Project for MSDM5003: Stochastic simulation for an active Brownian particle

Report due on December 6, 2023

1. Background

Self-propelled Brownian particles have come under the spotlight of the physical and biophysical research communities. These active particles are biological or man-made microscopic and nanoscopic objects that can propel themselves by taking up energy from their environment and converting it into directed motion. On the one hand, self-propulsion is a common feature in microorganisms and allows for a more efficient exploration of the environment when looking for nutrients or running away from toxic substances. On the other hand, tremendous progress has recently been made toward the fabrication of artificial microswimmers and nanoswimmers that can self-propel based on different propulsion mechanisms.

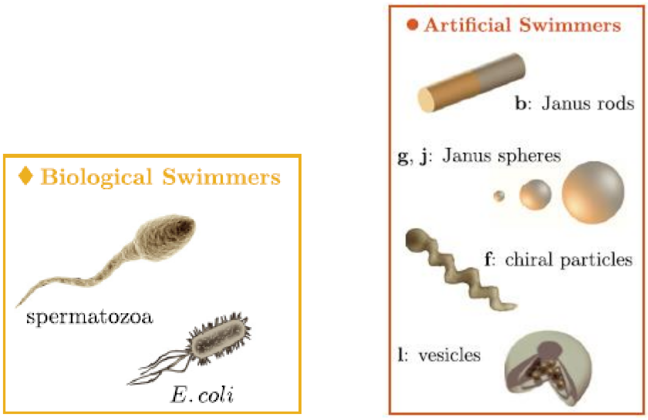

Figure 1. Self-propelled Brownian particles are biological or man-made objects capable of taking up energy from their environment and converting it into directed motion. They are microscopic and nanoscopic in size and have propulsion speeds (typically) up to a fraction of a millimeter per second.

2. Model: active Brownian motion

Consider a self-propelled particle with velocity v. The direction of motion is subject to rotational diffusion, which leads to a coupling between rotation and translation. The corresponding stochastic differential equations in 2-dimensional space are

$$\frac{dx}{dt} = v\cos\varphi, \qquad (1)$$

$$\frac{dy}{dt} = v\sin\varphi, \qquad (2)$$

$$\frac{d\varphi}{dt} = \sqrt{2D_R}\,\xi. \qquad (3)$$

Here the particle position is at $\mathbf{r}(t) = \left(x(t), y(t)\right)$ and the direction of motion is $\mathbf{n}(t) = \cos\varphi(t)\mathbf{i} + \sin\varphi(t)\mathbf{j}$ in two dimensions. The active velocity v is a positive constant, D_R is the rotational diffusion coefficient, and ξ is a Gaussian white noise satisfying $\langle \xi \rangle = 0$ and $\langle \xi(t_2)\xi(t_1) \rangle = \delta(t_2 - t_1)$ (i.e. with zero mean and correlation $\delta(t)$).

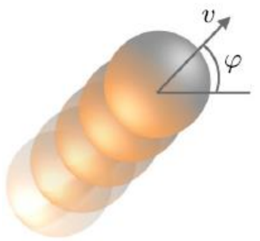

Figure 2. An active Brownian particle with velocity v and direction of motion φ in two dimensions.

3. Tasks

3.1 Autocorrelation of the direction of motion

The autocorrelation of the direction of motion is given by

$$\langle \mathbf{n}(s+t)\cdot\mathbf{n}(s) \rangle = \lim_{T\to\infty}\left[\frac{1}{T}\int_0^T \mathbf{n}(s+t)\cdot\mathbf{n}(s)ds\right] = \exp\left(-\frac{|t|}{\tau_R}\right), \quad (4)$$

where τ_R is the orientational persistence time. By carrying out the simulation for the stochastic equation (3), you will (i) compute $\langle \mathbf{n}(s+t)\cdot\mathbf{n}(s) \rangle$ as a function of t and (ii) show that τ_R depends on the rotational diffusion coefficient D_R through the relation $\tau_R = 1/D_R$.

Hint: The autocorrelation $\langle \mathbf{n}(s+t)\cdot\mathbf{n}(s) \rangle$ shall be numerically computed and fitted to an exponential function of t to determine τ_R. The dependence of τ_R on D_R shall be determined by carrying out the simulation for a set of selected values of D_R.

3.2 Effective diffusion coefficient in two dimensions

By carrying out the simulation for the stochastic equations (1), (2) and (3), you will compute the mean square displacement

$$\mathrm{MSD}(t) = \left\langle [\mathbf{r}(t)-\mathbf{r}(0)]^2 \right\rangle = \left\langle [x(t)-x(0)]^2 + [y(t)-y(0)]^2 \right\rangle, \quad (5)$$

which is analytically given by $2v^2\tau_R t$ for $t \gg \tau_R$. You are required to verify this theoretical result by computing $\mathrm{MSD}(t)$ for a set of selected values of v and $\tau_R = 1/D_R$. Here $\mathrm{MSD}(t) = 2v^2\tau_R t = 4D_{\mathrm{eff}}t$ in two dimensions gives the effective diffusion coefficient $D_{\mathrm{eff}} = v^2\tau_R/2$.

References

1. Romanczuk, P., Bär, M., Ebeling, W., Lindner, B., & Schimansky-Geier, L. (2012). Active Brownian particles. The European Physical Journal Special Topics, 202(1), 1-162.

2. Bechinger, C., Di Leonardo, R., Löwen, H., Reichhardt, C., Volpe, G., & Volpe, G. (2016). Active particles in complex and crowded environments. Reviews of Modern Physics, 88(4), 045006.

Note: These are long review articles. You only need to read a small part for this project.

Your report should include the following components:

1. A description of the dynamics governed by equations (1), (2), and (3).

2. Your understanding of equation (4), the behavior of the autocorrelation of the direction of motion.

3. The autocorrelation $\langle \mathbf{n}(s+t)\cdot\mathbf{n}(s)\rangle$ shall be numerically computed and fitted to an exponential function of t to determine τ_R. The dependence of τ_R on D_R, $\tau_R = 1/D_R$, shall be determined by carrying out the simulation for a set of selected values of D_R.

4. Your understanding of the behavior of $\mathrm{MSD}(t) \cong 2v^2\tau_R t$ for $t \gg \tau_R$.

5. You shall verify $\mathrm{MSD}(t) \cong 2v^2\tau_R t$ by computing $\mathrm{MSD}(t)$ for a set of selected values of v and $\tau_R = 1/D_R$.

Regarding the format of the midterm project report, please note the following:

1. A ***short*** report (two to three A4 pages, not including the source code) should be submitted.

2. The report should address all the ***five*** points listed in the end of the project assignment.

3. The numerical results (for the autocorrelation of $\mathbf{n}(t)$ and the mean square displacement $\mathrm{MSD}(t)$) need to be presented by using ***figures with caption***.

4. ***The source code*** needs to be included as the appendix to the report.