Microscopic models of active matter: Exercise set

October 23, 2025

1 A single Active Brownian particle

Consider an active Brownian particle in two dimensions, following the overdamped Langevin equations of motion

$$\zeta \dot{\mathbf{r}} = F_{\text{act}} \hat{\mathbf{n}} + \boldsymbol{\eta}^T \tag{1}$$

$$\dot{\theta} = \eta^r, \quad \hat{\mathbf{n}} = (\cos\theta, \sin\theta) \tag{2}$$

where F_{act} is the active force, η^T are the thermal fluctuations and η^r is rotational diffusion. Write a program to simulate such a particle in space and time, and extract its full trajectory data $x(t)$, $y(t)$ and $\theta(t)$. This is not very computationally intensive and your program should run in under a minute if written e.g. in python.

To do this effectively, we will work in simulation units. We choose a particle of radius 1, and we divide the first equation through by ζ. We then define the active velocity $v_0 = F_{\text{act}}/\zeta$, and the rescaled thermal noise $\tilde{\boldsymbol{\eta}}^T = \boldsymbol{\eta}^T/\zeta$. Using the fluctuation-dissipation theorem, the thermal noise has mean 0 and its x and y components separately have a variance $\langle(\tilde{\boldsymbol{\eta}}_i^T)^2\rangle = 2k_bT/\zeta$. We will assume that this is also 2, i.e. units where we measure energies in units of k_bT. Finally, we draw the rotational diffusion η^r from a Gaussian distribution with mean 0 and variance $2D_r$.

Use the slides on numerical simulations from the course material to implement your program. Then plot the trajectory for a couple of realisations of the system at different v_0 and D_r.

Use this information to compute several statistical quantities:

1. The angular mean square displacement, $\langle(\theta(t) - \theta(0))^2\rangle$. What is its scaling and prefactor?

2. The full mean square displacement $\langle(\mathbf{r}(t) - \mathbf{r}(0))^2\rangle$. Compare it to its theoretical prediction as a function of time, D_r and v_0.

Finally, to see much prettier ABP trajectories and MSDs, repeat your simulation for a system with zero temperature, i.e. where the thermal noise amplitude $\tilde{\boldsymbol{\eta}}_i^T = 0$.

Tip: To get better statistical results for your MSD, use a sliding window and the fact that things are time-translation invariant. Concretely, you want to average over all t_0 in your dataset where you can compute $\mathbf{r}(t+t_0) - \mathbf{r}(t_0)$, i.e. as long as $t + t_0$ is shorter than the simulation time.

2 Active colloid phases

Using the 'brownian.py' code that we discussed this week, investigate the phase diagram active and passive colloids in two dimensions.

For simplicity stay at $T = 0$, and vary packing fraction ϕ, active driving speed v_0 and rotational diffusion constant D_r. This makes a 3-dimensional phase diagram that you can't fully explore. Therefore, focus on two slices: 1. A diagram as a function of ϕ and v_0 at constant D_r as shown in the lecture slides. 2. If you have time, a diagram as a function of v_0 and D_r at constant ϕ - I suggest $\phi = 0.95$ so you can see the dense phases or $\phi = 0.5$ for the liquid phases.

Trace approximatively quantitative phase boundaries on your phase diagram. Note: To do this properly, one would need much more time and simulation data, not to mention quantitative analysis. Try to be within 10% on the ϕ axis and within a factor of 2 on the T axis.

Identify the following phases:

- The active gas phase, with no liquid structure and no motility induced phase separation
- The active liquid phase, with liquid structure and no phase separation
- The motility induced phase separation phase where the system clusters. Recall that this happens at large ($\gg 10$) dimensionless Peclet number, where $Pe = V_0/(rD_r)$, and r is the typical particle radius. Note that the system size and simulation speed here is not quite sufficient to see this phase very clearly.
- The active crystal phase
- The active glass phase, by changing polydispersity in the simulation