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Visualizing thermal equilibrium through a simple kinetic simulation

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Abstract

We present a simple simulation code that models, within a purely mechanical framework, the thermalization process between two ideal gases represented as kinetic billiards. The gases occupy adjacent compartments separated by a mechanically impermeable but ‘diathermic’ wall which mediates virtual exchanges of kinetic energy between particles approaching from opposite sides. The simulation shows the approach to a stationary equilibrium in which both gases attain the same average kinetic energy, thereby providing a microscopic visualization of the concept of thermal equilibrium and of the physical meaning of temperature. The model is fully mechanical, free from thermodynamic assumptions, and runs directly in the GlowScript VPython environment, making it suitable for classroom demonstrations and interactive learning activities at various educational levels.

Keywords: thermodynamics, macro-micro, v-python, zeroth law

Supplementary material for this article is available [online](#)

1. Introduction

As is well known, the notion of thermal equilibrium plays a central role in defining the concept of temperature and in formulating what is traditionally known as the Zeroth Law of Thermodynamics [1, 2]. In its classical wording, the law states that

if a system A is in thermal equilibrium with a system B, and B is in equilibrium with C, then A and C are also in equilibrium. This transitive property provides the logical basis for introducing temperature as a variable that remains constant among systems in mutual equilibrium.

In several introductory physics courses, however, the concept is presented only in verbal or macroscopic terms, without showing how the microscopic dynamics of two systems in thermal contact practically evolve toward a common equilibrium temperature. Making this microscopic link explicit can help students grasp the operational meaning of temperature and of thermal equilibrium [3, 4]: otherwise, naïve conceptions



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of thermal processes are retained and the connection of the idea of temperature with the kinetic behaviour of particles is hard to be constructed and understood [5].

In this work we present a minimal mechanical model of thermal contact between two ideal gases, implemented in GlowScript VPython. The simulation allows students to observe, at the particle level, how the average kinetic energies of the two systems converge toward equality while macroscopic quantities are displayed in real time. This provides a direct and more intuitive visualization of the thermalization process underlying the concept of temperature and, in a broader sense, also the spirit of the Zeroth Law.

The novelties of the approach lie in the micro-to-macro link explicitly embedded in the simulation and in the fact that the code—freely redistributable and modifiable—runs directly in a web browser without installation. From a physical viewpoint, this model realizes a simple yet effective diathermic-like wall interaction; moreover, it is easy to adjust physically meaningful parameters (number of particles, wall exchange efficiency, initial temperatures, etc). Finally, the approach to equilibrium is immediately visualized and there is wide flexibility to personalize the display for specific teaching aims.

2. The physical model and the code

In this simulation there are two equal compartments, each containing N identical ‘atoms’ of mass m , confined within a box. These compartments are divided by a perfectly rigid wall at the centre, preventing particle transfer: yet, it allows energy exchange by means of virtual collisions. In order to do so, the model is such that: (i) atoms move freely between collisions and interact through perfectly elastic collisions, according to the standard mechanical representation of an ideal gas; (ii) internal collisions within each compartment conserve total momentum and energy; (iii) the dividing wall is considered to be diathermic in the sense that it is modelled as a mechanism for exchanging kinetic energy between particles from opposite sides that are sufficiently close (within a distance $d_{\max}$ which can be changed by the user) to the wall and moving towards it; (iv) only the

component of velocity perpendicular to the wall, say, v_x , takes part in the exchange; (v) energy is transferred with a certain efficiency coefficient ε adjustable by the user which in this way can control the rate of thermalization. This coefficient simply tells how effective each wall contact is at exchanging energy: $\varepsilon = 0$ means no exchange, $\varepsilon = 1$ means very efficient exchange. This is the same idea as an ‘accommodation coefficient’ in more sophisticated and effective gas–surface models [6–8]. Our model is dimensionless in the present version, but physical units can be restored through appropriate scaling if desired.

A more detailed physical interpretation can be given of the parameter $d_{\max}$, which in the simulation defines the maximum distance from the wall within which particles are eligible for a virtual exchange. In practice, $d_{\max}$ represents an effective interaction thickness of the diathermic wall: the larger its value, the greater the number of particles per unit time that are eventually involved in virtual collisions, and hence the larger the microscopic flux of exchanged kinetic energy. We only consider particles within a thin layer next to the wall—often referred to as the Knudsen layer [9, 10]—in which non-equilibrium effects are confined; farther away the gas is already well mixed. In this sense, $d_{\max}$ plays a role similar to an effective cross section for wall–particle interaction. The actual amount of energy exchanged during each virtual collision is then scaled by the abovementioned efficiency parameter ε , which controls how much of the incoming kinetic energy is transmitted to the particle in the opposite compartment. The combination of these two parameters, $d_{\max}$ and ε , therefore determines the overall rate of thermalization and can be connected, in a coarse-grained sense, to the macroscopic thermal conductivity of the wall: a larger interaction region (higher $d_{\max}$) and/or a more efficient exchange (higher ε) both increase the effective conductive coupling between the two gases.

Another parameter with a direct physical meaning is the radius assigned to the atoms in the simulation. Although it is not directly relevant to the definition of temperature (which depends only on the average kinetic energy), the radius here has an important influence on the microscopic dynamics: particles with a larger radius collide more

frequently with each other and with the walls, reducing the mean free path and accelerating the redistribution of energy within each compartment. Conversely, a very small radius makes the behaviour closer to that of an ideal point-particle gas, where internal collisions are less frequent. Moreover, the radius also enters indirectly into the mechanism of exchange with the diathermic wall, since it determines the minimum effective distance an atom can approach the central plane: for the same value of $d_{\max}$, larger atoms have a greater geometric probability of being involved in a virtual collision. So, the atomic radius provides a bridge between a purely ideal model and a more realistic description in which the particle cross section plays a role in both the collision rates and the thermalization dynamics.

About the code: we choose to adopt the environment GlowScript-VPython since it offers several operational advantages: (i) it is freely accessible; (ii) it supports directly any contemporary web browser, without the need for installation or compilation; (iii) the programming syntax language is extremely similar to Python, reducing the learning curve for students who already have a basic programming experience and want to know the code functioning or even modify it; (iv) it embeds real-time 3D graphics and interactive controls at zero programming cost; (v) the apps developed and running in GlowScript are immediately shared with everyone possessing the link, as in the present work. Some performance variation of the code is expected across hardware—for example, a budget smartphone, the latest iPad, and a gaming desktop PC. Appropriate adjustments to the relevant parameters can reduce or eliminate these differences, as explained in the following brief presentation of the structure of the simulation code.

Initialization: Random non-overlapping positions are assigned to particles in each compartment. The Cartesian velocity components (v_x, v_y, v_z) are sampled independently from Gaussian distributions $N(0, \sigma^2)$ in which the variance is interpreted as the absolute temperature since $\sigma^2 = k_B T/m$. In the present dimensionless implementation $m = k_B = 1$, hence $\sigma^2 = T$. Consequently, the speed modulus automatically

will follow a Maxwell–Boltzmann distribution, $f(v) = \sqrt{2/(\pi T^3)} v^2 e^{-v^2/2T}$.

Main loop: At each time step dt , atom positions are updated, wall and boundary collisions are handled, and internal collisions within each compartment are accounted for.

Virtual diathermic exchange: As already said, this is quite a peculiar phase of the simulation. When an atom approaches close enough (within $d_{\max}$) the central wall in its motion towards it, another atom (a ‘partner’) from the opposite compartment is sampled with probability proportional to $|v_x|$. To pick a partner across the wall we weight candidates by how fast they head toward the wall (proportional to $|v_x|$). In kinetic theory this is the usual result: faster, wall-directed molecules hit a surface more often than slower, ‘wrongly’ directed ones [11]. Then, a fractional transfer of kinetic energy is performed between the partners: a portion ε of the kinetic energy difference associated with velocity in the normal direction is shifted from the higher-energy to the lower-energy particle, while the transverse components remain unchanged. This models non-elastic exchange processes whose strength are tuned by ε , whilst $d_{\max}$ sets how many opportunities occur: as already said, together, these parameters control the wall’s effective thermal conductance and drive the two gases toward a stationary regime which can be in retrospect named as thermal equilibrium. It is important to stress that the ‘partner’ particle selected on the opposite side is not a fixed counterpart of the ‘hitter’ particle. Rather, at each encounter with the wall a partner is randomly chosen among the particles in the neighbouring compartment, with a probability weighted by the magnitude of their normal velocity component $|v_x|$. This stochastic sampling ensures that particles moving faster towards the wall are more likely to take part in the exchange, while maintaining the probabilistic nature of microscopic interactions. In the meantime, elastic intra-side collisions redistribute energy in each compartment.

Graphical output: As depicted in figure 1, in the present version of the code, 3D visualization of the moving and colliding atoms in their compartments

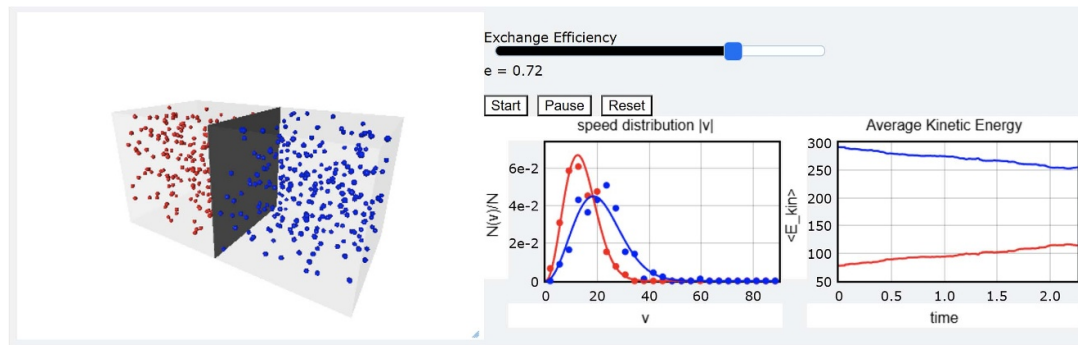


Figure 1. Snapshot of the simulation running within the GlowScript interface. The 3D view of the two compartments (left) can be rotated with the mouse or a touchscreen. The energy-exchange parameter ε can be adjusted with the slider during the run, and the simulation can be started, paused, or reset using the corresponding buttons. Speed distributions are computed and displayed in real time together with the theoretical Maxwell–Boltzmann curves, and the average kinetic energies of the two gases are plotted continuously.

is implemented. Moreover, the average kinetic energy (which is of course proportional to temperature) for each compartment is plotted in real time, so making the thermalization process evident. At the same time, also the speed modulus' of the gases are plotted along with the associated theoretical Maxwell–Boltzmann curves which necessarily have varying temperature during the simulation if the exchange coefficient is not zero. There is a slider that allows the parameter ε to be changed during the simulation, thereby reproducing a wall with varying thermal ‘conductivity’. Buttons are also provided to start, pause, and reset the simulation.

3. Connections between microscopic and macroscopic views and possible educational uses

In the simulation, the average kinetic energy per particle in each compartment is continuously computed according to the definition $\langle E_k \rangle = \frac{1}{2N} (\sum_{i=1}^N m v_i^2)$ and, in the present dimensionless implementation ($m = 1$, $k_B = 1$), the temperature is $T = \frac{2}{3} \langle E_k \rangle = \frac{1}{3} (v_{\text{RMS}})^2$ where we introduce the usual root mean square speed, $v_{\text{RMS}} = \sqrt{\langle v^2 \rangle}$. The histogram of $|v|$ is updated periodically and compared with this theoretical prediction (Maxwell–Boltzmann curve) using the instantaneous T estimated from the atom velocities.

This dual visualization—microscopic atom motion alongside macroscopic energy and

distribution plots—makes the approach to equilibrium and the convergence of the two speed distributions directly observable and easy to understand, in a purely mechanical framework.

The model here presented can be employed in a variety of teaching contexts, among which we suggest: (i) lecture demonstration, by projecting the simulation while discussing the microscopic meaning of temperature and the Zeroth Law; (ii) guided laboratory activity: in which students change initial temperatures, number of particles, and wall exchange efficiency, observe the general behaviour of atoms and record the time to equilibrium. For example, students choose initial temperatures $T_1(0)$ and $T_2(0)$ and set ε , d_{max} . They run the simulation and record the time to reach, as a possible equilibrium condition, $|T_1 - T_2|/T_{\text{av}} < 5\%$ where $T_{\text{av}} = [T_1(0) + T_2(0)]/2$ (of course 5% is just a possible criterion). By repeating with different ε values, they build a plot of equilibrium time vs wall efficiency and compare it with the expected inverse proportionality. This exercise allows a kind of hands-on exploration of Fourier’s heat law in a microscopic context; (iii) Conceptual exploration, by investigating for example the influence of wall interaction thickness d_{max} and, as already said, the weighting ε on the equilibrium dynamics: as an illustration, figures 2 and 3 show the relative differences of temperature between the two gases as a function of time for different values of ε and of d_{max} . As ε or d_{max} increase, the two temperatures meet faster.

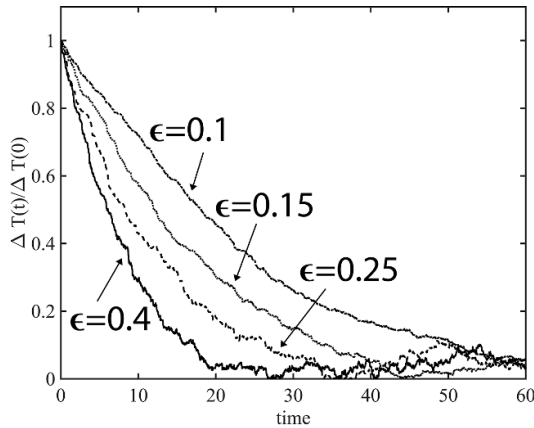


Figure 2. Relative differences of gas temperatures for some values of ε ($d_{\max} = 0.2$, $r = 0.2$, $\Delta T(0) = 220$, $N = 250$).

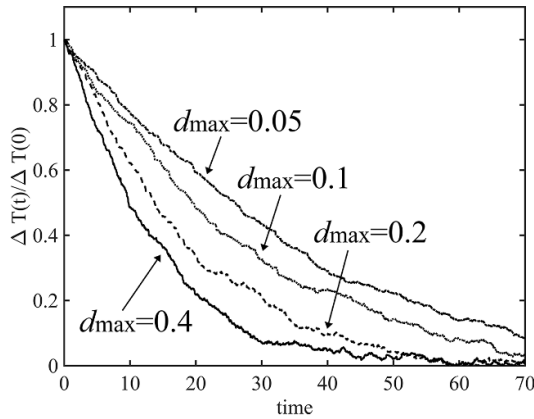


Figure 3. Relative differences of gas temperatures for some values of $d_{\max}$ ($\varepsilon = 0.15$, $r = 0.2$, $\Delta T(0) = 220$, $N = 250$).

A simple kinetic argument points the same way: stronger coupling at the wall and more ‘opportunities’ near it both raise the effective heat flow [12]; (iv) also, it is possible to further extend the experimentation by allowing for different particle masses in each compartment, varying the effective conduction mechanism of the centre wall during the simulation, including non-elastic collision to mimic energy loss and much more. When used as a classroom activity, the app plays a role similar to existing thermodynamics simulations—students can vary parameters and immediately see how microscopic interactions shape macroscopic variables [13, 14].

The simulation, as such, present both strengths and limitations. Points of favour include, as already mentioned, the direct, simultaneous view of microscopic dynamics and macroscopic trends with quite a simple implementation, accessible to instructors with minimal coding background and expertise, operating in a platform-independent and free to use environment. The used parameters are flexible in such a way that they can be tailored to various learning objectives. The visual link to the statistical mechanics concept in the form of the Maxwell-Boltzmann curve is another point in favour of this approach.

Concerning the limits of the simulation, we notice that atom number is obviously limited by computational speed in the browser: yet, with a standard laptop or an iPad, N values of the order of some hundreds are easily managed and the visualization is quite smooth. More importantly, it must be stressed that the diathermic wall model is definitely a phenomenological rendition of detailed, non-easily accessible and certainly computationally demanding microscopic interactions. Finally, units are in this version dimensionless and some extra work would be required for quantitative comparisons with real gases but we do not think that this can be seen as a major drawback (nor especially relevant in this educational context) of the simulation.

4. Conclusion and data availability statement

We have presented a minimal, interactive kinetic model that visualizes how two ideal gases reach thermal equilibrium through a purely mechanical exchange of kinetic energy. The simulation provides an intuitive connection between microscopic particle dynamics and macroscopic quantities such as average kinetic energy and temperature. Its simplicity and direct visualization make it a valuable educational tool for exploring the concept of temperature and the microscopic basis of thermal equilibrium, which in classical thermodynamics is formalized by the Zeroth Law. The code can be freely adapted, allowing instructors to design their own activities and students to explore a microscopically simulated thermalization beyond textbook descriptions. Because the

model runs directly in the GlowScript VPython environment without any installation, it can be easily used on a wide range of devices and platforms.

To execute the GlowScript code as provided, just go to <https://bit.ly/ZeroLawSim>; the simulation will start automatically. The source code may be viewed, downloaded, copied, modified and shared without any restriction. To run a modified version, sign in to the GlowScript environment (www.glowscript.org/) with a free account and upload the revised code in a directory created specifically for the purpose; then simply run the code as instructed. Further information for adjusting parameters and visualization settings are included as inline comments in the code.

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: <https://doi.org/10.5281/zenodo.17121841>.

Disclaimer

The author used the GPT-5 Chatbot by OpenAI [15] for spelling and grammar checks to ensure the clarity and readability of this manuscript. GPT-5 was also used to optimize some of the routines in the current version of the code which was manually tested across multiple devices.

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