Exercise III: Entropy and Entropy production

Background: In the lecture (Sec. 2.1), we considered N particles starting at time t=0 on the left side of the simulation box. Starting with random initial velocities, they evolve in time and are all over the box shortly. To study the entropy production of this nonequilibrium process, we calculate the Shannon entropy

$$S(t) = -\sum_{i=1}^{N} p_i(t) \ln p_i(t),$$

where $p_i(t)$ (i=1...N) is the probability that i particles are on the left side. That is, initially we have $p_N(0)$ = 1 and $p_N(0)$ = 1. At long times we expect $p_i(\infty)$ to be a Gaussian distribution peaked at $i = N/2$ (for large N). To calculate $p_i(t)$, we run k = 1...M simulations and compute for each simulation the number $n_k(t)$ of k particles being on the left side of the simulation box.

-Task I: simulation

- Create a 2D box with the dimensions 10 nm x 10 nm. The box walls are reflective, i.e., do not use the periodic boundary conditions implemented before.
- Create simulations with N = 5, 25 and 50 spherical particles with radius r = 0.2 nm (either at random positions or on s regular grid) and equal mass within the left half of the cell (i.e., between x = 0.2 and 4.8 nm).
- Generate M = 5, 25, 50 independent simulations for each arrangement by assigning a velocity $\boldsymbol{v}$ with $|\boldsymbol{v}|$=0.5 nm/step and random direction to each particle. The direction of velocity needs to be randomized for each simulation.
- For collisions, use the "hard spheres" collision method from the first exercise.
- Carry out simulations of 300 steps for each combination of i and k.
- *Addition*: in case your computer can stomach it, try 100 particles, as well. On my own laptop, 50 simulations with 100 particles each took ca. 6 minutes.

-Task II: Calculating the Entropy over time

Compute for each simulation the number $n_k(t)$ of particles being on the left side.

- Plot $S(t)$ for the given choices of N and M. How large do you need to choose N and M to get reasonable results?
- Using these values for N and M, plot $p_i(t)$ for a few representative choices of i.
- What is the time scale (counted in simulation steps) observed for the entropy production to take a (roughly constant) final value?