Gradient in a Region with a Temperature Difference

QR code linking to the simulation

1 System Model

We consider a two-dimensional region containing N particles of an ideal gas. The particles move in straight lines between collisions, and collide elastically with each other and with the boundaries. Interactions between particles occur only at the moments of collision.

The left and right walls are maintained at fixed temperatures T_ℓ and T_r. When a particle collides with a wall, it receives an amount of kinetic energy corresponding to the wall temperature. In two dimensions, the magnitude of the outgoing velocity is determined by

$$\frac{1}{2}mv^2 = kT_{\text{wall}}, \tag{1}$$

where m is the particle mass and k is the Boltzmann constant. The outgoing direction is chosen randomly, while the speed is fixed by the expression above.

2 Particle Mean Free Paths

The mean free path in a two-dimensional ideal gas is given by

$$\lambda = \frac{1}{\sqrt{2}\,\pi d^2 n}, \tag{2}$$

where d is the effective particle diameter and n is the local concentration.

In the region near the hot wall, particles possess higher average kinetic energy and thus higher speeds. This increases the mean time between collisions and leads to longer free paths. In the colder region, the free paths are shorter.
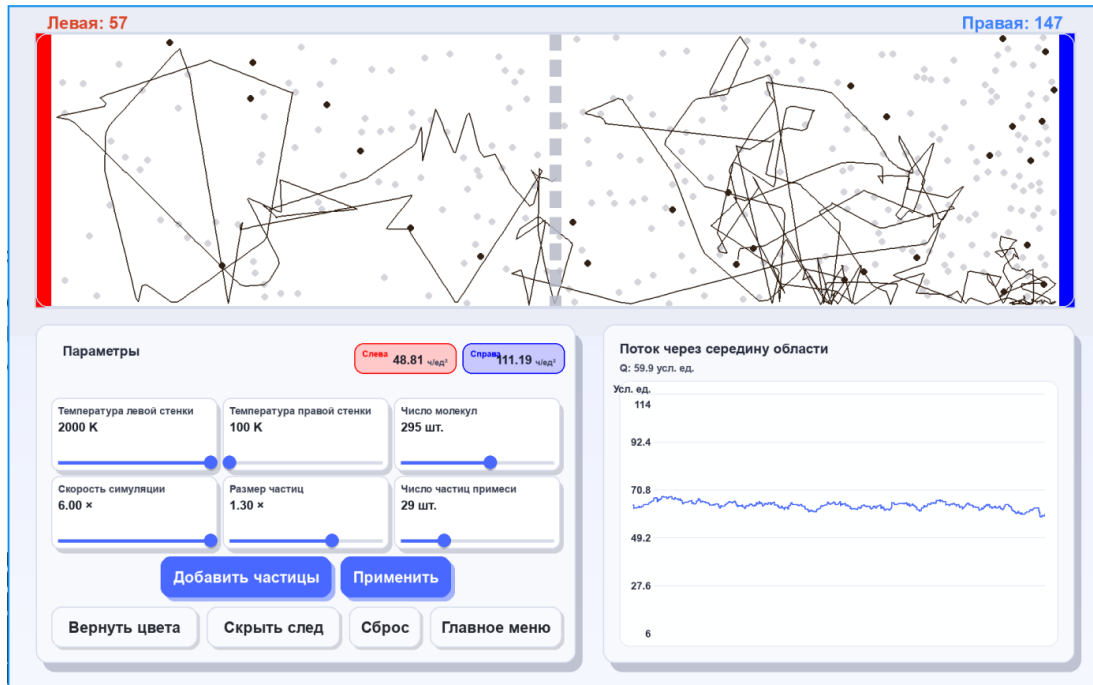

Figure 1: Illustration of differences in particle free paths: long trajectories in the hot region on the left and shorter trajectories in the cold region on the right.

The image shows a typical example of particle trajectories when the "trace" visualization option is enabled. One can clearly see the increase of free-path lengths in the hot part of the system and the decrease in the cold part.

3 Heat Conduction

At the macroscopic level, energy transport is described by the heat conduction equation:

$$\frac{\partial T(x,t)}{\partial t} = \kappa\, \frac{\partial^2 T(x,t)}{\partial x^2}, \tag{3}$$

where κ is the thermal conductivity coefficient. In the model, fast particles originating from the hot wall transfer energy toward the cold wall, producing a temperature gradient consistent with this equation.

4 The Mendeleev–Clapeyron Law and Its Realization in the Model

For an ideal gas, the Mendeleev–Clapeyron equation holds:

$$pV = \nu R T, \tag{4}$$

where p is the pressure, V the volume (in our two-dimensional system, the area), ν the amount of substance, T the thermodynamic temperature, and R the gas constant. Using the identity

$$R = N_{\mathrm{A}} k,$$

where N_{A} is Avogadro's number and k is the Boltzmann constant, one obtains an equivalent form in terms of particle concentration:

$$p = nkT, \tag{5}$$

where $n = N/V$ is the particle density.

From kinetic theory, pressure is related to the average kinetic energy via

$$pV = \frac{2}{f}\, N \left\langle \frac{1}{2} m v^2 \right\rangle, \tag{6}$$

where f is the number of degrees of freedom ($f = 2$ in two dimensions) and $\langle \cdot \rangle$ denotes averaging over particles in the volume. In local equilibrium,

$$\left\langle \frac{1}{2} m v^2 \right\rangle = \frac{f}{2} kT, \tag{7}$$

and thus the Mendeleev–Clapeyron law follows:

$$pV = NkT \qquad \Longleftrightarrow \qquad p = nkT. \tag{8}$$

Local Form and Relation to the Numerical Model

Consider a thin slice of width Δx. Its volume is

$$\Delta V = L_y\, \Delta x,$$

where L_y is the height of the domain. Let $N(x)$ be the number of particles in this slice, and let $T(x)$ denote the local temperature, defined through the average kinetic energy:

$$\left\langle \frac{1}{2} m v^2 \right\rangle_x = kT(x). \tag{9}$$

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The local concentration is then
$$n(x) = \frac{N(x)}{\Delta V},$$
and the local Mendeleev–Clapeyron law becomes

$$p(x) = n(x)\,k\,T(x). \tag{10}$$

This relation can be directly tested in the simulation:

- When $T_\ell = T_r$, after relaxation the average concentrations n_{left} and n_{right} coincide, meaning that pressures in the left and right halves match and the Mendeleev–Clapeyron law is satisfied.

- When a temperature gradient $T(x)$ is present, the system remains in a nonequilibrium steady state; however, in a *small local volume* where $T(x)$ and $n(x)$ vary slowly, the relation
$$p(x)\,\Delta V = N(x)\,k\,T(x)$$
continues to hold with good accuracy.

5 Energy Flux

The model records not the particle flux but the *energy flux* through a vertical boundary. Let a particle of mass m cross the boundary with velocity component v_x, where the sign of v_x indicates the direction:

$$v_x > 0 \quad \text{— particle crossing from left to right,}$$

$$v_x < 0 \quad \text{— particle crossing from right to left.}$$

Its kinetic energy is
$$E = \frac{1}{2}mv^2.$$
The contribution of this particle to the energy flux is

$$\Delta Q = \begin{cases} +E, & v_x > 0, \\ -E, & v_x < 0. \end{cases}$$

The total energy flux during time interval Δt is

$$J_E = \frac{1}{\Delta t} \sum_{i \in \Delta t} \Delta Q_i.$$

Thus:

- fast particles from the hot region contribute **positively**;

- slower particles moving from the cold region contribute **negatively**;

- for $T_\ell = T_r$ the average flux satisfies $J_E \approx 0$;

- for $T_\ell \neq T_r$ a steady nonequilibrium energy flux $J_E \neq 0$ is established.

In the steady state, the energy flux is constant, corresponding to a typical nonequilibrium condition sustained by external heat sources (the two walls).

6 Diffusion and Spatially Varying Diffusion

For impurity particles, the concentration $n(x, t)$ follows Fick's equation:

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial n}{\partial x}\right),\tag{11}$$

where the diffusion coefficient depends on temperature:

$$D(x) \propto T(x).\tag{12}$$

Diffusion is faster in the hot region, so an impurity cloud initially spreads preferentially toward the hot wall. Upon entering the colder region, the reduced value of $D(x)$ causes particles to remain there longer, resulting in a steady-state concentration profile shifted toward the cold wall.

7 Heat Conduction and Relation to Fick's Law

Microscopically, heat transfer in a gas occurs due to random motion of molecules carrying kinetic energy. Particles from the hot region have higher mean energy and transfer this energy into the colder region. This results in a heat flux.

In kinetic theory, the heat flux is defined as

$$j_Q = \frac{dQ}{dt\, dS},\tag{13}$$

where dQ is the energy crossing area dS during time dt.

Analyzing particle motion near an arbitrary surface yields Fourier's law:

$$j_Q = -\kappa\frac{dT}{dx},\tag{14}$$

where κ is the thermal conductivity. The minus sign indicates transfer from hot to cold regions.

The thermal conductivity of an ideal gas is

$$\kappa = \frac{1}{3}\lambda c_v \rho \bar{v},\tag{15}$$

where λ is the mean free path, ρ is density, c_v is heat capacity at constant volume, and $\bar{v}$ is the mean thermal speed. In two dimensions, the numerical factor becomes $1/2$ while the structure remains the same.

Writing the heat flux in gradient form yields full analogy with Fick's law:

$$j = -D\frac{\partial n}{\partial x},\tag{16}$$

with the diffusing quantity being thermal energy instead of particle density.

Relation to the Numerical Model

In the simulation, the energy flux is computed directly from the kinetic energies of particles crossing the vertical boundary:

$$\Delta Q_i = \begin{cases} +\dfrac{1}{2}mv_i^2, & v_{x,i} > 0, \\ -\dfrac{1}{2}mv_i^2, & v_{x,i} < 0. \end{cases}$$

The total flux is

$$J_E = \frac{1}{\Delta t} \sum_{i \in \Delta t} \Delta Q_i.$$

For equal temperatures,

$$J_E \approx 0,$$

corresponding to equilibrium.

For different wall temperatures, a nonequilibrium steady heat flux arises:

$$J_E \neq 0,$$

directly demonstrating Fourier's law and the kinetic origin of heat conduction.

8   Entropy and Nonequilibrium Steady States

For a normalized impurity density $p(x,t)$, entropy is defined as

$$S(t) = - \int p(x,t) \ln p(x,t) \, dx. \tag{17}$$

With equal wall temperatures, the system is closed and relaxes toward thermal equilibrium, where entropy reaches its maximum:

$$\frac{\partial S}{\partial t} = 0, \qquad J(x) = 0, \qquad n_{\text{left}} = n_{\text{right}}. \tag{18}$$

For $T_\ell \neq T_r$, the system becomes open: the hot wall injects energy, and the cold wall removes it. A nonequilibrium steady state is established:

$$\frac{\partial n}{\partial t} = 0, \qquad \frac{\partial T}{\partial t} = 0, \qquad J(x) \neq 0. \tag{19}$$

The entropy cannot reach a global maximum because external sources maintain a temperature gradient and a directed heat flux. Impurity spreading is accompanied by entropy growth $S(t)$, yet the steady-state distribution remains nonequilibrium due to spatially varying diffusion and the imposed temperature difference.