Exercise 1: Two-Dimensional Hard-Disc Gas in a Square Box

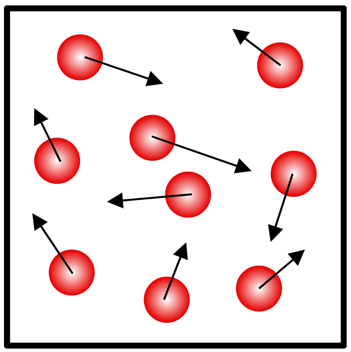
- In Exercise 1, you will **run**, **extend** and **apply** a small C-program I wrote for you to simulate a **two-dimensional hard-disc gas** confined in a **square box**

as a 2D model for a monoatomic gas (e.g. Argon)

Franz

Domen

→ Simulated system



Instantaneous Configuration Variables

t ***time in [ps]***

$x(t)$ ***2N-dim position vector in [nm]***

$v(t)$ ***2N-dim velocity vector in [nm/ps]***

Physical Input Parameters

N: Number of atoms

A: Box area in [nm^2]

T: Absolute temperature in [K]

m: Atomic mass in [g/mol]

r: radius in [nm]

R: Gas constant in [kJ / (K · mol)]

Numerical Input Parameters

K: number of time steps

Δt: time-step size [ns]

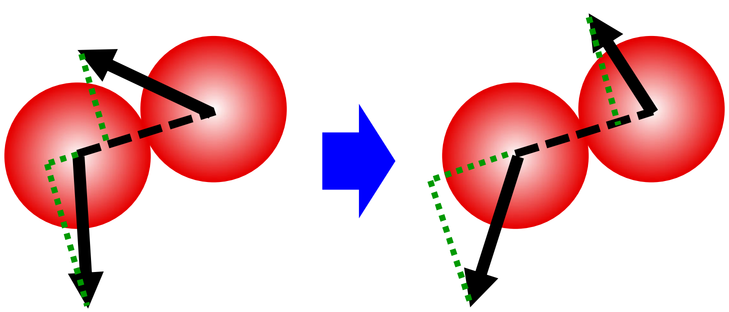
To be calculated

P: Average pressure in [kJ / (mol · nm^2)]

→ Collisions between **hard objects** are by definition **elastic**

i.e. they conserve both kinetic energy and momentum

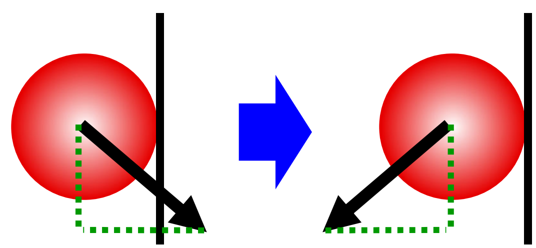
particle-particle collisions
[function process_atom_collisions()]



swap velocity components along the interatomic vector

(also reset positions to contact)

particle-wall collisions
[function process_wall_collisions()]

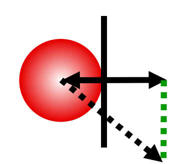


revert velocity components normal to the surface

(also reset positions to contact)

also calculate the "kick"

sum of outwards-directed normal velocities of all particles colliding with any of the four walls over a given time step



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- In this 2D case, the **ideal-gas law** reads

$$PA = NRT$$

The box area A replaces the 3D volume

The pressure is a line-pressure, i.e. force per unit length (and not per unit area)

The number of atoms is used here (and not of mols) because the pressure is defined in unit of [kJ / (K · mol)] that absorbs the Avogadro constant

→ The two-dimensional hard-disc gas is **always temperature-conserving** (zero temperature fluctuations) but **not necessarily ideal** (i.e. *PA=NRT* does not necessarily hold)

Do you see why? If not, the exercise will help you answer

- Note about the **units**

→ With the selected units, we can calculate the **kinetic energy** directly in [kJ/mol]

$$K = \sum \frac{mv^2}{2}$$

m in [g/mol]
v in [nm/ps]

× 10^6 for nm^2/ps^2 => m^2/s^2
× 10^-3 for g/mol => kg/mol
× 10^-3 for J/mol => kJ/mol

→ K is directly in [kJ/(mol)]

→ The conversion between kinetic energy in [kJ/mol] and **temperature** in [K] is given by the equipartition theorem with two degrees of freedom per atom in 2D

$$T = \frac{K}{NR}$$

K in [kJ/mol]
R in [kJ/(K mol)]

- Your task will be to:

→ (0) **Compile** and **run** the program ***(after downloading the tar-file at https://riniker.ethz.ch/education/StatPhysCSE)***

→ (1) **Read** and **understand** the program ***(first look at the README file)***

→ (2) **Implement** the functions **"calculate_temperature"** and **"calculate_pressure"**

→ (3) **Verify numerically** that the **ideal-gas equation** of state (approximately) holds