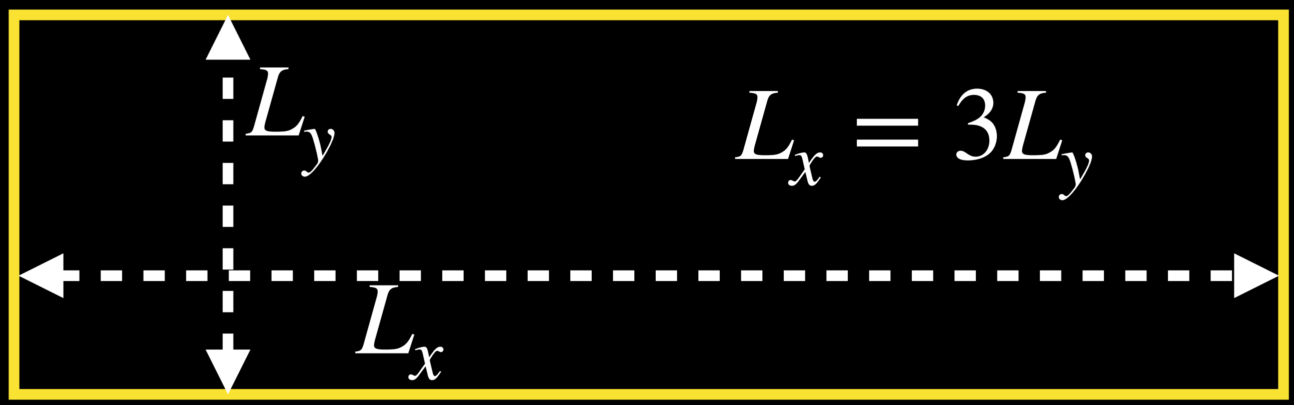
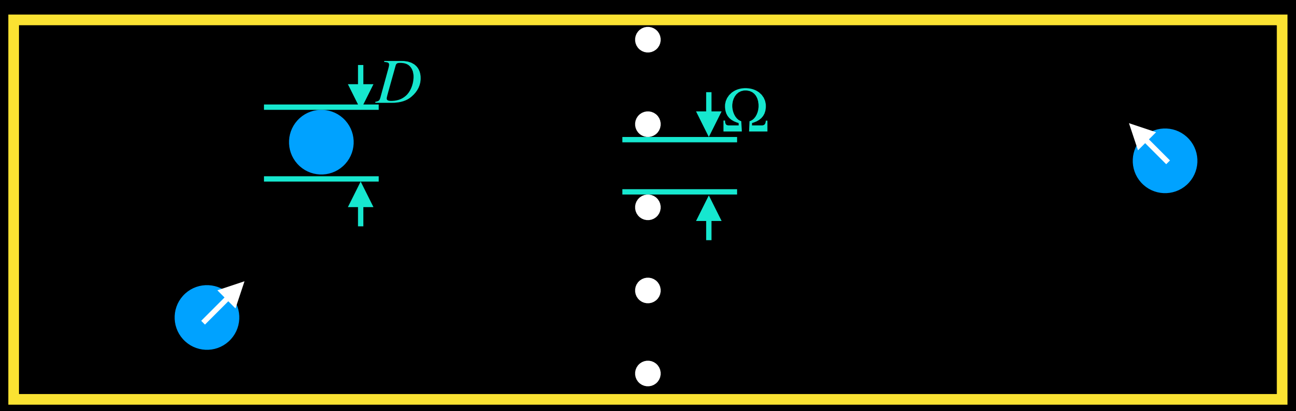
Project 4) Osmotic pressure

Choose an elongated box as shown in the picture below.



Place a vertical chain of infinitely heavy, but small particles inside the box (white particles in the following figure). The gap between those particles Ω should be variable.



We consider that those heavy particles do not move $v_x = v_y = 0$, but they interact with the other particles via elastic collisions.

Task: Chose an initial configuration, where all blue particles are on the right side of the white particle chain. Measure the time to reach the equilibrium steady state (equal density on right and left side) as a function of the particle spacing Ω. What it the minimal Ω to reach equal densities on the right and left? (You know the theoretical value, but does this value exists in practice ?)

Task: Measure the pressure on the right and left wall.

Hint: pressure is force per area and a force is nothing else than momentum transfer.

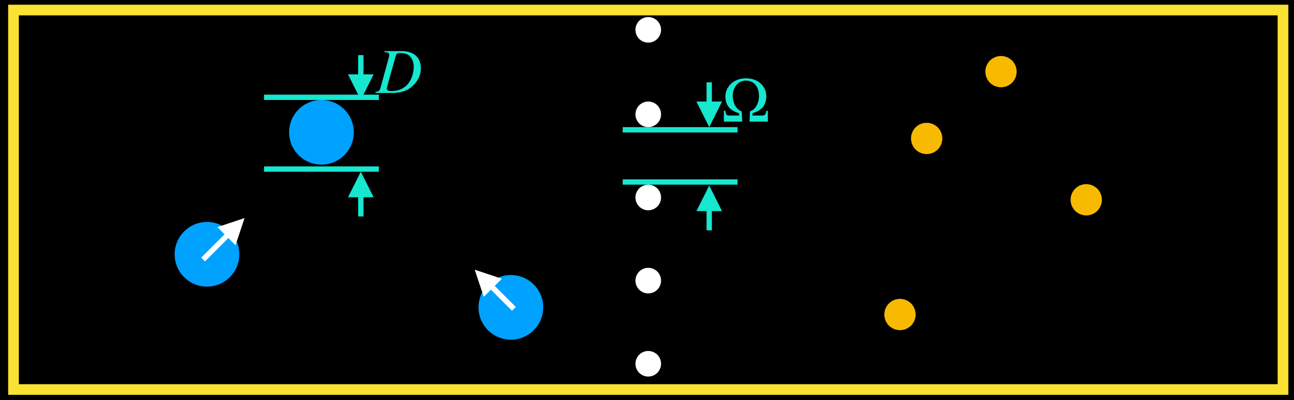
Check: In above setting the pressure on the right and left wall should be equal if the blue particles can cross the wall of white particles.

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

Project 4)

We want to study the osmotic pressure. Consider the white particles as the semi-permeable wall. Your system is composed of two kind of particles.
Blue: the diameter of the blue particles is larger than Ω, hence the blue particles can not cross the semi-permeable wall of white particles.
Orange: the diameter of the orange particles is sufficiently small compared to Ω, hence they can cross the Semin-permeable wall.

We choose an initial state, where blue particles are on the left and orange particles are on the right of the wall. We are interested in the osmotic pressure depending on the initial densities.



Velocity update after collision with membrane particles

velocity update with white particles

in general

$$\vec{v_1}' = \vec{v_1} - \frac{2m_2}{m_1+m_2}\left(\hat{\vec{\delta}} \cdot \vec{\Delta v}\right)\hat{\vec{\delta}} \text{ and}$$

$$\vec{v_2}' = \vec{v_2} + \frac{2m_1}{m_1+m_2}\left(\hat{\vec{\delta}} \cdot \vec{\Delta v}\right)\hat{\vec{\delta}}.$$

consider $m_1 \to \infty$ & m_2 finite

$$\Rightarrow \lim_{m_1 \to \infty} \frac{2m_2}{m_1+m_2} = 0, \quad \lim_{m_1 \to \infty} \frac{m_1}{m_1+m_2} = 1$$

in addition $\vec{V}_1 = (0,0)$

therefore

$$\vec{V}_1' = \vec{V}_1 = (0,0) \;\&\; \vec{V}_2' = \vec{V}_2 + 2\left(\hat{\vec{\delta}} \cdot \vec{\Delta V}\right)\hat{\vec{\delta}}$$

Thoughts about how to measure pressure

Force is an instantaneous quantity defined by $F(t) = m\,a(t) = m\,dv(t)/dt$. This means for every moment of time we can calculate the force. In this definition, you see that if $v(t) = const$, then $F(t) = 0$. This means for your simulation that only at the moment of a collision, i.e. when the particles change their velocity, you have forces that are non-zero. Why is this important?

Mechanical pressure is defined as the force particles exert on the confining wall per unit area. It is in principle also an instantaneous quantity. For example the pressure at time t on the right wall is defined as
$P_r(t) = F_{tot}(t) / A$, where $F_{tot}(t)$ is the total force particles exert on the right wall at time t and A is “the total area” of the right wall (we are in 2D, so that would be the length of the wall).

Consider the limit N -> infinity, V -> infinity, such that rho = N / V = constant. This is what we call the thermodynamic limit, which represents the real world. (Basically it just says that you have to consider a huge number of particles, if you want to approximate the real world in your simulation.) In a real-world system $F_{tot}(t) > 0$ at all times, because you would have so many particles (molecules in the air) such that there are always particles colliding with the wall, i.e. exerting a force on the wall. This means that pressure is indeed an instantaneous quantity in the real world.

Your simulation is far away from the thermodynamic limit. You have very few particles compared to the Avogadro number (number of particles in a mol). So you have to come up with a strategy of how to measure pressure. The basic problem is that you have so few particles, that a collision with the wall does not happen at every instant of time. The solution would be to average the total force exerted on the wall over time and then divide by the time interval of the measurement to obtain the averaged pressure.

Consider t is your total time and you start your measurement of pressure at t_start = 43 and you end it at t_end = 60.
This means you have measured pressure for total dt = t_end - t_start
At t = t_start you have a **global** variable which is initialised to zero
total_P = 0
For all t => t_start and t <= t_end: every time a particle collides with the right wall you do
total_P += mass[mono_1] * 2 * vel[mono_1, 0],
where vel[mono_1, 0] is the **old** velocity v_x of the particle that collided with the right wall. Why?
The force this particle exerts on the wall is
F = - m dv/dt = - m (v_x’ - v_x), where v_x’ is the velocity after the collision and v_x the velocity before the collision. You know that v_x’ = -v_x, thus the force the particle exerts on the right wall is
F = - m (-v_x - v_x) = 2 m v_x

At the end of your measurement, i.e. t = t_end you compute the average pressure on the right wall

total_P = total_P / ((t_end - t_start) * length)

where length is the length of the wall.

IMPORTANT: You should define your t_end and t_start in units of dt_frame (the constant time step unit).
For example t_start = 30 * dt_frame
This allows you to write something like

```
if frame == 30:
        total_P = 0
```

inside your function MolecularDynamicsLoop(frame)
Check your code for the variable frame! It is an integer that counts the number of frames you produce. It is increased from 0 to NumberOfFrames.

With the information, you understand that you could (not must) produce a graph of the evolution of pressure, but the recorded pressure would be a record of averages over a finite time interval (which needs to be sufficiently large). I do NOT expect that you have such a plot. However, if you measure only one pressure, I expect it is the one of the steady state, i.e. t_start must be sufficiently large.