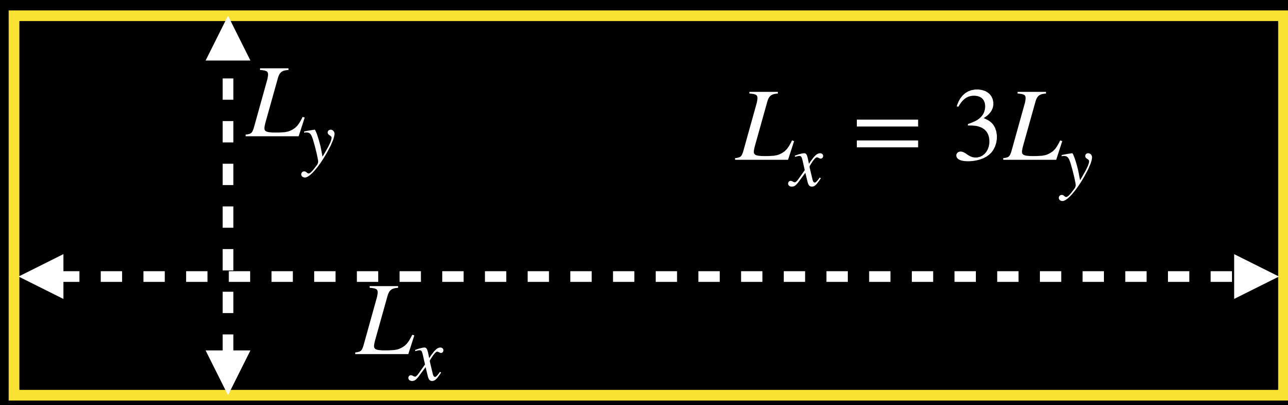
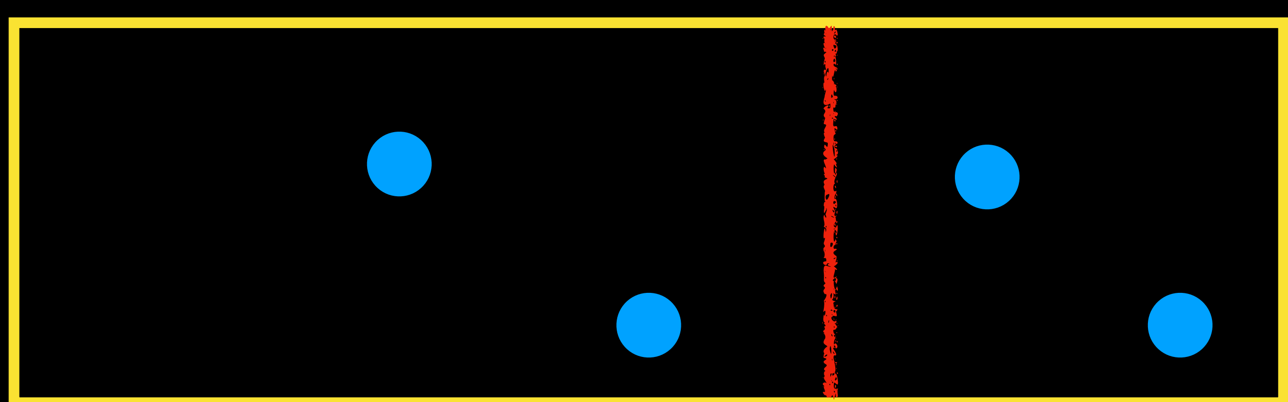
Project 1) Reaching the steady state

Choose an elongated box as shown in the picture below.



Separate the system by a vertical, moving wall.



This wall has $v_y = 0$ at all times, but $v_x \neq 0$ is non-zero and non-constant. Particles cannot cross this wall, but interact with purely elastic collisions. The wall has a finite mass and exchanges momentum with the particles following the rules of energy conservation and momentum conservation (in x direction).

Attention!!!

If v_W is the wall speed in x direction and $v_{i,x}$ is the velocity of particle i in x direction, then there is a condition which guarantees that the collision time between the moving wall and particle i is positive. You must find this conditions, otherwise particles cross the moving wall.

Note: It is not necessary, that one and the same code does everything. You can write several codes, which do one specific measurement.

Project 1)

Choose an initial configuration, where the moving wall is in the middle of the box but:

(A) density in chamber 1 $\gg$ density in chamber 2

(B) temperature in chamber 1 $\gg$ temperature in chamber 2

Note that the temperature in one chamber is set by the initial velocities you chose for the particles, as the total energy in one chamber is given by

$$E_j = \sum_{q=1}^{N_j} \frac{m_q}{2} \vec{v}_q^{\,2} = N_j k_B T_j$$

(Ensemble equivalence)

We do NOT define $k_B = 1.38 \cdot 10^{-23}$.
We rather work with a variable k_BT, which takes reasonable values, i.e. neither super large, nor super small.

(N_j, T_j number of particles and temperature in chamber $j = \{1,2\}$).

Task: Measure the position of the moving wall, the temperature in both chambers, and the density in both chambers as a function of time.

How long does it take for the system to reach a steady state (what characterises the steady state)?

How does the mass of the wall influence the time evolution of the system and the steady state?

Check if you reach the same steady state if you exchange the role of chamber 1 and 2!

How does the total number of particles influence the time evolution and the steady state? (If you increase the number of particles, you should increase the volume of you box such that $(N_1 + N_2)/(L_x L_y) = const.$.)

What would change, if you would put smaller & lighter particles in chamber 2?

e) Task (optional): In the system without moving wall, verify that the steady state distribution of the speed follows the Maxwell-Boltzmann distribution

$$P(|\vec{v}_i|) = \frac{m_i |\vec{v}_i|}{k_B T} \exp\left(-\frac{m_i \vec{v}_i^{\,2}}{2k_B T}\right).$$

You are simulating a constant energy ensemble, not a constant temperature ensemble. The Maxwell-Boltzmann distribution is derived for the constant temperature ensemble. Your constant energy ensemble follows the Maxwell-Boltzmann distribution only for large system sizes. This is because of ensemble equivalence. Measure the distribution $P(v_i)$ for $N = \{2, 3, 4, 10, 100\}$. What do you observe?