

QR code with a link to the program archive



# How to run the demonstration on macOS

Below is one possible way to launch the program on macOS. Unfortunately, this operating system is very protective about security, so before running the application you must execute a specific command inside the program folder. First, open the Terminal in the directory containing the unpacked program. Right-click the folder and choose the option “Open Terminal in the selected folder”. This process is illustrated in the images below.

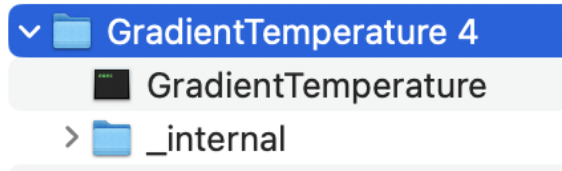


Figure 1: \*

Step 1. Right-click the folder after unpacking the archive

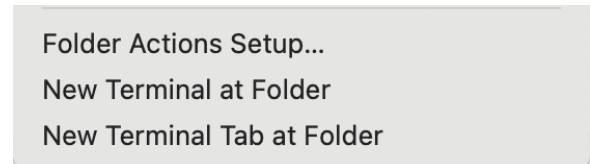


Figure 2: \*

Step 2. The option is located near the bottom of the list

Then, you must run the following command:

```
sudo xattr -cr .
```

After entering the command, type your user password. You may now close the Terminal. The program is ready to launch.

**Note.** The first launch may take some time because the application loads all the required libraries before starting.

# Diffusion and heat transfer in a domain with a temperature gradient: from particle simulation to stochastic equations

Probability is an honest confession that we do not know something for sure.

*from informal notes on statistical physics*

## 1 Problem setup and visualization of the temperature gradient

Consider a two-dimensional domain filled with an ideal gas with a cold left wall and a hot right wall. The wall temperatures are fixed and equal to  $T_\ell$  and  $T_r$ . In the numerical demonstration this is a rectangular container in which point particles of mass  $m$  move.

### 1.1 Visual representation of temperature

We observe the temperature gradient through the motion of the particles:

- particles that have recently collided with the hot wall have larger speeds; it is convenient to highlight them with “hot” colors;
- particles coming from the cold region move more slowly and are marked with “cold” colors;

For clarity we place impurity particles of black color in the centre of the domain. They do not affect the dynamics of the gas and simply move together with it, so that one can easily track the displacement of the centre of mass of the cloud and the growth of its dispersion.

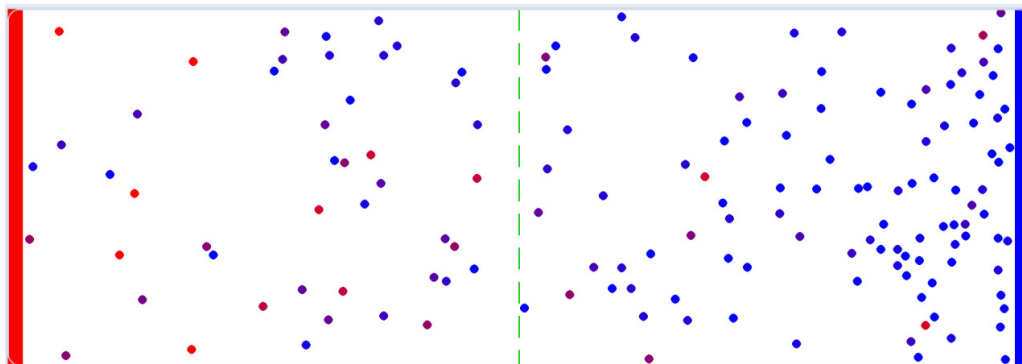


Figure 3: Geometry of the domain and visualization of the temperature gradient.

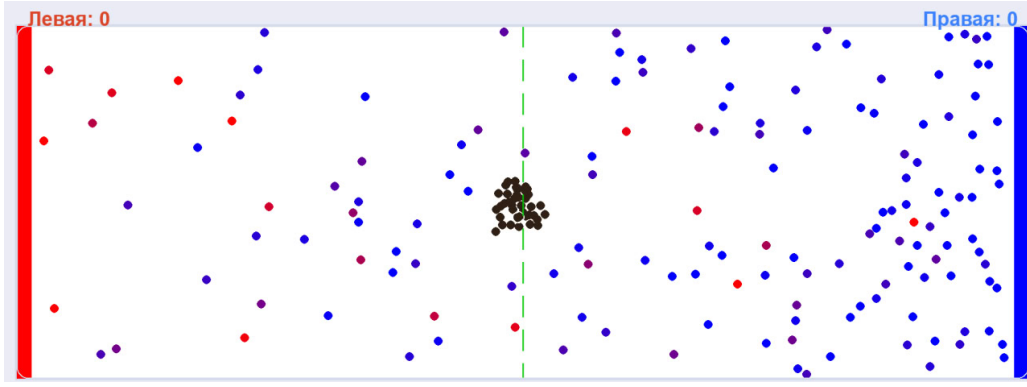


Figure 4: Adding impurity particles in the central region.

## 2 Microscopic model of the gas

### 2.1 Particle motion and collisions

The model is a two-dimensional gas of  $N$  point particles that interact via elastic collisions. Between collisions the particles move in straight lines with constant velocities. Collisions between particles and with the walls of the vessel are taken to be perfectly elastic.

The left and right walls play the role of thermostats. When a particle hits a wall, the modulus of its velocity is redefined according to the temperature of that wall:

$$\frac{1}{2}mv^2 = kT_{\text{wall}}, \quad (1)$$

where  $k$  is the Boltzmann constant. The direction of the velocity is chosen randomly, with the condition that the particle leaves the wall and returns back into the domain.

In this way the gas is kept in contact with two heat baths at different temperatures. Far from the walls the system relaxes due to collisions between particles, and a stationary temperature profile  $T(x)$  is formed, which interpolates between  $T_\ell$  and  $T_r$ .

## 3 Inhomogeneous diffusion and Fick's law

If you put a drop of perfume on the boundary between warm and cold air, the cloud will slowly drift toward the warm side: diffusion, in a sense, “votes” for the warm region.

*from FPAllbook*

Let us consider impurity particles (a cloud of a different color) that are convenient to treat as passive tracers. Their concentration  $n(x, t)$  obeys a diffusion equation. In the presence of a temperature gradient the diffusion coefficient  $D$  depends on the coordinate:  $D = D(x)$ . In a one-dimensional approximation Fick's equation reads

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left( D(x) \frac{\partial n}{\partial x} \right). \quad (2)$$

In kinetic theory the diffusion coefficient is related to the mean free path  $\lambda$  and the mean thermal speed  $\bar{v}$ :

$$D \sim \lambda \bar{v}. \quad (3)$$

For an ideal gas  $\bar{v} \propto \sqrt{T}$ , so to first approximation

$$D(x) \propto T(x). \quad (4)$$

Several important effects follow from this.

- In the hot part of the domain the diffusion coefficient is larger and the impurity cloud spreads faster.
- In the cold part, diffusion is slower and the concentration profile stays steeper for a longer time.
- If the cloud is initially placed near the boundary between hot and cold regions, then the higher diffusion in the hot region leads to an effective drift of the centre of mass toward the hot side.

We can think of a mental experiment: a drop of perfume is placed at the boundary between warm and cold air. Because diffusion is stronger in the warmer region, the cloud becomes asymmetric and its centre of mass moves toward the warm side. An observer will smell the perfume earlier on the warm side.

Exactly the same effect can be seen in our numerical demonstration: the cloud of black impurity particles slowly drifts toward the hot wall, even before a substantial part of the particles reaches the boundaries.

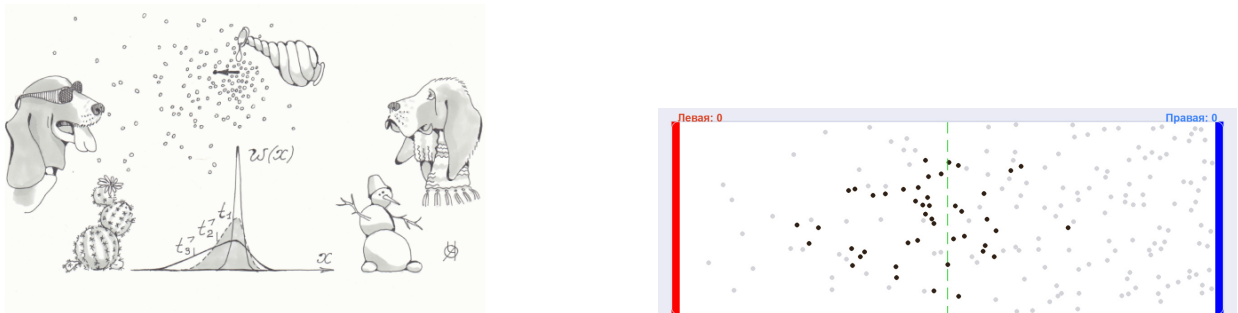


Figure 5: Analogy with a drop of perfume and demonstration of the drift of the impurity cloud.

## 4 Itô and Stratonovich stochastic equations

The same formula with different dots over the integral is enough to make two mathematicians argue: one insists on Itô, the other on Stratonovich.

*from a lecture on stochastic calculus*

The motion of a single impurity particle along the  $x$  axis in an inhomogeneous medium can be described, in the continuum limit, by a stochastic differential equation (SDE) with white noise:

$$dx_t = a(x_t) dt + b(x_t) \circ dW_t, \quad (5)$$

where  $a(x)$  is the deterministic drift,  $b(x)$  sets the amplitude of fluctuations, and  $dW_t$  is an increment of a Wiener process. The small circle indicates the **Stratonovich** interpretation.

The probability density  $w(x, t)$  satisfies the Fokker–Planck equation:

$$\frac{\partial w}{\partial t} = -\frac{\partial}{\partial x}(K_1(x)w) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(K_2(x)w). \quad (6)$$

The coefficients  $K_1, K_2$  are determined by the drift and noise intensity:

$$K_1(x) = -a(x) + D b(x)b'(x), \quad K_2(x) = 2D b^2(x), \quad (7)$$

where  $D$  is a constant setting the noise strength.

For the **Itô** interpretation the same SDE is written as

$$dx_t = a_{\text{Itô}}(x_t) dt + b(x_t) dW_t, \quad (8)$$

and the coefficients change:

$$K_1^{\text{Itô}}(x) = -a_{\text{Itô}}(x), \quad K_2^{\text{Itô}}(x) = 2D b^2(x). \quad (9)$$

Here the additional drift does not appear explicitly; it must be incorporated directly into the function  $a_{\text{Itô}}(x)$ .

In problems of statistical physics and non–equilibrium processes the Stratonovich interpretation is often more convenient, because it naturally corresponds to the limit of systems with finite correlation time of fluctuations and automatically produces the correct additional drift.

In our demonstration this effect is visible on the level of the cloud of particles: one can regard the random kicks due to collisions as noise, and the dependence  $D(x)$  on temperature generates an effective drift of the impurity.

## 5 Local equation of state of an ideal gas

On the macroscopic level an ideal gas satisfies the Mendeleev–Clapeyron equation

$$pV = \nu RT. \quad (10)$$

Switching to the number of particles  $N$  and the concentration  $n = N/V$ , we obtain

$$p = nkT. \quad (11)$$

In the demonstration this relation can be checked in two ways.

### 5.1 Global equilibrium

If the wall temperatures are equal ( $T_\ell = T_r$ ), then after sufficient time the system reaches equilibrium with uniform temperature  $T$  and pressure  $p$ . The relation  $p = nkT$  then holds for the whole container. By splitting the container into left and right halves one can verify that the same equation of state holds separately in each half.

### 5.2 Local form of the law

In the presence of a stationary temperature gradient the system is not in global equilibrium, but one can introduce local quantities. We divide the domain into narrow vertical stripes of width  $\Delta x$  and measure in each stripe the local temperature  $T(x)$ , mean concentration  $n(x)$  and pressure  $p(x)$ .

Exactly this dependence can be tested in the numerical model:

- for equal wall temperatures  $T_\ell = T_r$ , after relaxation the equation of state holds for each half of the container with good accuracy;
- when a temperature gradient  $T(x)$  is present, the system is in a non-equilibrium stationary state, but in sufficiently small subdomains (where  $T(x)$  and  $n(x)$  change little) the relation

$$p(x) \Delta V = N(x) kT(x)$$

remains valid.

Qualitatively, in the cold region the concentration is higher and the temperature is lower, whereas in the hot region the opposite is true; their product stays approximately constant. Thus the model makes it possible to observe the equation of state of an ideal gas both in global equilibrium and in its local form for small volumes in the presence of a temperature gradient.

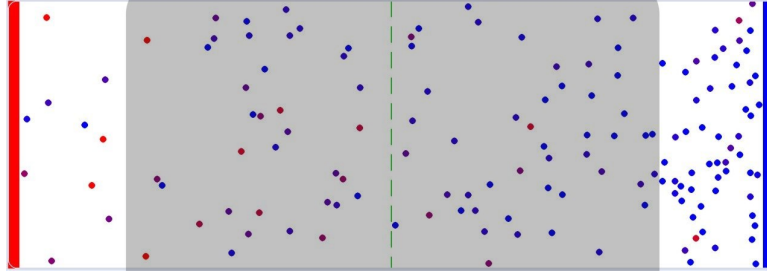


Figure 6: Schematic picture of the regions where the local relation  $p(x) = n(x)kT(x)$  holds.

## 6 Mean free path and transport coefficients

The mean free path in a gas is

$$\lambda = \frac{1}{\sqrt{2} \pi d^2 n}, \quad (12)$$

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

Close to the hot wall the actual free paths along trajectories are on average longer, because the particles move faster and the local concentration is slightly lower. Near the cold wall the situation is opposite: the trajectories are “chopped up” and the paths are shorter.

Transport coefficients such as the diffusion coefficient  $D$  and the thermal conductivity  $\kappa$  are expressed through  $\lambda$  and  $\bar{v}$ , so that spatial variations of the mean free path and temperature translate into variations of these coefficients. The simulation allows one to see this change directly at the level of particle trajectories.

## 7 Heat flux and Fourier’s law

In addition to diffusion of the impurity there is energy transport from the hot wall to the cold wall. To quantify this transport we fix an imaginary vertical boundary and count the energy flux through it.

If a particle of mass  $m$  crosses the boundary with velocity component  $v_x$ , its kinetic energy is

$$E = \frac{1}{2} m v^2. \quad (13)$$

The contribution of a particle to the energy flux is

$$\Delta Q = \begin{cases} +E, & v_x > 0 \quad (\text{particle moves from left to right}), \\ -E, & v_x < 0 \quad (\text{particle moves from right to left}). \end{cases} \quad (14)$$

Summing  $\Delta Q$  over all crossings per unit time and dividing by the area of the boundary we obtain the heat flux  $j_Q$ .

In a stationary regime, for small gradients, the heat flux is proportional to the temperature gradient. This is Fourier's law:

$$j_Q = -\kappa \frac{dT}{dx}, \quad (15)$$

where  $\kappa$  is the thermal conductivity. Structurally this law is similar to Fick's law for particle diffusion: the gradient of temperature plays the role of a "driving force" for energy transport.

## 8 Entropy and non-equilibrium stationary state

Let us recall that we consider a situation in which we add impurity particles in the central part of the domain and study the effects that arise. For the normalized impurity density  $p(x, t)$  the entropy is defined as

$$S(t) = - \int p(x, t) \ln p(x, t) dx. \quad (16)$$

- For equal wall temperatures the system is closed, and with time the impurity becomes uniformly distributed. The entropy approaches its maximum corresponding to a homogeneous state.
- For  $T_\ell \neq T_r$  the system is open: the hot wall constantly pumps energy into the gas, and the cold wall removes it. A non-equilibrium stationary state with a constant energy flux and a stable temperature profile is established.

The entropy of the impurity cloud grows as it spreads, but the global entropy production of the whole system does not vanish even in the stationary regime, because the external sources continually maintain the temperature gradient.

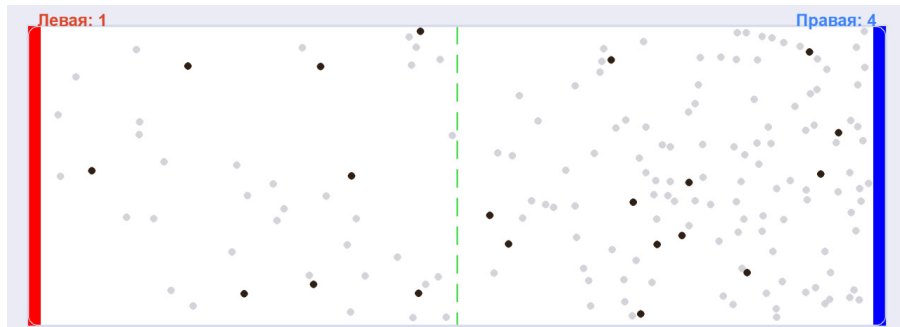


Figure 7: Growth of the impurity entropy and approach to the stationary regime.