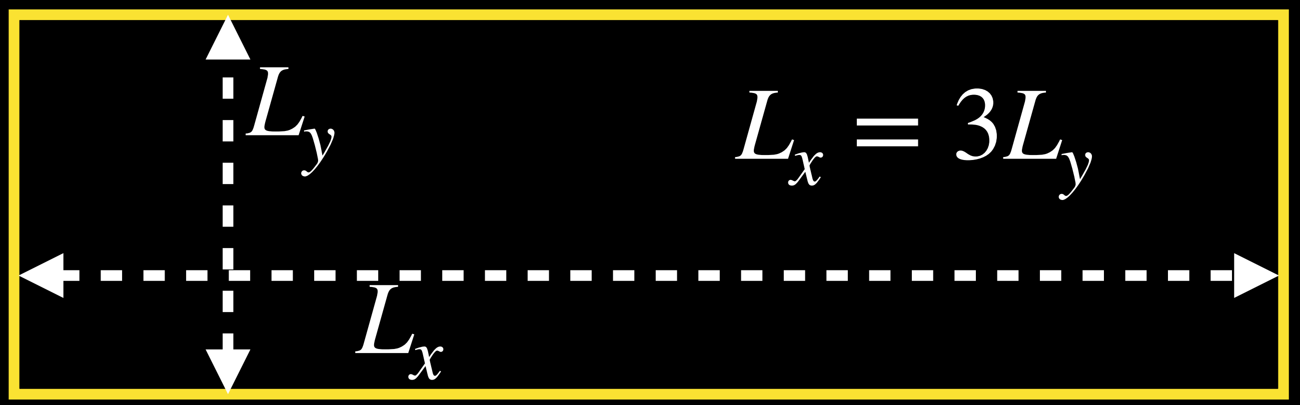
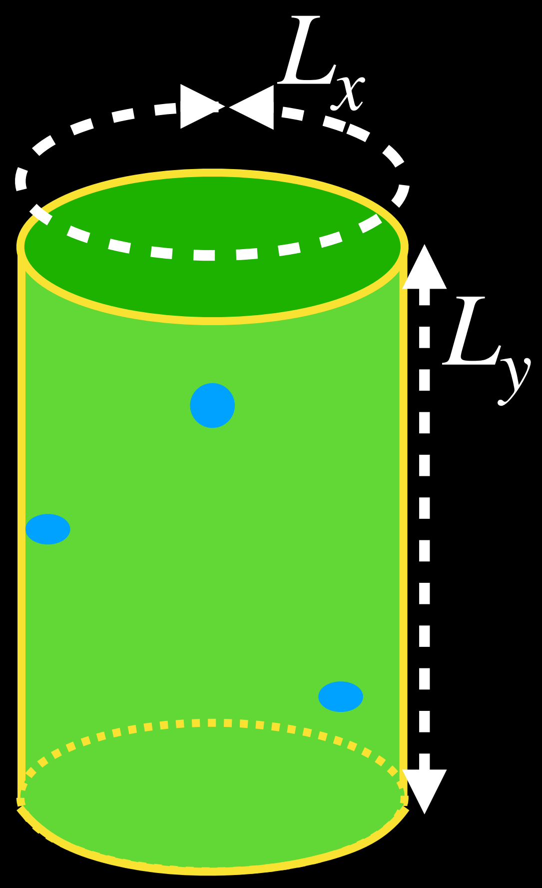
Project 3) Periodic boundary conditions - a fundamental tool in particle simulations

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 vise versa.
You MUST write a function which correctly calculates distances in x-direction under this periodic boundary conditions AND adjust the calculation of event times.



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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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.

(Ensemble equivalence)

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

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

Initialize 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

$$P(v_i) = \frac{m_i v_i}{k_B T} \exp\left(-\frac{m_i v_i^2}{2 k_B T}\right).$$

(this is NOT an event)

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. (Here we are really talking about the physical time. For example after 10 animations, your physical time should have involved by 10 dt.)

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

$$P_+(v_i) = \frac{m_i v_i}{k_B T_+} \exp\left(-\frac{m_i v_i^2}{2 k_B T_+}\right).$$

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

$$P\_(v_i) = \frac{m_i v_i}{k_B T\_} \exp\left(-\frac{m_i v_i^2}{2 k_B T\_}\right).$$

Please see here of how to sample a speed from the Maxwell-Boltzmann distribution:
https://github.com/JulianeUta/TP_Programmation2020_ForStudents/blob/master/Examples/MaxwellBoltzmann.zip

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?