11 Langevin and Brownian Dynamics

Brownian time and length scales (pen&paper)

- In the overdamped limit, the diffusion scale becomes the relevant time scale. Using the Stokes-Einstein formula, estimate the time scale of a particle of diameter $\sigma = 10^{-8}m$ to diffuse in water over a distance equal to its own diameter. Is this time scale compatible with the requirement of the Brownian description?
- Conversely, show that, above $\sigma = 5\mu m$, Brownian motion becomes negligible. Which other force becomes relevant?

(*Hint*: The energy scale is always the thermal energy at room temperature; for simplicity, the object has roughly the same density as water; also, the object is spherical.)

Brownian motion Consider an isolated particle (or an "ideal gas" of non interacting Brownian particles). Set $m = 1$, $\sigma = 1$ and $\epsilon = 1$ as units of mass, length, energy. Set $L = 20\sigma$ and apply periodic boundary conditions. Choose initial conditions as you prefer; the most convenient choice is to set all the starting positions in the origin.

- Brownian motion in the bulk: Simulate this system in the overdamped limit (first order integrator) or in the "underdamped" limit (Stochastic Velocity Verlet or with the second order integrator). Compute the mean square displacement and discuss what happens upon varying the temperature (0.1< T^* <2, $\gamma = 1\tau^{-1}$) and the friction coefficient (0.1< $\gamma\tau$ <100, $T^* = 1$). Pick 5-10 values in each case. Compare the results with the theory. Further measure the distribution of the displacement of the particle(s) along one axis at different times: what changes to the distribution as time progresses?
- Brownian motion in an harmonic trap: consider single overdamped particle (or, again, an ideal gas of non-interacting overdamped particles) in an harmonic trap, centred in a certain point of the box $\vec{r}_0$ (for simplicity, choose the origin of the reference frame or the centre of the box).

  $$V(r) = \frac{1}{2}K(\vec{r} - \vec{r}_0)^2 \tag{1.25}$$

  Set $L = 20\sigma$ and apply periodic boundary conditions. Fix the initial conditions in the centre of the trap. Compute the average and the variance of the position along one axis as a function of $0.1 < K\sigma^2/\epsilon < 10$, $0.1 < \gamma\tau < 100$, 0.1< T^* <2 (Note: when varying one quantity, keep the others fixed to unitary value). Measure both the mean square displacement and the displacement distribution along one axis. Discuss the result, in comparison to the bulk case.