1.14 Langevin simulation of many particles

This exercise is based on the C code provided in the previous lesson.

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?

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.

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?

Plausible or mandatory $(*)$ parameters .

```
nstep_save=0; // saving configs if >0 (e.g. =10 saves every 10 Dt)
N=2000;       // nr of small particles
Lp=2;         // length of each dumbbell
box[0]=40;    // box size, x
box[1]=40;    // box size, y
T=1;          // temperature (kB=1)
v_trap_ini=...; // smallest velocity of the trap. NOT USED
Nv=...;              // number of velocities. NOT USED
v_per_decade=...;    // velocities per decade. NOT USED
(*) k_trap=0; // stiffness of the trap
k_pol=10;     // stiffness of the polymer bonds
(*) R=0.125;  // "radius" of each particle
eps=10;       // repulsive energy of particles
R0=1.25;      // "radius" of the probe
eps0=20;      // repulsive energy of the probe
dt=1e-3;      // integration time step
tt=10000;     // total time of the simulation

---ADD---
Lambda=0.5
f_active=....
```

To generate an mp4 video from the folder containing the png frames, a command might look like:

```
ffmpeg -r 10 -f image2 -pattern_type sequence -start_number 100001 -i fr_%06d.png -s 500x500 video.mp4
```