Simulating Active Brownian Motion

Project Report

Fidha Nazreen K M

Introduction

Unlike passive Brownian particles, active Brownian particles are able to propel themselves which drive them to the state of non-equilibrium. Understanding the motion of the active particles (micro-swimmers) provide insights into the non-equilibrium phenomena and is key to the development of its numerous applications.

This project is based on the paper 'Simulation of the active Brownian motion of a micro swimmer' [American Journal of Physics 82, 659 (2014)]. In this work, 2-dimensional active Brownian motion was modelled using a set of stochastic equations. The system of equations was solved by employing finite-difference algorithm. The motion of the particles was first modelled in a homogeneous environment and further extended to complex environments where the particles encountered an obstacle.

In this project, following the methods in the paper, several results were reproduced. The programming part was done using Python. The following sessions illustrate the mathematical model, implementation of the algorithms and discuss the results in detail.

Model

Passive Brownian motion of a spherical particle of radius R can be expressed as a sum of random diffusion processes with a translational diffusion constant,

$$D_T = \frac{K_B T}{6\pi\eta R}$$

and a rotational diffusion constant,

$$D_R = \frac{K_B T}{8\pi\eta R^3}$$

where, K_B is the Boltzmann Constant, T the temperature, η the fluid viscosity.

When it comes to active particles, a velocity component v, that corresponds to the self-propulsion part is added. In the case of chiral particles, the torque which is represented by an angular velocity component Ω, also comes into the picture.

The final set of Langevin equations that describes how the particle orientation $\varphi(t)$ and the position of the particle $[x(t), y(t)]$ change with respect to time in two-dimension is given by,

$$\frac{d}{dt}\varphi(t) = \Omega + \sqrt{2D_R}W_\varphi$$

$$\frac{d}{dt}x(t) = vcos\varphi(t) + \sqrt{2D_T}W_x$$

$$\frac{d}{dt}y(t) = vsin\varphi(t) + \sqrt{2D_T}W_y$$

where, W_φ, W_x and W_y are the terms that correspond to the independent stochastic processes with mean 0 and standard deviation 1. To solve the above set of stochastic differential equations, finite difference algorithm can be used. Discretizing the continuous time solutions $[\varphi(t), x(t), y(t)]$ by doing the following substitutions,

$$\varphi(t) = \varphi_i$$

$$x(t) = x_i$$

$$y(t) = y_i$$

$$\frac{d}{dt}\varphi(t) = \frac{\varphi_i - \varphi_{i-1}}{\triangle t}$$

$$\frac{d}{dt}x(t) = \frac{x_i - x_{i-1}}{\triangle t}$$

$$\frac{d}{dt}y(t) = \frac{y_i - y_{i-1}}{\triangle t}$$

we arrive at the following set of finite difference equations,

$$\varphi_i = \varphi_{i-1} + \Omega \triangle t + \sqrt{2D_R \Delta t} w_{\varphi,i}$$

$$x_i = x_{i-1} + v \cos \varphi_{i-1} \triangle t + \sqrt{2D_T \Delta t} w_{x,i}$$

$$y_i = y_{i-1} + v \sin \varphi_{i-1} \triangle t + \sqrt{2D_T \Delta t} w_{y,i}$$

Here, the values of $w_{\varphi,i}$, $w_{x,i}$ and $w_{x,i}$ can be taken randomly from a normal distribution of mean 0 and standard deviation 1.

A particle with radius $R = 1\ \mu m$, temperature $T = 300\ K$, and immersed in a medium of viscosity $\eta = 0.001\ Ns/m^2$ is considered throughout.

Homogeneous Environment

Achiral Particles

First, to simulate the motion of achiral particles (with angular velocity Ω= 0 rad/s^2), for a fixed velocity and the initial conditions $[\varphi(0), x(0), y(0)]$ = $[0, 0, 0]$, the finite difference equations were solved for each time step $t_i = i\triangle t$ for the duration of 10 s in increments of $\triangle t$ = 0.01 s. The simulations were carried out four times to obtain four different particle trajectories. This method was repeated for v = 0, 1, 2 and 3 $\mu m/s$ and the trajectories were plotted to obtain fig.0.0.1.

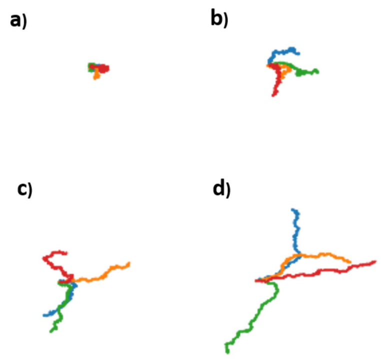

Figure 0.0.1: Achiral Particles in Homogeneous Environment. a), b), c) and d) are the trajectories for the velocities 0, 1, 2 and 3 $\mu m/s$ respectively. Marked in green, red, orange and blue are the four different particle trajectories with the same initial condition (0,0,0).

In the fig. 0.0.1 a) we can see that the position of the particles are concentrated around their initial position when v = 0 $\mu m/s$. As the velocity increases, we can see that the particle is traversing longer distances and the trajectories are becoming spread (b) - d)).

Chiral Particles

Choosing the angular velocity, Ω to be 3.14 or -3.14 rad/s^2, the velocity to be 31 $\mu m/s^2$ and the initial conditions $[\varphi(0), x(0), y(0)] = [0,0,0]$, the finite difference equations were solved for each time step $t_i = i\triangle t$ for the duration of 0 to 10 s in increments of 0.01 s and the trajectories were plotted to obtain fig. 0.0.2.

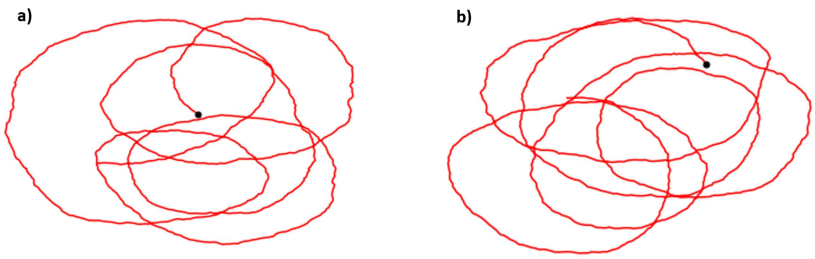

Figure 0.0.2: Chiral Particles in Homogeneous Environment. a) Trajectory of a particle with Ω = 3.14 rad/s^2 b) Trajectory of a particle with Ω = - 3.14 rad/s^2. Marked in black dot is the final position of the particle.

From fig.0.0.2 , we can see that when the angular velocity, Ω = 3.14 rad/s^2, the particle moves in anti-clockwise direction and when Ω = - 3.14 rad/s^2 the particle moves in clockwise direction in an almost spiral manner.

Mean Square Deviation

Mean square deviation (MSD) is a measure of how much a particle gets displaced from its initial position. It is expressed as ,

$$MSD(\tau) =< [x(t+\tau) - x(t)]^2 + [y(t+\tau) - y(t)]^2 >$$

In discrete time scales, MSD can be calculated from the trajectory $[x_n, y_n]$, at a time t_n with a time step of $\triangle t$ as,

$$MSD(m\triangle t) =< [x_{n+m} - x_n]^2 + [y_{n+m} - y_n]^2 >$$

Theoretically, MSD can be calculated as,

$$MSD(\tau) = [4D_T + v^2\tau_R]\tau + \frac{v^2\tau_R^2}{2}[\exp^{-2\tau/\tau_R} - 1]$$

where, $\tau_R = 1/D_R$, is the time scale of the rotational diffusion. From the equation, we can see that in shorter time scales, the motion of the particles is dominated by self propulsion and is ballistic with a τ^2proportionality. When it comes to longer time scales ($\tau > \tau_R$), the motion becomes diffusive and MSD becomes linearly proportional to τ.

Keeping the values of Ω as 0, a single trajectory was generated for velocities v = 0, 1, 2 and 3 $\mu m/s$ each using the finite difference method. For each of these trajectories, for τ values ranging from 0 to 10 s in increments of $\triangle t = 0.01$ s, MSD was calculated using the discrete time scale formula. MSD values were plotted against time and both the axes were converted to log scale to obtain fig. 0.0.3 a).

Theoretical values of MSD were calculated by substituting the τ values ranging from 0 to 10 s in increments of 0.01 s in the above formula for velocities v = 0, 1, 2 and 3 $\mu m/s$. The MSD values were plotted against time and both the axes were converted to log scale to obtain the graph as shown in fig. 0.0.3 b).

In both the plots, a vertical line was drawn at the rotational diffusion time scale to illustrate the transition from ballistic regime to diffusive regime.

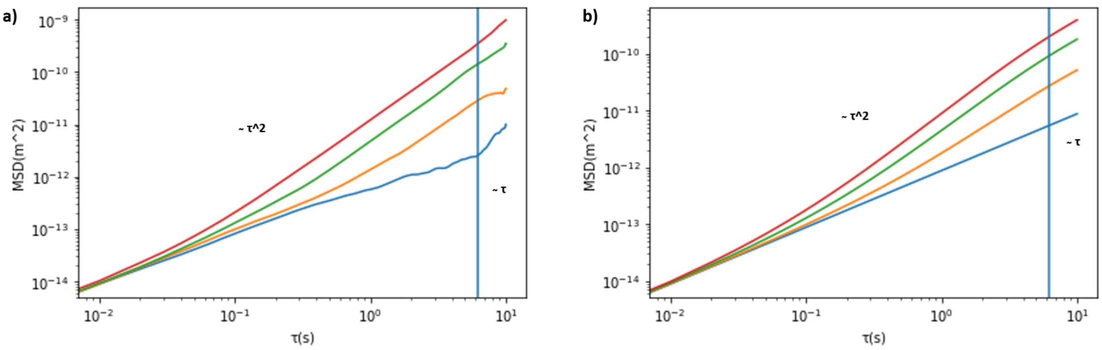

Figure 0.0.3: Mean Square Deviation Plots a) Numerical value of MSD from the trajectories generated. b) Theoretical Value of MSD. Blue, orange, green and red lines corresponds to velocities 0, 1, 2 and 3 $\mu m/s$ respectively. The vertical line shows the rotational diffusion time scale.

From the fig. 0.0.3, we can see that the numerical calculation of MSD from the generated trajectory is similar to the theoretical values. For $v > 0$ $\mu m/s$, we can see that in shorter time scales, the motion is ballistic, while for larger time scales, the motion is dominated by diffusion.

Complex Environment (Circular Pore)

Whenever an active particle encounters a barrier in its path, it slides along the surface of the barrier. To model this process the reflective boundary conditions can be implemented. This ensures that the particle is confined within the boundaries.

Inorder to confine a particle inside a circular pore of radius R_c, the algorithm used to implement the reflective boundary conditions is applied as given below,

- When a particle moves from its previous position $\mathbf{r}_{i-1} = [x_{i-1}, y_{i-1}]$ within the circle to its new position $\tilde{\mathbf{r}}_\mathbf{i} = [x_i, y_i]$, check if the new point is within the circle, employing the condition $||\tilde{\mathbf{r}}_\mathbf{i}|| \leqq R_c$.

- If the new position lies within the circle, then the new point $\tilde{\mathbf{r}}_\mathbf{i}$ becomes $\mathbf{r_i}$.
- If the new point lies outside the circle, then find the point $\mathbf{p}$, where the line drawn between the points $\tilde{\mathbf{r}}_\mathbf{i}$ and $\mathbf{r_{i-1}}$ intersects the circle.
- Once we have the point $\mathbf{p}$, find the line l in the direction of the unit tangent vector $\hat{\mathbf{t}}$ and unit vector $\hat{\mathbf{n}}$ normal to the circle at point $\mathbf{p}$.
- The point $\tilde{\mathbf{r}}_\mathbf{i}$ is then reflected on the tangent line l. Then the reflected point given by,

  $$\mathbf{r_i} = \tilde{\mathbf{r}}_\mathbf{i} - 2[(\tilde{\mathbf{r}_i} - \mathbf{p}).\hat{\mathbf{n}}]\hat{\mathbf{n}}$$

  becomes the new point.

To find the point $\mathbf{p}$, vector algebra was employed as follows,

- Let $\mathbf{q}$ be the centre. Here a circle centred at origin is considered. Hence $\mathbf{q} = [0,0]$
- Let $\mathbf{v1}$ be the vector from $\mathbf{q}$ to $\mathbf{r_{i-1}}$.
- Let $\mathbf{v2}$ be the vector from $\mathbf{q}$ to $\tilde{\mathbf{r}}_\mathbf{i}$.
- Let λ be any scalar, $\mathbf{v1} + \lambda(\mathbf{v2} - \mathbf{v1})$ gives any point on the line between $\tilde{\mathbf{r}}_\mathbf{i}$ and $\mathbf{r_{i-1}}$, for varying λ. Substituting the x and y components in the equation of circle, $x^2 + y^2 = R_c^2$ and solving the quadratic equation in λ, two solutions will be obtained.
- Substituting the values of λ in the equation $\mathbf{v1} + \lambda(\mathbf{v2} - \mathbf{v1})$, gives two points $p1$ and $p2$.
- From $\mathbf{v1}$ or $\mathbf{v2}$, the closest point among $p1$ and $p2$ was found. This will be the point $\mathbf{p}$.

Once $\mathbf{p}$ is obtained, only the unit normal is required to find the reflected point $\mathbf{r_i}$. Since the unit normal lies in the same direction as that of the vector from $\mathbf{q}$ to $\mathbf{p}$, this vector was normalised to obtain $\hat{\mathbf{n}}$.

The radius of the circular pore was taken to be 20 μm. Employing the method mentioned above, fixing the angular velocity Ω at 0 rad/s^2 and the velocity v, choosing the initial conditions to be random within the μm range (chosen from a random distribution with mean 0 and standard deviation 1) , the finite difference equations were solved for each time step for the duration of 10 s in increments of $\triangle t$ = 0.01 s. The simulations were carried out four times to obtain four different particle trajectories.

The probability disribution inside a circle is symmetric and therefore the probability disribution across the radius will give the same results as that across the diameter. Here, the probability distribution across the radius was calculated. For a fixed velocity, points from all the four trajectories simulated in the previous step were taken. The entire circle was divided into circular strips of width $\triangle r$ = 0.1 μm. The number of points in each of these strips were counted and were plotted against the corresponding radii i.e. $r_i = i\triangle r$, where r_i takes values from 0 to 20 μm.

Both the particle trajectories with reflective boundary conditions and the probability distribution of points across the radius were found for v = 0, 5 and 10 $\mu m/s$ and plotted to obtain the results shown in fig. 0.0.4.

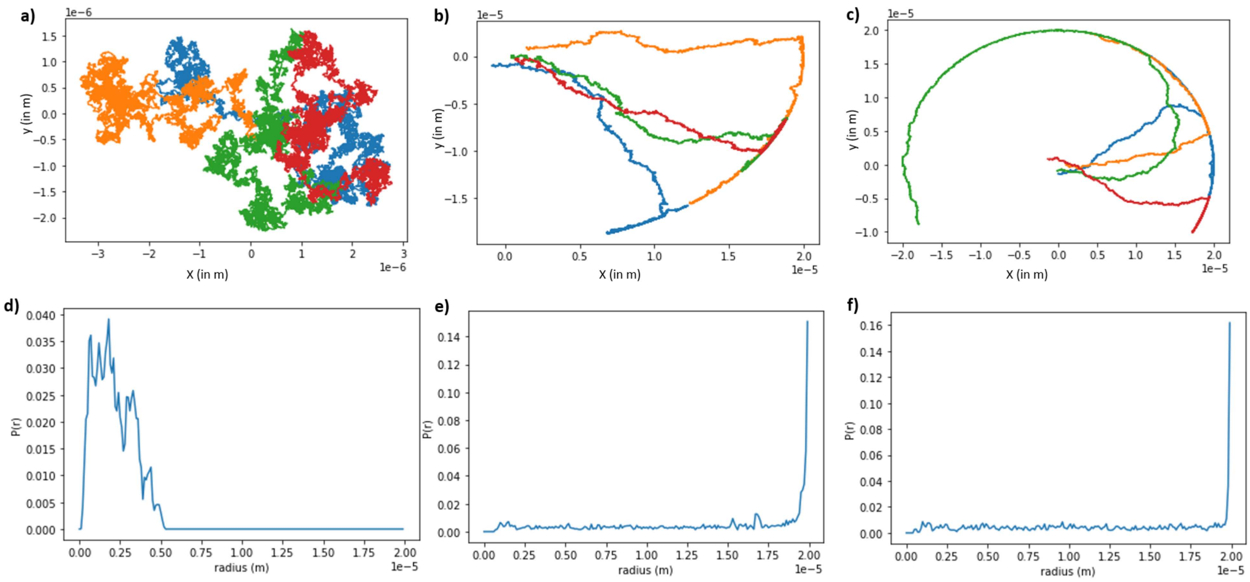

Figure 0.0.4: Trajectories confined in a circular pore and the corresponding radial probability distribution points. a) and d), b) and e) and, c) and f) corresponds to the particle trajectories confined in a circle of radius 20 μm and the corresponding probability distribution of finding the particle at a particular radius, where velocity v = 0 , 5 and 10 $\mu m/s$ respectively. Marked in green, red, orange and blue are the four different particle trajectories with different random initial conditions.

From the fig. 0.0.4, a) and d), we can see that when the velocity is 0 $\mu m/s$, the particle positions are clustered around their initial position. As the velocity increases, the particles reach the circular boundary and the trajectories form along them. We can also see that the probability of finding the particle at the circular boundary is increasing with the increase in velocity as shown in the fig. 0.0.4 e) and f).

The particles moving along the circular boundary and the maximum probability of finding the particle at the boundaries suggests the out of equilibrium nature of the active particles, as they show a clear deviation from the Maxwell - Boltzmann distribution.

Summary

Langevin equations that define two-dimensional active Brownian motion were solved using the finite-difference algorithm, for particles in homogeneous as well as complex environments (circular pore). In the homogeneous environment, in case of achiral particles, they travelled longer distances with larger velocities. In the case of chiral particles, depending upon the sign of the angular velocity, the particles formed almost spiral trajectories that bent in the clockwise or anti-clockwise direction. The mean square deviation for achiral particles with different velocities was calculated both theoretically and numerically. For non-zero velocities, it was seen that in shorter time scales, the motion is ballistic and for larger time scales, the motion becomes diffusive. Furthermore, the particles were confined inside a circle using reflective boundary conditions and the radial probability distribution of points were found. With the increase in velocity, particle trajectories were formed along the boundary, in turn increasing the probability of finding the particles near the edges of the circle. This finding validated their non-equilibrium character.