Exercise 1. Event-driven Molecular Dynamics

Goal: So far in our MD simulations we were using particles interacting with each other via a continuous potential. Event-driven simulations are able to model particles interacting by hard core potentials considering binary collisions (i.e. no lasting contacts). Between these binary collisions the trajectories of the particles can be calculated analytically. In systems without external forces (e.g. gravity) the particles follow straight paths between collisions.

The collision time between pairs of particles can be calculated as follows

$$|\boldsymbol{r}_{ij}(t_0) + \boldsymbol{v}_{ij}(t_0)t_{ij}| = R_i + R_j$$

where $\boldsymbol{r}_{ij}$ is the distance vector between particles i and j, $\boldsymbol{v}_{ij}$ their velocity difference, t_{ij} the collision time and R_i, R_j the radii of the hard spheres. t_0 is the time at which the last collision occurred. In this method one has to calculate the collision time between all particle pairs to get the "global" collision time $t_C = \min_{ij}(t_{ij})$.

Task 1: *Implement the event-driven dynamics either in $1D$ or $2D$.*

Hint: In the $1D$ case: No quadratic equation has to be solved. Only neighboring particles interact with eacht other. The sphere radii can be set to 0. Assume that all particles have the same mass m.

Hint: In the $2D$ case: Consider collisions with perfect slip. Assume that all particles have the same mass m and the same radius R.

Task 2: *Solve some simple problems with different initial conditions. For example:*

- *Consider a $1D$ chain of N beads in a box with restitution coefficient $e = 1$ (such that the total energy is conserved).*
- *Consider a $1D$ chain of N beads with restitution coeeficient $e < 1$ hitting a resting wall. What is the effective restitution coefficient $e_{\mathit{eff}} = \sqrt{E_f/E_i}$ where E_i and E_f are the initial and final kinetic energies of the chain, respectively. Vary N at fixed e. Above which N does the effective restitution coefficient practically vanish, i.e. the cluster does not re-bounce anymore?*

Task 3 (OPTIONAL): *Speed up your code by storing the events for each particle in a priority queue (see lecture notes). While checking all particle pairs requires $\mathcal{O}(N^2)$ operations, generating events only for the colliding particles and inserting them in the queue is only $\mathcal{O}(N\log(N))$.* [1]

Hint: Only the interacting particles need to be advanced but keep in mind that the collision can invalidate previously predicted events. You can either remove them manually from the queue in time $\mathcal{O}(N)$ or, more efficiently, keep a counter of each particle's collisions and identify an event as invalid only when resolving it.

Solution. We implemented a 2D system of spherical particles with diameter d and mass $m = 1$ in a box with side length L assuming perfect slip. Thus, we have to consider two types of collisions:

- Particle-wall collisions: Given the position $\boldsymbol{r}$ and the velocity $\boldsymbol{v}$ of a particle, we compute

[1] The bound is even tighter in $1D$. Also methods for an insertion time of $\mathcal{O}(1)$, i.e. $\mathcal{O}(N)$ in total, have been proposed: https://arxiv.org/pdf/physics/0606226.pdf.

four different times:

$$t_1 = \frac{L - d/2 - r_x}{v_x} \quad t_2 = \frac{d/2 - r_x}{v_x} \quad t_3 = \frac{L - d/2 - r_y}{v_y} \quad t_4 = \frac{d/2 - r_y}{v_y}$$

The collision time t_C is then given by the smallest positive of these.

- Particle-particle collisions: Given $\boldsymbol{r} = \boldsymbol{r}_i - \boldsymbol{r}_j$ and $\boldsymbol{v} = \boldsymbol{v}_i - \boldsymbol{v}_j$ for two particles i and j, we can compute the times:

$$t_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

where $a = \langle \boldsymbol{v} | \boldsymbol{v} \rangle$, $b = 2 \langle \boldsymbol{r} | \boldsymbol{v} \rangle$ and $c = \langle \boldsymbol{r} | \boldsymbol{r} \rangle - d^2$. If $a = 0$ (particles do not move relative to each other) or $b^2 < 4ac$ (particles cross their trajectories but at different times), no collision occurs and we set $t_C = \infty$. Otherwise we choose the smallest positive solution as the collision time.

A screenshot of a system with $N = 20$ particles with diameter $d = 2$ in a box with side length $L = 30$ can be observed in Fig. 1.

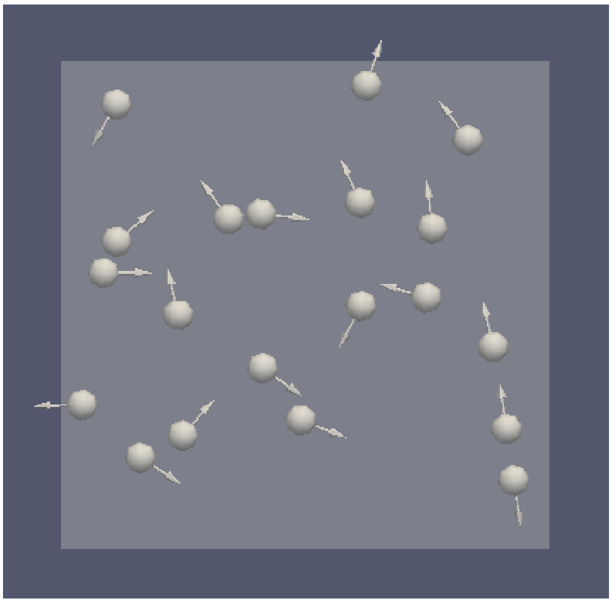

Figure 1: Screenshot of an event-driven MD simulation with 20 particles in a box.