Osmosis in a 2D gas solution
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Synopsis
In this applet, the osmosis effect (see references 1 and 2) is described and simulated for the case of a 2D gas solution. In an orthogonal container divided into two chambers D1 and D2 with a semi-permeable barrier, N disk-like particles are moving. The particles are discriminated into two classes: The "red" particles which cannot pass through the barrier and they are always trapped in chamber D1 and the "blue" particles which can pass through the barrier and move everywhere in the container. The number of "red" particles is $n_r = N/3$ and that of the "blues" is $n_b = 2N/3$. The particles interact with the walls of the container by elastic collisions. The particles interact with each other by pairs (p-p interaction). In the p-p interactions, the linear momentum and the energy of the pair are conserved; the directions of the velocities just after any p-p interaction are random and independent of their directions just before the interaction (see paragraph: "The particles' interactions"). The system is isolated. At time $t=0$, the mean energy of the particles is everywhere the same; there are equal numbers of particles in D1 an D2: $N/3$ "reds" and $N/6$ "blues" in D1 and N/2 "blues" in D2. Hence the pressure of the gas in each chamber is the same. But, because of the inability of the red particles to pass through the barrier, the number of particles in D1 gradually increases, and that of the particles in D2 decreases. As a result, the pressure in D1 increases with time, and the pressure in D2 decreases by the same amount. This process continues until the system reaches in a state of **dynamical equilibrium**, achieved when the number of "blue" particles is the same in both chambers. In the state of dynamical equilibrium, the total numbers of particles in each chamber are different. This implies that the final pressure in D1 is different than the pressure in D2; their difference is defined as the **osmotic pressure** of the system.

The program of the simulation counts the **actual** number of particles in each chamber, at a specific sequence of time moments, and calculates the corresponding pressures. These values which are been obtaining in real-time, consist of the experimental data concerning the evolution of the 2D gas in the container. In parallel, for every time-step of the simulation, the program calculates the theoretical values of the particles' numbers and the pressures in D1 and D2 derived by the theoretical model, and the corresponding graphs are composed. The theoretical graphs and the experimental points are plotted on the same system of axes so that the user can check the agreement of the theoretical predictions with the experimental data.

Finally, the user is prompted to carry out a set of recommended activities.

Objectives of the application
1. The user is getting acquainted with a theoretical model, aiming at the description of the osmosis effect, for the case of a 2D gas solution. He makes predictions concerning the evolution of the system and confirms or disconfirms them in the virtual environment of the simulation.
2. The user compares the theoretical predictions derived by the model, with the experimental data obtained in real-time by the evolution of the virtual gas. He can evaluate the reliability of the model and the technical details of the virtual environment.

Key concepts and relations
2D gas – Semipermeable barrier – Elastic collisions – p-p interactions – Linear momentum and energy conservation in the p-p interactions – Random variable – Distribution density function of a random variable – Distribution function of a random variable – Forces exerted by the particles on the walls of the container – Pressure of the 2D gas – Mean energy of the particles – Thermodynamic equilibrium – Maxwell-Boltzmann distribution – Boltzmann H-theorem – Variation of the particles' number in the chambers of the container with time – Dynamical equilibrium – Gas pressure in each chamber in the equilibrium state – Osmotic pressure

Description of the device and the theoretical model

An orthogonal plane container of width $2L$ and height L is divided into two equal chambers D1 (the left one) and D2 (the right one) by a barrier B, as shown in figure 1. In the container, there are N disk-like particles, each of mass m and radius r. The particles are discriminated into two classes: The "red" particles which cannot pass through the barrier and they are always trapped in chamber D1 and the "blue" particles which can pass through the barrier and move everywhere in the container. The total number of the "red" particles is $n_r = N/3$ and that of the "blue" ones is $n_b = 2N/3$. The container is thermally isolated, and its walls are rigid.
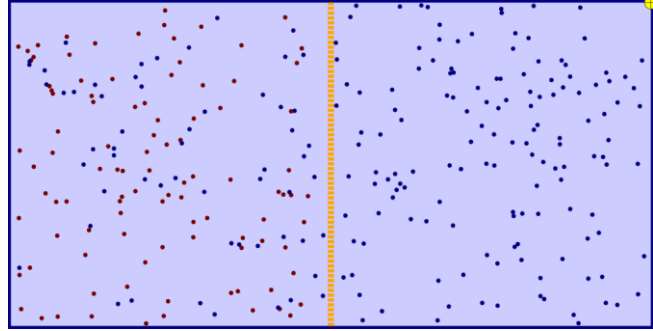
At time $t{=}0$, there are $n_{b1} = N/6$ "blue" particles in D1 and $n_{b2} = N/2$ in D2. Hence in each chamber, there is the same number of particles: $n_{1r} + n_{1b} = \frac{N}{3} + \frac{N}{6} = \frac{N}{2}$ in D1, and $n_{2b} = \frac{N}{2}$ in D2. According to equations 7a and 7b (see paragraph: "*Variation of the pressure in each chamber with time according*

Figure 1

to the theoretical model"), the pressure of the gas in each chamber at any time t, is proportional to the number of particles contained in it; hence, in the initial state, the pressures in D1 and D2 are equal.

The initial positions of the particles are random: the probability distributions of the X and Y particles' positions are uniform (see reference 3); they are calculated by the program of the simulation, using the random method of JavaScript. Given that the energy and linear-momentum conservation equations in the p-p interactions are independent of the particles' positions, the chaotic character of the particles' positions is maintained with time.
The directions of the velocities in the initial state are random. The velocity magnitudes are random, taking values at certain intervals determined in the program, in accord to the energy level chosen by the user. This distribution is very "near" to the Maxwell-Boltzmann one (see Appendix). Nevertheless, according to the Boltzmann H-theorem, because of the p-p interactions the velocity magnitude distribution converges fast-enough to the M-B distribution (see references 2 and 3).

The particles' interactions
The particles interact with the walls and the barrier (the "reds" only) via elastic collisions.
In every p-p interaction, the linear momentum and the total kinetic energy of the interacting particles are conserved. The direction of the velocities just after every interaction is random, independent of the velocity directions just before the interaction. Between two successive interactions, each particle moves with constant velocity. Finally, the duration of any interaction is negligible, compared with the time between two successive interactions of any particle in the system.

Now, we shall relate the velocities of the interacting particles just before and just after their interaction.
Consider that at time t, the j-particle interacts with the k-particle. Let us symbolize $\vec{r}_j, \vec{v}_j, \vec{r}_k, \vec{v}_k$ the positions and the velocities of the particles just before their interaction, in the inertial reference frame Oxy, fixed to the container (figure 2).
In the simulation, the interaction moment t of the two particles is determined by the following two conditions:
a) $\left| \vec{r}_j - \vec{r}_k \right| < s \cdot r$ (The parameter s is determined in the program)
b) $\frac{d}{dt}\left[(\vec{r}_j - \vec{r}_k)(\vec{r}_j - \vec{r}_k) \right] < 0$ or: $(\vec{v}_j - \vec{v}_k) \cdot (\vec{r}_j - \vec{r}_k) < 0$

Figure 2

(The two particles are moving so that, in the infinitesimal time interval $[t, t + \Delta t)$ their centers-distance decreases)
Symbolize $K_{jk} \equiv K$ the **center of mass** of the j and k-particles at the interaction moment t and Kxy, their center-of-mass inertial reference frame (figure 2).
We implement the following steps:
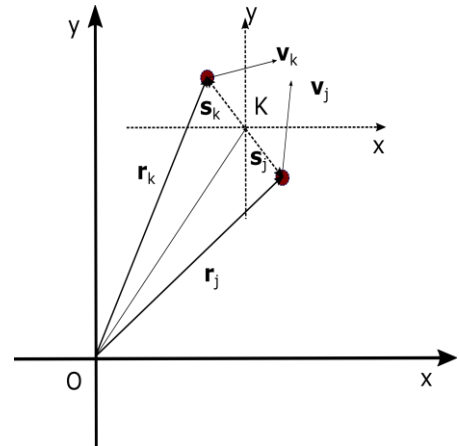1) Find the relations of the j and k-particle velocities in the frames Oxy and Kxy.

2) Calculate the velocities just after the interaction in the center of mass frame Kxy.
3) Calculate the velocities just after the interaction in the frame Oxy.

1) The particles have equal masses. Hence:
$$\overrightarrow{OK} = \tfrac{1}{2}(\vec{r}_j + \vec{r}_k), \vec{V}_K = \tfrac{1}{2}(\vec{v}_j + \vec{v}_k) \tag{1a}$$
$\vec{V}_K$ is the center of mass velocity in Oxy. The velocities of the j and k-particle, in the Kxy system, are symbolized: $\vec{u}_j, \vec{u}_k$

According to figures 2 and 3, the following relations are true:
$$\vec{s}_j = \vec{r}_j - \overrightarrow{OK} = \tfrac{1}{2}(\vec{r}_j - \vec{r}_k), \vec{s}_k = \tfrac{1}{2}(\vec{r}_k - \vec{r}_j) = -\vec{s}_j \tag{1b}$$
$$\vec{u}_j = \tfrac{1}{2}(\vec{v}_j - \vec{v}_k), \ \vec{u}_k = \tfrac{1}{2}(\vec{v}_k - \vec{v}_j) = -\vec{u}_j \tag{1c}$$
$$\vec{r}_j = \vec{s}_j + \overrightarrow{OK}, \ \vec{r}_k = \vec{s}_k + \overrightarrow{OK} \tag{1d}$$
$$\vec{v}_j = \vec{u}_j + \vec{V}_K, \ \vec{v}_k = \vec{u}_k + \vec{V}_K \tag{1e}$$

2) Just after the interaction of the j and k-particle, their velocities $\vec{u}'_j, \vec{u}'_k$ in the Kxy frame are calculated from the linear momentum and energy conservation (figure 3):
$$\vec{u}'_j + \vec{u}'_k = \vec{u}_j + \vec{u}_k = 0 \tag{2a}$$
$$u'^2_j + u'^2_k = u_j^2 + u_k^2 \tag{2b}$$

Equations 2a and 2b imply that:
$$u'^2_j = u'^2_k = u_j^2 = u_k^2 \tag{2c}$$

We infer that $\vec{u}'_j, \vec{u}'_k$ have mutually opposite directions and equal magnitudes. Their magnitude is the same as the common velocity magnitude of j and k-particle just before their interaction (relation 2c). But in general, the axis defined by $\vec{u}'_j, \vec{u}'_k$ is different from the axis defined by the velocities just before the interaction (figure 3). The directions of $\vec{u}'_j, \vec{u}'_k$ are determined by a rotation angle θ formed with $\vec{u}_j, \vec{u}_k$ respectively (figure 3).

In the present model, the value of theta (θ) is random; it is determined by the JavaScript random values method.

According to figure 3, the x and y-components of $\vec{u}'_j, \vec{u}'_k$ in the Kxy frame, are calculated as a function of the x and y-components of the velocities $\vec{u}_j, \vec{u}_k$ and the angle θ, by the equations:
$$\begin{pmatrix} u'_{jx} \\ u'_{jy} \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} u_{jx} \\ u_{jy} \end{pmatrix} = \begin{pmatrix} u_{jx}\cos\theta + u_{jy}\sin\theta \\ -u_{jx}\sin\theta + u_{jy}\sin\theta \end{pmatrix} \tag{3a}$$
$$\begin{pmatrix} u'_{kx} \\ u'_{ky} \end{pmatrix} = -\begin{pmatrix} u'_{jx} \\ u'_{jy} \end{pmatrix} \tag{3b}$$

3) The velocities $\vec{v}'_j, \vec{v}'_k$ of the j and k-particle just after their interaction, in the Oxy reference frame are calculated by equations 1e, 3a, and 3b:
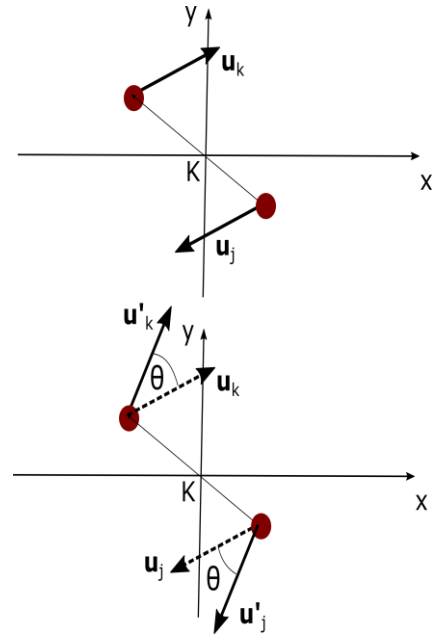$$\vec{v}'_j = \vec{u}'_j + \vec{V}_K, \vec{v}'_k = \vec{u}'_k + \vec{V}_K \tag{4}$$

Figure 3

Some more features of the model and the virtual environment of the simulation

A) In the simulation program, the value of the parameter s has been chosen so that the gas, because of the p-p interactions, gets fast enough the M-B velocity distribution (Boltzmann H-theorem, see reference2 and 3) and then, stays at this state. It is a particularly good approximation to assume that at any time, the temperature of the gas is constant and equal to the inverse of the particles' mean energy (see references 2 and 3).

B) At any time, the gas pressure in each chamber is calculated by the mean force exerted by the particles on some rigid wall of the chamber, divided by the length of the corresponding wall. According to equations 7a and 7b of the next paragraph, at $t=0$ the pressures in D1 and D2 are equal: for $t = 0: P_1 = P_2$

C) Nevertheless, just after the user starts the simulation, the "blue" particles' number is greater in D2 than in D1. Hence the flow of "blue" particles from D2 to D1 is greater than in the opposite direction. The result of this situation is that the number of "blue" particles increases in D1 with time, and decreases by the same amount in D2. Consequently, the pressure in D1 increases, and in D2 decreases. The system converges to a steady-state when the number of "blue" particles in D1 and D2 reaches the same value. When the system obtains this state of dynamical equilibrium, the flow of "blue" particles is the same to both directions; the mean number of particles and the pressure in each chamber do not change with time. At the equilibrium state, the total

number of particles in D1 is different from the one in D2. Hence, the pressure in D1 is different from the pressure in D2. In the context of the present model, the difference of the gas pressure in chambers D1 and D2, at the equilibrium state, is called "**osmotic pressure**": $\Delta P = P_1 - P_2$.

D) In the virtual environment of the simulation, the user can watch the motion of the particles, their interactions, and the function of the semi-permeable barrier. In the graph-window, the user can watch the variation of the actual gas pressure in both chambers, in real-time: the program measures both pressures in a sequence of time moments (red, zigzagged lines). In the same window, the corresponding theoretical graphs are drawn, in real-time again, according to the prediction of the model (blue, continuous lines). So, the user can compare the theoretical predictions with the experimental data and evaluate the whole application. The calculation of the osmotic pressure is accomplished from the graphs when the system has approached the state of equilibrium.

Variation of the "blue" particles' number in each chamber with time according to the theoretical model
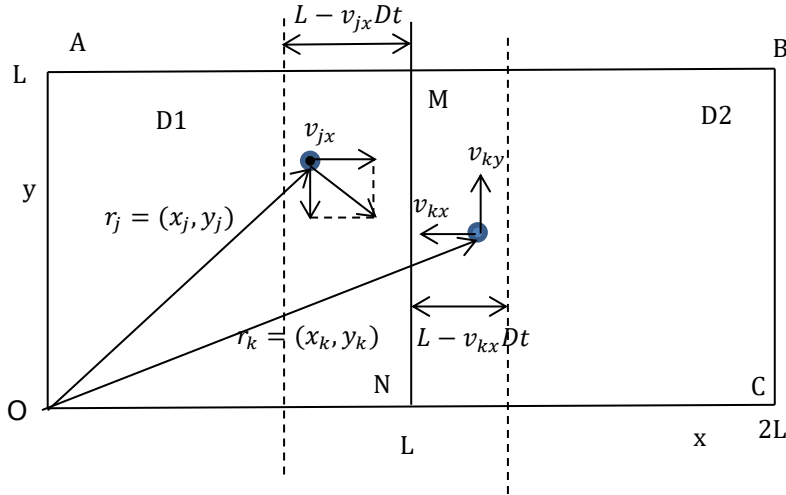

Figure 4

Symbolize $n_{b1}(t), n_{b2}(t)$ the number of "blue" particles at time t, in chambers D1 and D2, respectively. Let $\Delta n_{b1\to2}$ be the number of the "blues" that in the time interval $[t, t + Dt), Dt \to 0$ move from D1 into D2 and $\Delta n_{b2\to1}$ the number of "blues" that move from D2 into D1, in the same interval. According to the present model and with the help of figure 4, the following equations describe the variation of the particles' number with time:

$$\Delta n_{b1\to2} = Dt \sum_{j=0}^{n_{b1}-1} P\left[\left(L > x_j > L - |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} > 0\right)\right] \tag{5a}$$

$$\Delta n_{b2\to1} = Dt \sum_{j=0}^{n_{b2}-1} P\left[\left(L < x_j < L + |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} < 0\right)\right] \tag{5b}$$

With $P\left[\left(L < x_j < L + |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} < 0\right)\right]$ is symbolized the probability of the composite fact: "At time t, the x-position of the "blue" j-particle is between L and $L + |v_{jx}|Dt$ and its x-velocity is negative". Similarly, $P\left[\left(L > x_j > L - |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} < 0\right)\right]$ is the probability of the composite fact: "At time t, the x-position of the "blue" j-particle is between $L - |v_{jx}|Dt$ and L, and the value of x-velocity is positive".

The individual facts: "At time t, the x-position of the "blue" j-particle is between $L - |v_{jx}|Dt$ and L", and: " At time t, the x-velocity of the "blue" j-particle is positive", are mutually independent and time-independent. Hence, given that the position distribution of the particles is uniform, we write:

$$P\left[\left(L > x_j > L - |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} > 0\right)\right] = P\left[L > x_j > L - |v_{jx}|Dt\right] \cdot P\left[v_{jx} > 0\right] = \frac{|v_{jx}|Dt}{L} \cdot \frac{1}{2}$$

Similarly:

$$P\left[\left(L < x_j < L + |v_{jx}|Dt\right) \text{ AND } \left(v_{jx} < 0\right)\right] = P\left[L < x_j < L + |v_{jx}|Dt\right] \cdot P\left[v_{jx} < 0\right] = \frac{|v_{jx}|Dt}{L} \cdot \frac{1}{2}$$

The flow of the "blue" particles takes place from D2 to D1 and vice-versa. Assume that:

$\Delta n_{b1 \to 2} < 0$ and $\Delta n_{b2 \to 1} > 0$

The number of "blues" is constant: $n_{b1} + n_{b2} = \frac{2N}{3}$; hence the following equation is true:

$\Delta n_{b2 \to 1} + \Delta n_{b2 \to 1} = 0$

Equations 5a and 5b are written as follows:

$$\Delta n_{b1 \to 2} = -\frac{Dt}{2L}\sum_{j=0}^{n_{b1}-1}|v_{jx}| = -n_{b1}(t)\frac{Dt}{2L}\frac{1}{n_{b1}(t)}\sum_{j=0}^{n_{1b}-1}|v_{jx}| = -Dtn_{b1}(t)\frac{\overline{|v_x|}}{2L} \qquad (5c)$$

$$\Delta n_{b2 \to 1} = Dtn_{b2}(t)\frac{\overline{|v_x|}}{2L} \qquad (5d)$$

The mean value of the x-velocities absolute-values is determined by the relations:

$\overline{|v_x|} = \frac{1}{n_{b1}}\sum_{j=0}^{n_{b1}-1}|v_{jx}| = \frac{1}{n_{b2}}\sum_{j=0}^{n_{b2}-1}|v_{jx}| = \frac{1}{N}\sum_{j=0}^{N-1}|v_{jx}|$

According to 5c and 5d, the variations of the "blues" number in each chamber, at the time interval $[t, t + Dt)$ are determined by the equations:

$$n_{b1}(t + Dt) = n_{b1}(t) + (\Delta n_{b1 \to 2} + \Delta n_{b2 \to 1}) = n_{b1}(t) + Dt\frac{\overline{|v_x|}}{2L}(-n_{b1}(t) + n_{b2}(t)) \qquad (6a)$$

Or:

$$\frac{dn_{b1}(t)}{dt} = \frac{\overline{|v_x|}}{2L}(-n_{b1}(t) + n_{b2}(t)) \qquad (6b)$$

And:

$$n_{b2}(t) = \frac{2N}{3} - n_{b1}(t) \qquad (6c)$$

Notice that because of the randomness of the velocity directions after any p-p interaction, the 2D gas does not lose its homogeneous and isotropic character with time. The mean value of a vector quantity along some direction is independent of the reference frame it is used. Hence, we can write: $\overline{|v_x|} = \overline{|v_y|}$, or even: $\overline{v_x^2} = \overline{v_y^2}$, for every time moment t.

Nevertheless, if the particles' velocity distribution is different from the Maxwell-Boltzmann (M-B), it changes with time and converges to the M-B (Boltzmann H-theorem, see references 2 and 3). *Hence, in general, the mean values of microscopic quantities depend on the velocity distribution, and consequently, on time. They are stabilized when velocity distribution becomes identical to the Maxwell-Boltzmann, i.e. when the system obtains the state of thermodynamic equilibrium (see "Appendix").*

The consequence of this fact is that $\overline{|v_x|}$ changes with time until the system reaches the state of thermodynamic equilibrium. As a result, many difficulties arise with the treatment of differential equations 6, where $\overline{|v_x|}$ appears as an unknown function of time. The theoretical value of $\overline{|v_x|}$, appearing in equations 6 is calculated in the appendix, for two cases: a) when the system has reached the M-B velocity distribution, and b) for the case of the step-function distribution.

In the simulation, at $t=0$ the system is "near" the state of thermodynamic equilibrium. The velocity magnitude of each particle is a random number in the interval $[0, v_{in.})$, where $v_{in.}$ is determined by the program for every selection of the energy level by the user. This state, although not identical to the thermodynamic equilibrium state, it is extremely near to this and moves rapidly to this. A criterion for this "nearness" is the comparison of the actual value of $\overline{|v_x|}$, corresponding to this initial state with the theoretical value of $\overline{|v_x|}$ corresponding to the M-B distribution. The user can see both values in the simulation environment for any choice of the initial energy level of the system (see also, reference 3).

Variation of the pressure in each chamber with time according to the theoretical model

Let $P_1(t)$ be the pressure of the 2D-gas in D1 at time t. The pressure is calculated by the total force perpendicular to a rigid wall of D1 -say OA in figure 4- exerted by the particles during their collision with this wall at an infinitesimal interval $[t, t + Dt)$, divided by the length of the wall.

The force exerted on the wall during the collision of one particle with it is calculated by the 2nd Newton-law. In the infinitesimal time-lap Dt, the total force on the wall OA is due to the number of particles that strike on OA in the time interval $[t, t + Dt)$:

$$f(t) = \sum_{j=0}^{n_{1b}+n_r-1}\frac{2m|v_{jx}|}{Dt}P\big[(0 < x_j < |v_{jx}|Dt)\ AND\ (v_{jx} < 0)\big] =$$

$$= \frac{2m}{Dt}\frac{1}{2}\sum_{j=0}^{n_{b1}+n_r-1}|v_{jx}|\frac{|v_{jx}|Dt}{L} = \frac{m}{L}(n_{b1} + n_r)\frac{1}{n_{b1}+n_r}\sum_{j=0}^{n_{b1}+n_r-1}|v_{jx}|^2 = \frac{m}{L}(n_{b1} + n_r)\overline{v_x^2}$$

Hence, $P_1(t)$ is calculated by the analytical expression:

$$P_1(t) = \frac{f(t)}{L} = \frac{m}{L^2}(n_{b1}(t) + n_r)\overline{v_x^2} \qquad (7a)$$

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Similarly, the pressure in D2 is given by the expression:

$$P_2(t) = \frac{m}{L^2} n_{b2}(t)\overline{v_x^2} \tag{7b}$$

The mean energy of the 2D-gas is:

$$E = \frac{1}{N}\sum_{j=0}^{N-1}\frac{1}{2}m\left(v_{jx}^2 + v_{jy}^2\right) = \frac{1}{2}m\left(\overline{v_x^2} + \overline{v_y^2}\right) = m\overline{v_x^2} = m\overline{v_y^2} \tag{8}$$

Hence, 7a and 7b can be written as follows:

$$P_1(t) = \frac{E}{L^2}\left(n_{1b}(t) + n_r\right) \tag{9a}$$

$$P_2(t) = \frac{E}{L^2}n_{2b}(t) \tag{9b}$$

Appendix: Variation of the mean values of microscopic quantities with time, when the 2D gas is not in thermodynamic equilibrium

Let $P_t[(v \leq V < v + Dv) \; AND \; (\theta \leq \Theta < \theta + D\theta)]$ be the probability of the event: "At time t, the velocity magnitude of any, specific particle of the 2D gas is in the infinitesimal interval $[v, v + Dv)$ and the angle of its velocity with the x-axis is in $[\theta, \theta + D\theta)$". Symbolize:
$Dn_t = N_t(v \leq V < v + Dv; \theta \leq \Theta < \theta + D\theta)$

the number of particles which at time t their velocity magnitudes is in the interval $[v, v + Dv)$, and the angles of their velocities with the x-axis is in $[\theta, \theta + D\theta)$. For the 2D gas, the following relations hold (see reference 3):
$P_t[(v \leq V < v + Dv) \; AND \; (\theta \leq \Theta < \theta + D\theta)] = \frac{1}{N}Dn_t = \frac{1}{2\pi}p_t(v)vDvD\theta$

The function $p_t(v)$ is called "**the velocity distribution density function**" at time t. According to the Boltzmann H-theorem, because of the p-p interactions, $p_t(v)$ converges to the M-B velocity distribution density function (reference 3):

$$\lim_{t\to+\infty} p_t(v) = \beta m e^{-\beta\frac{mv^2}{2}} = p_{MB}(v) \tag{A1}$$

Consider a microscopic quantity q which is a function of the particle velocity: $q_j = q(v_j, \theta_j)$, $j = 0,1,\dots N-1$. Its mean value at the time moment t is calculated by the equations:

$$\langle q \rangle = \frac{1}{N}\sum_{j=0}^{N-1} q(v_j, \theta_j) = \frac{1}{2\pi}\int_0^{+\infty} dv \int_0^{2\pi} d\theta v p_t(v)q(v,\theta) \tag{A2}$$

In general, $\langle q \rangle$ is changing with time until the system reaches the M-B velocity distribution:

$$\frac{d}{dt}\langle q \rangle = \frac{1}{2\pi}\int_0^{+\infty} dv \int_0^{2\pi} d\theta \; v \; \frac{\partial}{\partial t}p_t(v) \; q(v,\theta) \tag{A3}$$

The M-B distribution $p_{MB}(v)$ determines the stable state of the system and is characterized by the condition:
$\frac{\partial}{\partial t}p_{MB}(v) = 0$

Hence, if the system is at the state of thermodynamic equilibrium, it is true that $\frac{\partial}{\partial t}\langle q \rangle = 0$ for any microscopic quantity q. In the present model, there are two exceptions: The mean energy and the mean linear momentum of the system are conserved even if the system is not at the state of thermodynamic equilibrium; this is caused by the conservation of these quantities along with any p-p interaction. The following conditions are fulfilled, for any time moment t:

$$\frac{d}{dt}\langle E \rangle = \frac{1}{N}\frac{d}{dt}\sum_{j=0}^{N-1}\frac{1}{2}mv_j^2 = \frac{1}{2\pi}\int_0^{+\infty} dv \int_0^{2\pi} d\theta v \frac{\partial p_t(v)}{\partial t}\frac{1}{2}mv^2 = 0 \tag{A4}$$

$$\frac{d}{dt}\langle mv_x \rangle = \frac{1}{N}\frac{d}{dt}\sum_{j=0}^{N-1}\frac{1}{2}mv_{jx} = \frac{1}{2\pi}\int_0^{+\infty} dv \int_0^{2\pi} d\theta v \frac{\partial p_t(v)}{\partial t}\frac{1}{2}mv_x = 0 \tag{A5}$$

$$\frac{d}{dt}\langle mv_y \rangle = \frac{1}{N}\frac{d}{dt}\sum_{j=0}^{N-1}\frac{1}{2}mv_{jy} = \frac{1}{2\pi}\int_0^{+\infty} dv \int_0^{2\pi} d\theta v \frac{\partial p_t(v)}{\partial t}\frac{1}{2}mv_y = 0 \tag{A6}$$

Application for the cases of the step-function distribution and the M-B distribution
Assume that the initial velocity distribution density function of the 2D gas is a delta function:
$p_{t=0}(v) = A\delta(v - v_{in.})$
The constant A is calculated by the condition:
$\frac{1}{2\pi}\int_0^{2\pi}\int_0^{+\infty} A\delta(v - v_{in.})vDvD\theta = 1$

It is implied that $A = \frac{1}{v_{in.}}$ and: $p_{t=0}(v) = \frac{1}{v_{in.}}\delta(v - v_{in.})$

The corresponding velocity distribution function is a step-function:

$$P_{t=0}(v) = P[0 \leq V < v] = \frac{1}{2\pi}\int_{u=0}^{v}\int_{\theta=0}^{2\pi}\frac{1}{N}Dn_{t=0} =$$

$$= \frac{1}{2\pi}\int_{u=0}^{v}\int_{\theta=0}^{2\pi}p_{t=0}(u)ududu\theta = \frac{1}{v_{in.}}\int_{0}^{v}u\delta(u-v_{in.})du =$$

$$= \begin{cases} 0 \text{ if } v < v_{in.} \\ 1 \text{ if } v \geq v_{in.} \end{cases}$$

That is, the velocity magnitude for every particle at $t=0$ equals to $v_{in.}$.

The mean energy of the system, calculated in the state corresponding to the step-function velocity distribution is:

$$\langle E \rangle = \frac{1}{N}\sum_{j=0}^{N-1}\frac{1}{2}mv_{in.}^{2} = \frac{1}{2}mv_{in.}^{2}$$

Or:

$$\langle E \rangle = \frac{1}{2\pi}\int_{0}^{+\infty}dv\int_{0}^{2\pi}d\theta v\frac{1}{v_{in.}}\delta(v-v_{in.})\frac{1}{2}mv^{2} = \frac{1}{2}mv_{in.}^{2} \qquad (A7a)$$

When the system reaches the state of thermodynamic equilibrium, the velocity distribution density function is given by A1. The mean energy is calculated by A2:

$$\langle E \rangle = \frac{1}{2\pi}\int_{0}^{+\infty}dv\int_{0}^{2\pi}d\theta vm\beta e^{-\beta\frac{1}{2}mv^{2}}\frac{1}{2}mv^{2}$$

One can find that:

$$\langle E \rangle = \frac{1}{\beta} \qquad (A7b)$$

From A7a, A7b, and the energy conservation theorem, it is obtained that:

$$\frac{1}{\beta} = \frac{1}{2}mv_{in.}^{2} \qquad (A8)$$

The mean absolute value of the x-velocity, contrary to the energy, is not conserved during the system evolved from its initial state up to the state of thermodynamic equilibrium.

In the initial state (corresponding to the step-function velocity distribution):

$$\overline{|v_x|}_{in.} = \frac{2}{2\pi}\int_{0}^{+\infty}dv\int_{-\pi/2}^{\pi/2}d\theta v\frac{1}{v_{in.}}\delta(v-v_{in.})v\cos\theta = \frac{2}{\pi}v_{in.} = \frac{2\sqrt{2}}{\pi}\sqrt{\frac{\langle E \rangle}{m}} \qquad (A9)$$

In the state of thermodynamic equilibrium:

$$\overline{|v_x|}_{MB} = \frac{2}{2\pi}\int_{0}^{+\infty}dv\int_{-\pi/2}^{\pi/2}d\theta vm\beta e^{-\beta\frac{1}{2}mv^{2}}v\cos\theta = \sqrt{\frac{2}{\beta m\pi}} = \sqrt{\frac{2}{\pi}}\sqrt{\frac{\langle E \rangle}{m}} \qquad (A10)$$

Activities

It is given that $N = 300, n_r = \frac{N}{3}, L = 10\,sim.\,units$

The user can choose the level of the particles' mean energy E among three alternatives: "low energy" - "mid energy" - "high energy".

A) By using the theoretical model, developed in the previous paragraphs, demonstrate that the system reaches its state of dynamical equilibrium when the numbers of the "blue" particles in both chambers are equal. In that state, show that the difference of the pressure in D1 and D2 is given by the equation:

$P_{1eq} - P_{2eq} = \frac{E}{L^2} n_r$

Confirm this relation in the virtual environment. Run the simulation successively, for every level of the mean energy E.

B) In the context of the developed theoretical model, demonstrate that the pressure in each chamber converges exponentially to the corresponding equilibrium value, with a time-constant calculated by the equation:

$\tau = \frac{\overline{|v_x|}}{L}$

Run the simulation by selecting successively all the available alternatives of the mean energy E. For every case, proceed to an estimation of the time constant value. From this, calculate the corresponding value of $\overline{|v_x|}$. Compare the result with the theoretical value of $\overline{|v_x|}$ displayed by the relative counter in the virtual environment of the application.

C) Demonstrate that the "equation of state" of the 2D-gas described in the context of the developed theoretical model, is expressed by the equation:

$PL^2 = NE$

P denotes the pressure of the gas in a plane orthogonal container of width L and height L, consisting of N particles. E is the mean energy of the particles. Notice that the system is in thermodynamic equilibrium state: the particles' velocity distribution is the Maxwell-Boltzmann one. For a 2D gas (see reference 3):

$N_{MB}(v) = N \left(1 - e^{-\beta \frac{mv^2}{2}} \right)$

The temperature T of the gas is determined by the parameter β: $\frac{1}{\beta} = k \cdot T$, k is a constant depending on the system of units. For the case of the 2D gas β is related to the mean energy E, by the relation (reference 3):

$\beta = \frac{1}{E}$

D) Which parameter the user must change in the virtual environment of the simulation, to alter the gas temperature? If he manages to increase the temperature, then answer the following questions (demonstrate your assumptions).
   a. Does the system reach the state of dynamical equilibrium in less, greater, or the same time?
   b. The absolute value of the final difference of the pressure in D1 and D2 increases, decreases, or remains unaltered?
   Check your predictions in the virtual environment of the simulation.

E) Write down your thoughts about the reliability of the model and the functionality of the virtual environment. What would you propose to get the model more reliable and the virtual environment more functional?

k_pm

References
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3) http://users.sch.gr/kostaspapamichalis/ejss_model_approachingEquilibrium_a/index.html
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