# 13.0 Langevin simulation of many particles

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## 13.1 Cell list

Comment on the two implementations of the cell list, namely the version for particle 0 and the version for smaller particles. Which is the best algorithm?

The provided code features two implementations of the cell list algorithm: one for particle 0 and another for smaller particles. During initialization, the particle position matrix $x$ situates the big particle 0 at the center of the box, while randomly placing all other smaller particles. Simultaneously, the trap, which affects only the big particle and follows deterministic dynamics, is positioned at the box's center and moves linearly with velocity $v_{\text{trap}}$.

**Particle 0**

The force acting on the big particle, $\vec{F}_0$, comprises two primary components. Firstly, there is the harmonic trap force given by $\vec{F}_{\text{trap}} = k_{\text{trap}} \cdot (\vec{x}_{\text{trap}} - \vec{x}_0)$, where $\vec{x}_{\text{trap}}$ and $\vec{x}_0$ are the positions of the trap and particle 0, respectively.

The second component arises from interactions with smaller particles within a specified cutoff distance. Specifically, we consider smaller particles located in neighboring cells denoted as $Dv_0$. These interaction forces stem from an exponential potential dependent on the distance between particle 0 and each smaller particle. Mathematically, this component is expressed as $\vec{F}_{\text{int}} = f_{p0} \cdot \exp(-r^2 \cdot \text{inv}_0)$, where $r^2$ represents the distance squared between particle 0 and the periodic image of the smaller particle $i$, and the constants involved are defined as $f_{p0} = \frac{Q \cdot \epsilon_0}{\sigma_0^2}$ and $\text{inv}_0 = \frac{1}{2\sigma_0^2}$.

It's important to note that the force applied to particle 0, $\vec{F}_0$, is subtracted from the force applied to the smaller particles, ensuring that the forces are equal in magnitude and opposite in direction.

**Small particles**

Small particles also undergo interactions among themselves, which are characterized by a Gaussian repulsion term similar to the one we have already described: $\vec{F}_{\text{int,ss}} = f_p \cdot \exp(-r^2 \cdot \text{inv})$, where $r^2$ represents the distance squared between two smaller particles $i$ and $ii$ in neighbouring cells.

The special case where small particles are organized into polymers of length $L_p$ warrants separate discussion. Specifically, when $L_p > 1$, small particles experience polymer bond interactions characterized by a spring-like force between adjacent particles in the polymer chain. Mathematically, this interaction is expressed as:$F_{\text{poly}} = k_{pol} \cdot v$, where $v$ is the shortest distance vector between consecutive particles $ii$ and $i$, considering periodic boundary conditions.

All particle positions, including the big particle, undergo a numerical integration step using the Euler method. This step adds the contribution of deterministic forces and stochastic noise ( particle 0: $stoch0 \cdot \mathcal{N}(0,1)$ and small particles: $stoch \cdot \mathcal{N}(0,1)$) to each particle's position update, introducing thermal fluctuations.

## 13.2 Active matter

We aim to use the $N$ small particles to implement $N/2$ "active dumbbells", each one representing a bacterium with propulsion. Each one is composed of particles $i$ and $i+1$. They are kept apart by a harmonic spring of rest length $\Lambda = 1/2$. Moreover, particles $i$ and $i+1$ feel a propulsive force $\vec{f}$ oriented as the vector $\vec{r_i} \to \vec{r_i}+1$. and of magnitude $f$. Implement this system. To study the active Matter and diffusion of the probe, remove the harmonic trap that would keep the probe confined and study the diffusion of the probe in the bath of $N/2$ active dumbbells. Focus on the mean square displacement as a function of time. Study it for different values of $f$, starting from $f = 0$ (equilibrium) . How does the probe's mean square displacement change with $f$?

To solve this exercise, I made two primary modifications to the provided code:

1. I altered the polymer bond by incorporating a harmonic potential with a rest length $\Lambda$ between the two units of the dumbbell. This modification results in a spring force given by $\vec{F_{\text{spring}}} = k_{\text{pol}} \left(|r| - \Lambda\right) \frac{r}{|r|}$.

2. I introduced an active force acting on the second unit of each dumbbell, represented by $\vec{F_{\text{active}}} = k_{\text{active}} \frac{r}{|r|}$.

| $nstep\_save$ | $N$ | $L$ | $Bx$ | $By$ | $T$ | $v\_ini$ | $Nv$ | $v\_x\_dec$ |
|---|---|---|---|---|---|---|---|---|
| 100 | 500 | 2 | 20 | 20 | 1 | 0 | 1 | 0 |
| $k$ | $kp$ | $R$ | $eps$ | $R0$ | $eps0$ | $\Lambda$ | $k\_active$ | |
| 0 | 10 | 0.125 | 10 | 1.25 | 20 | 0.5 | [1,4,6,8] | |

Table 1: Parameters used in the simulation, where $N$ is the number of small particles, $L$ is the polymer lenght, $B_x$ and $B_y$ are the box sizes, $T$ is the temperature, $k_{trap}$ is the stiffness of the trap, $k_{pol}$ is the stiffness of the polymer bonds, $R/R_0$ is the radius of each particle/probe, $eps/eps_0$ is the repulsive energy of particles/probe, $\Lambda$ is the rest lenght of the spring between dumbells and $k_{\text{active}}$ is the constant of the active force of each dumbell.

I studied the diffusion of the probe in a bath containing $N/2$ active dumbbells for various values of the active force constant $k_{\text{active}}$ and for the remaining parameters reported in the above figure.. The plot clearly shows that as the value of the active force increases, the probe spreads in space more quickly. The same plot, when considering just the small particles, yields more defined lines, showing a linear trend in time.

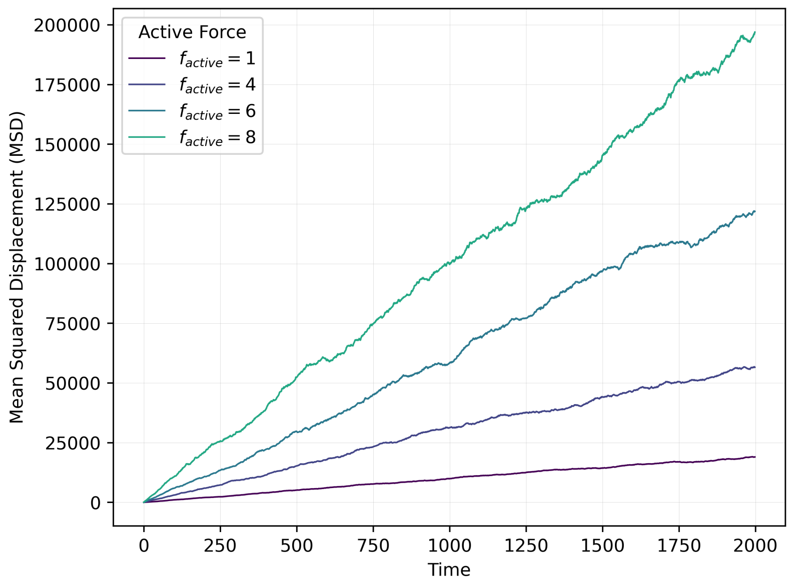


Figure 1: All small particles diffusion for different values of $k_{\text{active}}$.

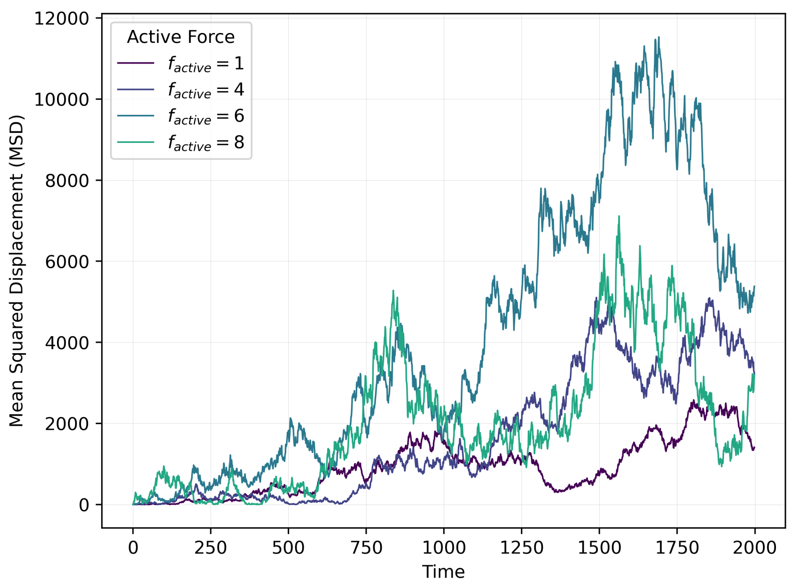


Figure 2: Probe diffusion for different values of $k_{\text{active}}$.

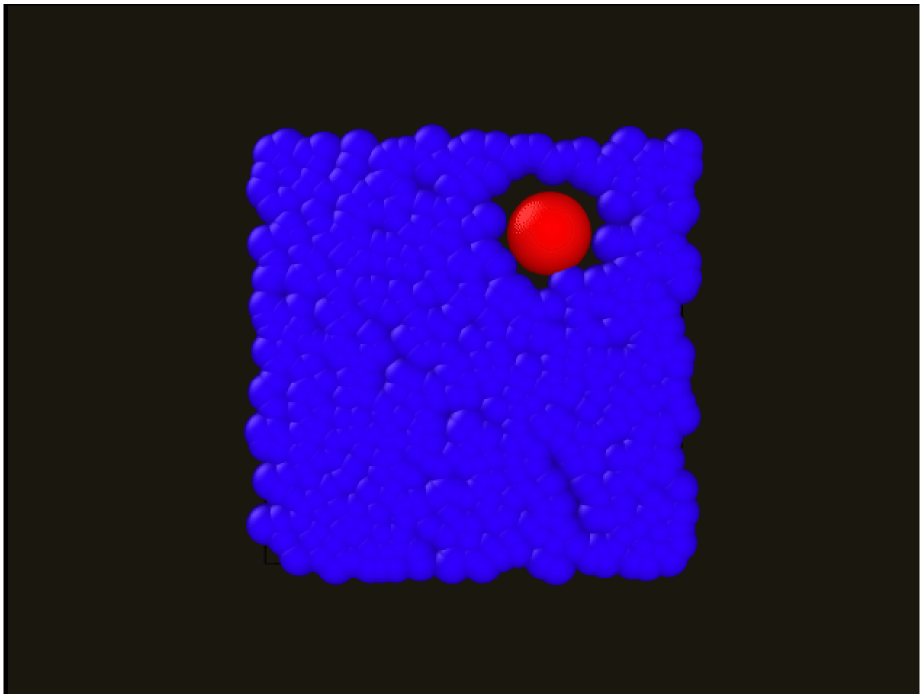

Figure 3: A single frame of the gif showing the diffusion of the probe in the bath of $N/2$ active dumbells. The **complete gif** can be found in the directory of the exercise 13.

I used the OVITO software to create some GIFs that show the diffusion of the probe in the bath of active dumbbells. For the GIFs, I used the same simulation data as reported in the table with $k_{active} = 1$. Additionally, I used the probe's radius as $R0$, while the radius of the dumbbells was increased by 200% to ensure the small particles were visible. I also created a version with the radius of the small particles increased even more. Both versions of the GIFs can be found in the folder chapter 13, and here is a frame.