Lecture 13: Exercise on the cell list

Simulate N Brownian particles in a two-dimensional box of size $B \times B$, with reflective boundary conditions. Each particle has position $\vec{x}_i = (x_i^0, x_i^1)$ and follows the time-discretized Euler-Maruyama dynamics with increments

$$d\vec{x}_i = \mu_i \vec{F}_i(x)dt + \sqrt{2D_i}\vec{\mathcal{B}}_i$$

with time step dt, mobility μ_i, diffusion constant D_i, force $\vec{F}_i(x)$ depending on all particles' positions $x = (\vec{x}_0, \ldots, \vec{x}_{N-1})$. Each component of the Gaussian white noise term $\mathcal{B}_i^\alpha$ ($\alpha = 0, 1$) is drawn from a zero-mean normal distribution with variance $\sqrt{dt}$.

Each pair of particles interacts with a repulsive potential energy depending on their distance $r_{ij} = |\vec{x}_i - \vec{x}_j|$ and a reference distance σ_{ij},

$$U(r_{ij}) = \varepsilon\, e^{-r_{ij}^2/(2\sigma_{ij}^2)}$$

We assign a radius R_i to each particle and set $\sigma_{ij} = R_i + R_j$. Note that $U(|\vec{r}|)$ yields a central force $\vec{F}_U(|\vec{r}|)\hat{r}$. We cutoff this force at $r_c = 4\sigma_{ij}$ (i.e., it is set to zero for $r > r_c$). The total force F_i on each particle is a sum of F_U pairwise forces with other particles in its surroundings.

To introduce thermodynamics and physics at a temperature T (with $k_B = 1$), we set $D_i = \mu_i T$, and mimic Stokes' law by setting $\mu_i = 1/R_i$.

The goal of this exercise is simulating this system also for large N values. To this end, implement the cell list algorithm.

With everything in place, study the diffusivity as a function of the number density $\rho = N/B^2$. Specifically, study the mean square displacement along the x-direction, $\Delta(t) = \left\langle [x^0(t) - x^0(0)]^2 \right\rangle$, for different ρ values. Usually, such quantity is plotted as a function of t in a log-log diagram. For low ρ, the mean square displacement should follow $2D_i t$ up to a saturation due to the finite box size. For large ρ, the behavior should be more complex, effectively with lower diffusivity and possibly with plateaus due to particles' caging. Such effect emerges if neighboring particles do not move much due to the high density and constrain the observed particle to remain caged for some time in a region.

For large ρ, the system would cristallize if all R_i are the same. We avoid this by choosing $R_i = R^A$ for half of the particles and $R_i = R^B \neq R^A$ for the other ones.

Parameters

- $B = 100$
- $R_i = R^A = 1.25$ for $0 \leq i < N/2$ (particles of kind A)
- $R_i = R^B = 1$ for $N/2 \leq i < N$ (particles of kind B)
- $T = 1$
- $\varepsilon = 10$
- A possible list of N to have ρ over some orders of magnitude is $N = 2, 10, 50, 200$ and maybe 500.

1. Which side ℓ for the cell in the cell list do you choose with these parameters?
2. Is $\Delta^A(t)$ for particles A different from $\Delta^B(t)$ for particles B?
3. How do Δ's change with ρ?