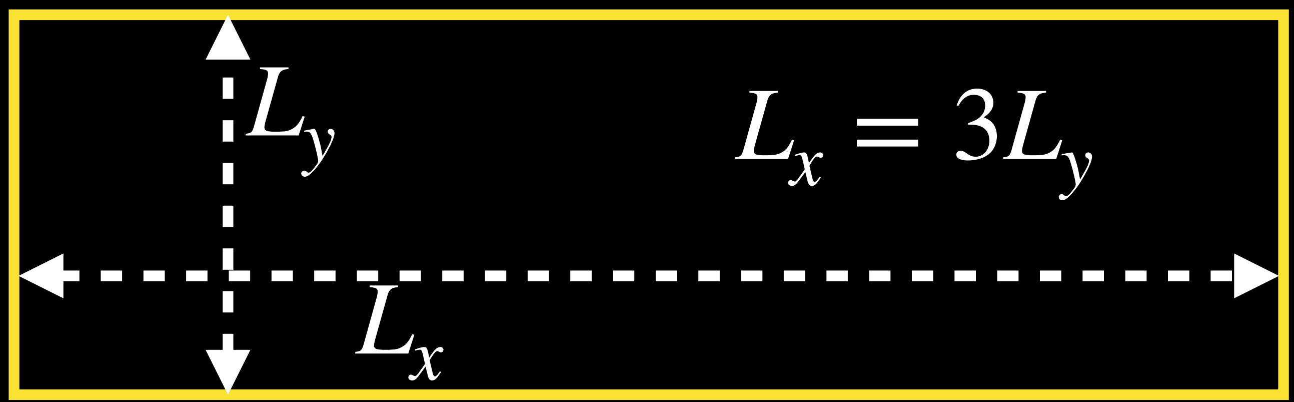
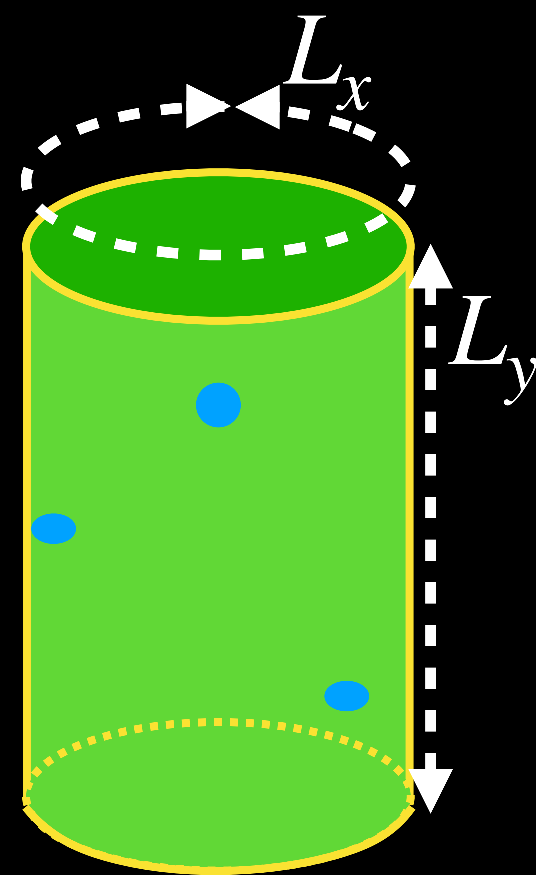
Project 3) Periodic boundary conditions - a fundamental tool in particle simulations

Choose an elongated box as shown in the picture below.





Implement periodic boundary conditions in x-directions, i.e.:
Remove collisions with vertical (right and left) walls.
If $\epsilon > 0$, then the following equality for the positions applies $x = L_x + \epsilon = \epsilon$ and equivalently $x = -\epsilon = L_x - \epsilon$.
This means we consider that the vertical walls are glued together, such that the particles move on the surface of a cylinder (see figure). Do NOT implement the graphic representation of the cylinder! We only want to see that a particle, which leaves the box on the right wall, reenters the system at the position of the left wall and vice versa.

You should define functions which calculate the absolute and vectorial distances in x-direction under this periodic boundary conditions. These functions should be used for the calculation of the event times and the update of the velocities after a collision.

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

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(Ensemble equivalence)

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

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

Initialise the velocities of the particles at a temperature of your choice. For this, chose random directions and the speed $v_i = |\vec{v}_i| = const$. 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

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

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.

Now, we imagine that there is a demon watching the system from the outside. Each time a particle with $v_x > 0$ passes the position $x = 0$, the demon changes the speed of the particle (direction unchanged). The demon draws the speed from

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

Equivalently, each time a particle with $v_x < 0$ passes the position $x = 0$, the demon draws the speed from

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

Task: Measure the particle flux as a function of $\Delta T = T_+ - T_-$.

Task: Add one big, heavy particle in the system, which the demon does not see (i.e. its speed is unchanged at $x = 0$). What do you observe?

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Advanced project inspired by the work of Anke Lindner et al. at ESPCI:
Flexible filaments buckle into helicoidal shapes in strong compressional flows,
Nature Physics volume 16, pages 689–694 (2020)
https://www.nature.com/articles/s41567-020-0843-7

Task (advanced): With the dimer class, you can create a chain of particles. You can consider this particle chain as a model for filaments and study the behaviour of your filament in the flow of the bath.
Again, the demon cannot see the blue particles composing the chain, but only the red particles.