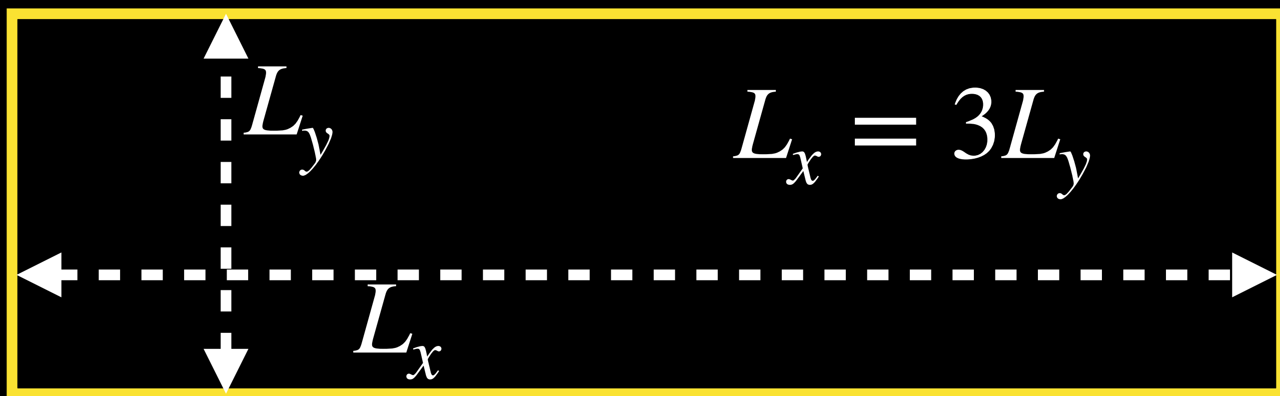
Project 2) Heat conduction - a non-equilibrium steady state

Choose an elongated box as shown in the picture below.



(Ensemble equivalence)

The temperature is set by the velocity of the particles. The total energy of the system is given by

$$E = \sum_{i=1}^{N} \frac{m_i}{2} \overrightarrow{v}_i^2 = N k_B T. \tag{1}$$

Initialise the velocities of the particles at a temperature of your choice. For this, chose random directions and the speed $v_i = |\overrightarrow{v}_i| = const$. Because of (1), the chosen constant initial speed fixes the temperature.
Task (optional): Verify that the steady-state distribution of the speed follows the Maxwell-Boltzmann distribution

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

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?

Task: Confirm that the particle flux in x direction is zero $J_x(x) = 0$. For this: Chose a vertical line at x^*. Each time a particle crosses x^* with $v_x > 0$: $J_x += 1$ and for $v_x < 0$: $J_x -= 1$, respectively. The particle flux at x^* is then given by $J_x(x^*) = J_x / t_{measure}$, where $t_{measure}$ is the time interval of the measurement. Note that crossing x^* is NOT an event.

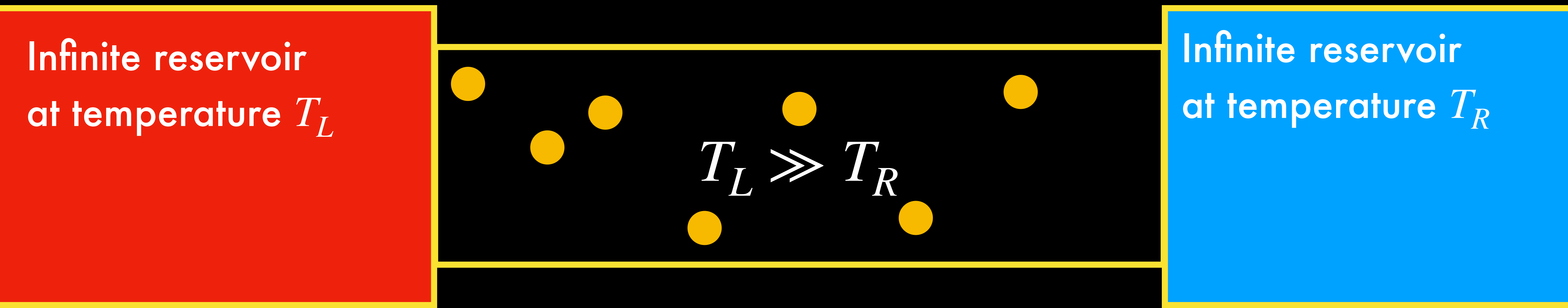
Project 2)

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.

Implement temperature reservoirs:
The right and left wall of the box are in contact with infinite reservoirs at different temperatures (see picture). Particles perform elastic collisions with ALL four walls. However, each time a particle collides with the left (right) wall, it leaves the wall with a new, random speed $v_i = |\vec{v}_i|$ (does not affect, the direction) drawn from the Maxwell-Boltzmann distribution at T_L (or T_R)

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

Please see here of how to sample a speed from the Maxwell-Boltzmann distribution: https://github.com/JulianeUta/simul2021Student



Tasks:

- Repeat the measurement of the particle flux $J_x(x^*)$. What changes if you wait for some time until you start your measurement (remember: if you don't wait until you reach the steady state, your measurements can be influenced by the initial conditions).
- Measure the temperature as a function of the x-position. Draw $T(x)$! What is the functional dependence? Does your result agrees with Fourier's law?
- Create one big and heavy particle, which does not feel the temperature reservoirs (i.e. ordinary elastic collisions with all walls). Place it **close** to the hot wall (not touching it). Trace the x-position of the particle as a function of time! You may want to repeat this experiment to obtain some statistics.

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