\left(h-2r\right)}\sqrt{\frac{\pi m}{2\langle E\rangle}}\qquad(10a)$$

How do particles interact?

At time *t*=0 all *N* particles of the virtual gas are in compartment D1. The interactions of particles with the walls of the container are elastic collisions. The particles interact with each other in pairs.

The directions and the magnitudes of the velocities immediately after each interaction, satisfy the conservation laws of the linear momentum and energy of the pair. They are completely determined by an additional random parameter: the angle θ formed by the velocities after, with the velocities before the interaction, in the pair's center-of-mass reference frame (Figure 3). The value of θ is independent of the velocity directions before the p-p interaction (the successive p-p interactions form Markov processes).
Between two successive interactions, each particle moves at a constant velocity. The time that each interaction lasts is negligible to the time-lap between any two successive interactions.

Suppose that at a time moment *t*, the j-particle interacts with the k-particle. Symbolize $\vec{r}_j, \vec{v}_j, \vec{r}_k, \vec{v}_k$ the corresponding positions and velocities of these particles in the Oxy inertial system of the container (Figure 2).
The moment *t* of the interaction is determined by the simultaneous conditions:

$$\left|\vec{r}_j - \vec{r}_k\right| < s \cdot r$$

(the centers of the two particles are less than $s \cdot r$ - parameter *s* is determined in the program of the simulation)

$$\frac{d}{dt}\left[\left(\vec{r}_j - \vec{r}_k\right)\left(\vec{r}_j - \vec{r}_k\right)\right] < 0$$

Or:

$$\left(\vec{v}_j - \vec{v}_k\right) \cdot \left(\vec{r}_j - \vec{r}_k\right) < 0$$

(the two particles are moving so that in the infinitesimal time interval $[t, t + \Delta t)$ the distance of their centers is decreasing)

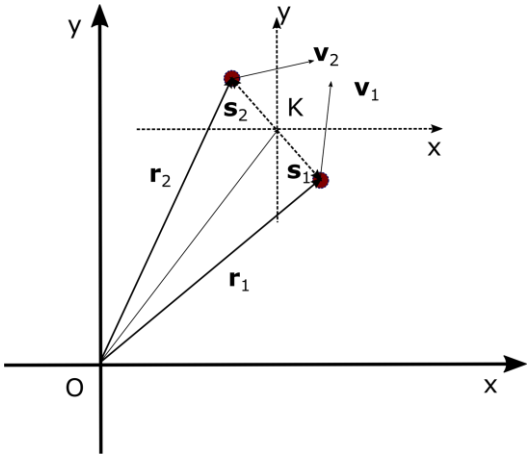

Figure 2

Let $K_{jk} \equiv K$ be the center of mass of the j and k-particles at the time *t* of their interaction. In the following steps, it is obtained:
a) A relation of the particles' velocities in two inertial reference frames: The Oxy and the center-of-mass frame Kxy.
b) A derivation of the particles' velocities after their interaction, in the Kxy reference frame.
c) A derivation of the particles' velocities after their interaction, in the Oxy reference frame.

(a) The particles have equal masses (m=1mass-unit), therefore:

$$\overrightarrow{OK} = \frac{1}{2}\left(\vec{r}_j + \vec{r}_k\right), \vec{V}_K = \frac{1}{2}\left(\vec{v}_j + \vec{v}_k\right) \qquad (11a)$$

$\vec{V}_K$ is the center of mass velocity in the Oxy-frame (Figure 2)
It is true that:

$$\vec{s}_j = \vec{r}_j - \overrightarrow{OK} = \frac{1}{2}\left(\vec{r}_j - \vec{r}_k\right)$$
$$\vec{s}_k = \vec{r}_k - \overrightarrow{OK} = \frac{1}{2}\left(\vec{r}_k - \vec{r}_j\right) = -\vec{s}_j \qquad (11b)$$

$$\vec{u}_j = \frac{1}{2}\left(\vec{v}_j - \vec{v}_k\right)$$
$$\vec{u}_k = \frac{1}{2}\left(\vec{v}_k - \vec{v}_j\right) = -\vec{u}_j \qquad (11c)$$

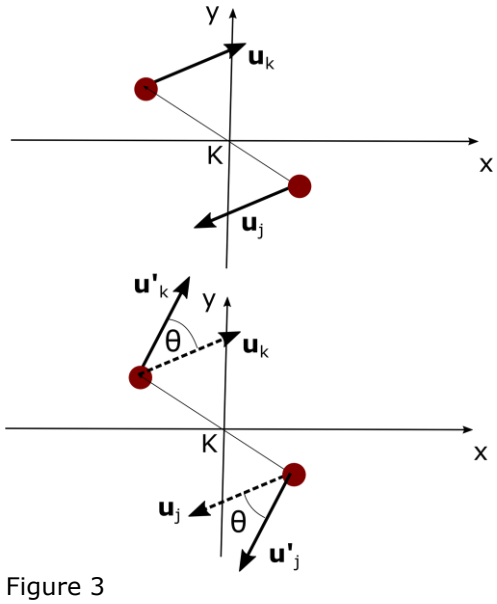

Figure 3

$\vec{u}_j$, $\vec{u}_k$ are the j and k-particle velocities in the Kxy-frame (Figure 2).

$$\vec{r}_j = \vec{s}_j + \overrightarrow{OK}$$
$$\vec{r}_k = \vec{s}_k + \overrightarrow{OK} \quad (12a)$$
$$\vec{v}_j = \vec{u}_j + \vec{V}_K$$
$$\vec{v}_k = \vec{u}_k + \vec{V}_K \quad (12b)$$

(b) Let $\vec{u}'_j$, $\vec{u}'_k$ be the j and k-particles velocities just after their interaction, in their center-of-mass reference frame Kxy. They are derived by applying the linear momentum and energy conservation laws (Figure 3):

$$\vec{u}'_j + \vec{u}'_k = \vec{u}_j + \vec{u}_k = 0 \quad (13a)$$

$$u'^2_j + u'^2_k = u_j{}^2 + u_k{}^2 \quad (13b)$$

From 13a and b, it is implied that:

$$u'^2_j = u'^2_k = u_j{}^2 = u_k{}^2 \quad (13c)$$

The velocities $\vec{u}'_j$, $\vec{u}'_k$ in Kxy-frame have the same magnitudes as the velocities $\vec{u}_j$, $\vec{u}_k$ just before the interaction, and their directions are opposite to each other. However, in general, the axis that is determined by $\vec{u}'_j$, $\vec{u}'_k$ forms an arbitrary angle θ with the axis of $\vec{u}_j$, $\vec{u}_k$ (Figure 3). The angle θ is determined in the program of the simulation, by the JavaScript random variables method, in the interval $[0, 2\pi)$. In Kxy-frame, the coordinates of the velocities $\vec{u}'_j$, $\vec{u}'_k$ are calculated by the equations:

$$\begin{pmatrix} u'_{jx} \\ u'_{jy} \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} u_{jx} \\ u_{jy} \end{pmatrix} = \begin{pmatrix} u_{jx}\cos\theta + u_{jy}\sin\theta \\ -u_{jx}\sin\theta + u_{jy}\sin\theta \end{pmatrix} \quad (14a)$$

$$\begin{pmatrix} u'_{kx} \\ u'_{ky} \end{pmatrix} = -\begin{pmatrix} u'_{jx} \\ u'_{jy} \end{pmatrix} \quad (14b)$$

(c) The coordinates of the j and k-particle's velocities, just after the interaction, in the Oxy-frame shall be calculated by 11e and 14a, b:

$$\vec{v}'_j = \vec{u}'_j + \vec{V}_K \text{ , } \vec{v}'_k = \vec{u}'_k + \vec{V}_K \quad (15)$$

Characteristics of the simulation

At time t=0 all N particles of the virtual gas are confined in chamber D1 of the container. The energy level of the system can be selected by the user. The particles' positions, the directions, and the magnitudes of the particles' velocities are random. The velocity magnitudes are random numbers produced by the JavaScript random number method in the interval $[0, v_{in.})$, where $v_{in.}$ is related to the chosen mean energy level E. The initial velocity distribution of the virtual gas, although is not identical to the M-B distribution, is very "near" to it [(1)]. Extremely fast, the virtual gas converges to the M-B velocity distribution [(1,2,3)], according to the Boltzmann's H-theorem.

The gap is initially closed by a barrier. The program imposes a delay of 2 time-units for the barrier to be removed after the user starts the simulation. Aiming at a better perception of the formation of the particles' trajectories under the successive p-p interactions, one specific particle, and its path has been colored red.

The user controls three parameters: the energy level of the gas, the length h of the gap, and the probability P_{pass} of passing a particle from D1 to D2 or back, if all the other conditions for that, predicted by the theoretical model, are satisfied. P_{pass} is a phenomenological parameter taking values in the interval $(0,1]$ used to obtain the best agreement of the theoretical graphs with the experimental.

In the energy graphs window, it is depicted the actual gas's energy in each chamber and the total gas's energy, in a sequence of time moments (they are measured in real-time by the program).

In addition, at each moment of this time-sequence the program counts in real-time the actual number of particles in each chamber and draws the corresponding experimental graphs (reddish curves, in the number-of-particles window). In the same window, the theoretical graphs are also depicted for the chosen by the user parameters (bluish curves).

The user is prompted to adjust the value of the parameter P_{pass}, so that to succeed the best agreement of the theoretical graph with the experimental.

Remark: A change of P_{pass} implies a change of time constant only; it does not affect the other characteristics of the theoretically derived functions $n_1(t)$, $n_2(t)$ (relations 9a, 10a).

The user compares the theoretical predictions with the actual particles' number over time in each compartment and evaluates both the theoretical model and the virtual environment.

Activities

In the virtual environment of the simulation, the mass of each particle is m=1mass-units, the length of each container wall is L=20length-units, the radius of each particle is r=0.12length-units.

1. Run the simulation for different values of the parameters E and h. Choose the value of P_{pass} to obtain the best agreement of the theoretical graphs with the experimental. What are the causes for any observed discrepancies between theoretical and experimental graphs? Please indicate at least two.

2. Keep the length *h of the* gap constant and for three different values of the mean energy E, run the simulation.
    a. In each case, select and write down the optimum value of P_{pass} to have the best agreement of the theoretical graphs with the experimental. Write down the time constant of the system. How much time is needed to reach the system the equilibrium state?
    b. Compare the time constants to each other. Explain.
    c. Compare the values of P_{pass} you selected in each case. Formulate an empirical rule.

3. For a certain energy level and three different values of the length h of the gap run the simulation.
    a. In each case, select and write down the optimum value of P_{pass} to have the best agreement of the theoretical graphs with the experimental. Write down the time constant of the system. How much time is needed to reach the system the equilibrium state?
    b. Compare the time constants to each other. Explain the result of the comparison.
    c. Compare the values of P_{pass} you selected in each case. Formulate an empirical rule.

References

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k_pm