# Collective motion of squirmers in confined environments

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#### 1 Introduction

This internship is the continuation of a project realised last semester. The aim of the project was to develop numerical methods for modeling the dynamics of interacting squirmers. The squirmer is a model for active particles imitating the propulsion of bacteria.

A python code to simulate the behaviors of two interacting squirmers has been implemented during the project.

These interactions are governed by steric and lubrification forces. Test cases were conducted to validate our model. Moving forward, we plan to adapt this model to simulate interactions among a large number of squirmers.

#### 2 Context

The collective behavior of active particles is well studied in the literature. Various models exist to simulate these active particles, such as the Vicsek model[3] and the Squirmer model.

The squirmer model initially proposed by Lighthill in 1952[6], represents a spherical Stokesian swimmer with a surface that undergoes small-amplitude deformations to achieve propulsion. This model has been applied to a range of microswimmer dynamics in both biological and artificial contexts. Blake[6] later refined the model, adapting it to describe a spherical microswimmer covered with a dense array of beating cilia. Instead of representing individual cilia, the model uses a continuous, deformable layer that propagates the wave.

The aim of this internship is to study squirmers, in a confined domain and to compare their collective motion with that of the active particles using the Vicsek model. The motion of the squirmers is described by a continuous model that approximates lubrification and steric forces[1][5].

# 3 Objectives

The main goal is to model the dynamics of a group of squirmers within confined environments and to study the influence of numerical parameters on their collective behavior.

To achieve this objective, the following tasks will be carried out:

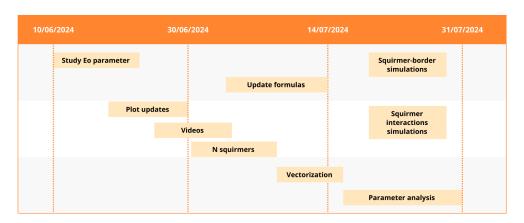
- Validate the formulas of the steric and lubrification forces from the previous project.
- Investigate the impact of altering the parameter  $\beta$ , which defines the type of squirmers (pusher, puller, neutral swimmer), on the interaction between two squirmers.
- Conduct a comparative analysis of the interaction between a squirmer and a boundary of the domain by varying the initial angle of the squirmer and

the parameter  $\beta$ , to comprehensively understand their influence on the system dynamics.

- Update and vectorize the code to enable a simulation of a larger number of squirmers.
- Examine the impact of numerical parameters on the collective behavior of squirmers.

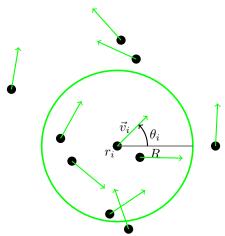
All of these steps are consolidated in the following roadmap:

# Roadmap



### 4 Vicsek model

In this section a detailed overview of the Vicsek model will be provided.



The Vicsek model consists of N particles with  $r_i(t)$  in  $\mathbb{R}^2$  and  $\theta_i(t) \in [0, 2\pi]$  their mass center and orientations.

All particles have the same velocity  $v_0$  and radius. The evolution of the orientation  $\theta_i(t)$  at each time step  $\Delta t$  is given by:

$$\theta_i(t + \Delta t) = \langle \theta_j(t) \rangle_{|r_i(t) - r_j(t)| \le R} + \epsilon_i(t),$$

with

$$\langle \theta_j(t) \rangle = \arctan\left(\frac{\sin(\theta_j(t))}{\cos(\theta_j(t))}\right).$$

R is the range of interaction,  $\langle \theta_j(t) \rangle_{|r_i(t)-r_j(t)| < R}$  the average orientation of the particles in the range R of the i-th particle (including itself) at the time t and  $\epsilon_i(t)$  represents the noise. It is a random number taken from a uniform probability distribution over  $\left(-\frac{\eta}{2}, \frac{\eta}{2}\right)$  where  $\eta$  is the main tool that counteracts the alignment of the particles.

The evolution of the position  $r_i(t)$  at each time step  $\Delta t$  is described by:

$$r_i(t + \nabla t) = r_i(t) + v_0 \Delta t \begin{pmatrix} \cos(\theta_i(t)) \\ \sin(\theta_i(t)) \end{pmatrix}.$$

The velocity  $\vec{v}_i(t)$  is defined by:

$$\vec{v}_i(t) = v_0 \begin{pmatrix} \cos \theta_i(t) \\ \sin \theta_i(t) \end{pmatrix}.$$

The collective behavior of the particles are quantified by the polar order parameter  $v_a$  which is given by:

$$v_a = \frac{1}{Nv_0} \left| \sum_{i=1}^N \vec{v}_i \right|.$$

The boundary conditions are reflective, if a particle is outside of the domain after computing  $r_i(t + \Delta t)$ , the new coordinates and orientations of the particle are given by:

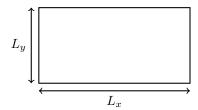
For the x-boundary:

$$|x_i(t + \Delta t)| = 2L_x - |x_i(t + \Delta t)|,$$
  
$$\theta_i(t + \Delta t) = \pi - \theta_i(t + \Delta t).$$

For the y-boundary:

$$|y_i(t + \Delta t)| = 2L_y - |y_i(t + \Delta t)|,$$
  
$$\theta_i(t + \Delta t) = -\theta_i(t + \Delta t).$$

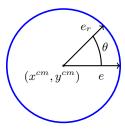
Where  $L_x$  represents the length of the domain, and  $L_y$  represents the width of the domain.



These conditions ensures that the particles reflect off the boundaries. We will compare our results with those obtained using a similar model.

# 5 Squirmer model

I will continue by detailing the squirmer model as well as the interactions between such active particles. This model uses lubrification forces and torques to describe particle behavior, while the Vicsek model focuses more on collective behavior to model particle movement.



The time-independent velocity u defined on the surface of the squirmer is given in polar coordinates by :

$$\begin{cases} u_r(R,\theta) = 0 \\ u_{\theta}(R,\theta) = B_1 \sin(\theta) + B_2 \sin(\theta) \cos(\theta) \end{cases} [5];$$

With R denoting the particle's radius, and  $B_1$  and  $B_2$  being constants. By setting  $\beta = \frac{B_2}{B_1}$ , we have :

$$u_{\theta}(R, \theta) = B_1(\sin(\theta) + \beta\sin(\theta)\cos(\theta)),$$

where  $\beta$  is the type of the squirmer :

$$\left\{ \begin{array}{l} \beta = 0 : \text{neutral swimmer} \\ \beta < 0 : \text{pusher} \\ \beta > 0 : \text{puller} \end{array} \right.$$

and  $B_1$  describes the swimming velocity  $v_0 = \frac{2B_1}{3}$ . Now let us put u in cartesian coordinates:

$$u = \begin{pmatrix} u_x \\ u_y \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} u_r \\ u_\theta \end{pmatrix},$$
$$= B_1 (1 + \beta \cos(\theta)) \begin{pmatrix} -\sin^2(\theta) \\ \sin(\theta) \cos(\theta) \end{pmatrix}.$$

We define  $e_r$  the unit vector pointing from the center to the surface

$$e_r = \begin{pmatrix} \frac{x - x^{cm}}{R_{cm}} \\ \frac{y - y^{cm}}{R} \end{pmatrix} = \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix}$$

and  $e = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix}$  the swimming direction of the squirmer.

By fixing  $\theta = 0$ , one has  $e = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and one finds the following expression for the velocity field in cartesian coordinates:

$$u = B_1 (1 + \beta \cos(\theta)) \begin{pmatrix} -\sin^2(\theta) \\ \sin(\theta) \cos(\theta) \end{pmatrix},$$

$$= B_1 (1 + \beta \cos(\theta)) \begin{pmatrix} \cos^2(\theta) - 1 \\ \sin(\theta) \cos(\theta) \end{pmatrix},$$

$$= B_1 \left( 1 + \beta \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} \right) \left[ \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} \right) \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right],$$

$$= B_1 (1 + \beta(e \cdot e_r)) [(e \cdot e_r) e_r - e].$$

Thus, u in cartesian coordinates is given by :

$$u_r = B_1(1 + \beta(e \cdot e_r))[(e \cdot e_r)e_r - e].$$

# 6 Dynamics of two interacting squirmers

#### 6.1 The evolution of the mass center

The evolution of the mass center  $r_i = (X_i, Y_i)$  of one squirmer i in presence of another squirmer j and rigid boundaries, is given by the Langevin equation:

$$\frac{dr_i}{dt} = v_0 p_i - \sum_{i \neq j} \nabla_{r_{ij}} V_{ij} - \sum_i \nabla_{r_i} V_i + \sum_{i \neq j} \left[ F_{i(j) \to i} + F_{j(i) \to i} \right] + \sum_{k \in w} F_{k \to i}^w + \sqrt{2D} \eta_i(t)$$

We have:

- $v_0$  the particle velocity,
- $p_i = (\cos(\theta), \sin(\theta))^T$  orientation,
- $F_{i(j)\to k}$  the lubrification forces applied on the  $k^{th}$  squirmer and generated by the  $i^{th}$  squirmer in presence of the  $j^{th}$  one [1],
- $F_{k \to i}^w$  the lubrification forces exerted on the  $i^{th}$  squirmer due to the presence of the  $k^{th}$  wall[1],
- $V_{ij}$  and  $V_i$  are the Weeks-Chandler-Andersen potential use to define a repulsive steric force avoiding the overlapping of two squirmers or of one squirmer and a rigid boundary. The force is activated when the distance between two surfaces is small,
- D the translational diffusivity,

•  $\eta_i$  are independent noises.

The second law of Newton states[7]:

$$m\vec{a} = \sum_{i} \vec{F}_{i}.$$

The force of viscosity on a small sphere moving through a viscous fluid is given by the Stokes-Einstein relation[8]:

$$F_d = 6\mu\pi R v_0 \frac{dr_i}{dt}.$$

We consider the squirmers propulsion in absence of inertia:  $m\vec{a}=0$ . Hence one has:

$$0 = -F_d + \sum_{i \neq d} F_i,$$

we have:

$$\frac{dr_i}{dt} = \frac{1}{6\mu\pi R} \sum_{i \neq d} F_i.$$

The Weeks-Chandler-Andersen potential is given by:  $V_{ij} = \frac{E_s}{6\pi\mu R} \left[ \left( \frac{2R}{|r_{ij}|} \right)^{12} - \left( \frac{2R}{|r_{ij}|} \right)^6 \right]$  and  $V_i = \frac{E_s}{6\pi\mu R} \left[ \left( \frac{R}{|r-r_i|} \right)^{12} - \left( \frac{R}{|r-r_i|} \right)^6 \right]$ 

With:

- $r_{ij} = \sqrt{D_x^2 + D_y^2}$ ,  $|r_{ij}|$  the distance between the centers of two squirmers,
- $|r-r_i|$  the distance between the wall and the squirmer center,
- $E_s$  a positive constant,
- R the radius of a squirmer,
- $\mu$  the dynamic viscosity.

We want to compute the steric force applied between two squirmers, given by  $\nabla_{r_{ij}} V_{ij}$ :

$$\begin{split} \frac{\partial V_{ij}}{\partial D_x} &= \frac{\partial}{\partial D_x} \frac{E_s}{6\pi \mu R} \left[ \left( \frac{2R}{|r_{ij}|} \right)^{12} - \left( \frac{2R}{|r_{ij}|} \right)^6 \right] \\ &= \frac{E_s}{6\pi \mu R} \left[ \frac{\partial}{\partial D_x} \left( \frac{2R}{|r_{ij}|} \right)^{12} - \frac{\partial}{\partial D_x} \left( \frac{2R}{|r_{ij}|} \right)^6 \right] \\ &= \frac{E_s}{6\pi \mu R} \left[ \frac{-12D_x (2R)^{12} (r_{ij})^{10}}{(r_{ij})^{24}} - \frac{-6D_x (2R)^6 (r_{ij})^4}{(r_{ij})^{12}} \right] \\ &= \frac{-12E_s}{2r6\pi \mu R} \left[ \frac{D_x (2R)^{13}}{(r_{ij})^{14}} - \frac{D_x (2R)^7}{2(r_{ij})^8} \right] \\ &= -\frac{E_s}{2R^2\pi \mu} \frac{D_x}{r_{ij}} \left[ \frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7} \right]. \end{split}$$

Equivalently, we have :  $\frac{\partial V_{ij}}{\partial D_y} = -\frac{E_s}{2R^2\pi\mu} \frac{D_y}{r_{ij}} \left[ \frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7} \right]$ 

We find:

$$\nabla_{r_{ij}} V_{ij} = \begin{pmatrix} -\frac{E_s}{2R^2\pi\mu} \frac{D_x}{r_{ij}} \begin{bmatrix} \frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7} \\ -\frac{E_s}{2R^2\pi\mu} \frac{D_y}{r_{ij}} \begin{bmatrix} \frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7} \end{bmatrix} \end{pmatrix}$$

In addition, we need to compute  $\partial_{r_i}V_i$  to obtain the force applied between a squirmer and a rigid boundary.

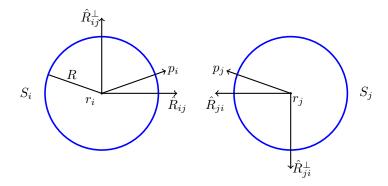
$$\begin{split} \frac{\partial V_{i}}{\partial X} &= \frac{\partial}{\partial X} \left( \frac{E_{s}}{6\pi\mu R} \left[ \left( \frac{R}{|r - r_{i}|} \right)^{12} - \left( \frac{R}{|r - r_{i}|} \right)^{6} \right] \right) \\ &= \frac{\partial}{\partial X} \left( \frac{E_{s}}{6\pi\mu R} \left[ \left( \frac{R}{\sqrt{(X_{box} - X)^{2} + (Y_{box} - Y)^{2}}} \right)^{12} - \left( \frac{R}{\sqrt{(X_{box} - X)^{2} + (Y_{box} - Y)^{2}}} \right)^{6} \right] \right) \\ &= \frac{E_{s}}{6\pi\mu R} \left[ 12(X_{box} - X) \frac{R^{12}}{|r - r_{i}|^{14}} - 6(X_{box} - X) \frac{R^{6}}{|r - r_{i}|^{8}} \right] \\ &= -\frac{E_{s}(X_{box} - X)}{\pi\mu R^{2}|r - r_{i}|} \left[ 2\left( \frac{R}{|r - r_{i}|} \right)^{13} - \left( \frac{R}{|r - r_{i}|} \right)^{7} \right]. \end{split}$$

Equivalently, we have :  $\frac{\partial V_i}{\partial Y} = -\frac{E_s(Y_{box} - Y)}{\pi \mu R^2 |r - r_i|} \left[ 2 \left( \frac{R}{|r - r_i|} \right)^{13} - \left( \frac{R}{|r - r_i|} \right)^7 \right]$ .

We have:

$$\nabla_{r_i} V_i = \begin{pmatrix} -\frac{E_s(X_{box} - X)}{\pi \mu R^2 |r - r_i|} \left[ 2 \left( \frac{R}{|r - r_i|} \right)^{13} - \left( \frac{R}{|r - r_i|} \right)^7 \right] \\ -\frac{E_s(Y_{box} - Y)}{\pi \mu R^2 |r - r_i|} \left[ 2 \left( \frac{R}{|r - r_i|} \right)^{13} - \left( \frac{R}{|r - r_i|} \right)^7 \right] \end{pmatrix}$$

These steric forces are applied on two squirmers when  $r_{ij} < R2^{\frac{7}{6}}.$ 



The figure shows the different vectors involved in the computations which will follow.

We define:

• 
$$W_n(x) = \frac{2}{n(n+1)} P'_n(x)$$
 [1],

•  $P_n(x)$  the Legendre polynomials [6] given by:

$$- P_1(x) = x,$$
  
-  $P_2(x) = \frac{1}{2}(3x^2 - 1),$ 

- $p_i = (\cos \theta_i, \sin \theta_i),$
- $\hat{R}_{ij} = \frac{r_{ij}}{|r_{ij}|}$ ,
- $\hat{R}_{ij}^{\perp} = rot(\frac{\pi}{2})\hat{R}_{ij}$ .

The tangential lubrication forces acting on the two spheres, depending on

the direction of the vectors 
$$\hat{R}_{ij}$$
 and  $\hat{R}_{ij}^{\perp}$ , are defined by[1]: 
$$F_{i(j)\to i}^y = 9\mu\pi R \frac{\lambda^2}{(\lambda+1)^2} \sum_n \left[ B_n W_n(p_i \hat{R}_{ij})(-p_i \hat{R}_{ij}) + \frac{1}{2} B_n W_n'(p_i \hat{R}_{ij})(p_i \hat{R}_{ij}^{\perp})^2 \right] (ln\epsilon + O(1)).$$
 For  $n=1$ :

$$\begin{split} W_1(p_i\hat{R}_{ij}) &= 1, \\ W_1'(p_i\hat{R}_{ij}) &= 0, \\ -B_1W_1(p_i\hat{R}_{ij})p_i\hat{R}_{ij} + \frac{1}{2}B_1W_1'(p_i\hat{R}_{ij})(p_i\hat{R}_{ij}^{\perp})^2 &= -B_1p_i\hat{R}_{ij}. \end{split}$$

For n=2:

$$\begin{split} W_2(p_i\hat{R}_{ij}) &= p_i\hat{R}_{ij},\\ W_2'(p_i\hat{R}_{ij}) &= 1,\\ -B_2W_2(p_i\hat{R}_{ij})p_i\hat{R}_{ij} + \frac{1}{2}B_2W_2'(p_i\hat{R}_{ij})(p_i\hat{R}_{ij}^\perp)^2 &= -B_2(p_i\hat{R}_{ij})^2 + \frac{1}{2}B_2(p_i\hat{R}_{ij}^\perp)^2. \end{split}$$

Since all squirmers share the same radius R, we have  $B_1 = \frac{3}{2}v_0$ ,  $B_2 = B_1 \cdot \beta$  and  $\lambda = 1$ , so:

$$6\mu\pi R F_{i(j)\to i}^{y} = 9\mu\pi R \frac{\lambda^{2}}{(\lambda+1)^{2}} \left[ -B_{1}p_{i}\hat{R}_{ij} - B_{2}(p_{i}\hat{R}_{ij})^{2} + \frac{1}{2}B_{2}(p_{i}\hat{R}_{ij}^{\perp})^{2} \right] (\ln\epsilon + O(1))$$

$$= 9\mu\pi R \frac{1}{4} \cdot \frac{3}{2}v_{0} \left[ -p_{i}\hat{R}_{ij} - \beta(p_{i}\hat{R}_{ij})^{2} + \frac{1}{2}\beta(p_{i}\hat{R}_{ij}^{\perp})^{2} \right] (\ln\epsilon + O(1))$$

$$F_{i(j)\to i}^{y} = -\frac{9}{16}v_{0} \left[ (p_{i}\hat{R}_{ij})(1+\beta p_{i}\hat{R}_{ij}) - \frac{1}{2}\beta(p_{i}\hat{R}_{ij}^{\perp})^{2} \right] (\ln\epsilon + O(1))$$

The normal forces acting on the two spheres can be calculated explicitly by [1]:

$$F_{i(j)\to i}^x = -\frac{4}{5}\mu\pi R \frac{\lambda(\lambda+4)}{(\lambda+1)^2} \sum_n B_n W_n(p_i \hat{R}_{ij}) (ln\epsilon + O(1))$$

So:

$$6\mu\pi R F_{i(j)\to i}^x = -\frac{4}{5}\mu\pi R \frac{5}{4}p_i \hat{R}_{ij}^{\perp} (B_1 + B_2 p_i \hat{R}_{ij}) (ln\epsilon + O(1)),$$

$$= -\mu\pi R \frac{3}{2}v_0 p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

$$F_{i(j)\to i}^x = -\frac{1}{4}v_0 p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1))$$

The effect of a wall can be calculated by replacing one of the spheres with one of infinite diameter, so  $\lambda \to \infty$ :

$$F_{w \to i}^{y} = -\frac{9}{4}v_{0} \left[ (p_{i}\hat{R}_{ij})(1 + \beta p_{i}\hat{R}_{ij}) - \frac{1}{2}\beta(p_{i}\hat{R}_{ij}^{\perp})^{2} \right] (ln\epsilon + O(1))$$

$$F_{w \to i}^{x} = -\frac{1}{5}v_{0}p_{i}\hat{R}_{ij}^{\perp}(1 + \beta p_{i}\hat{R}_{ij})(ln\epsilon + O(1))$$

#### 6.2 The evolution of the orientation

The evolution of the orientation of one squirmer is given by:

$$\frac{d\theta_i}{dt} = \sum_{i \neq j} \left[ \Gamma_{i(j) \to i} + \Gamma_{j(i) \to i} \right] + \sum_{k \in w} \Gamma_{k \to i}^w + \sqrt{2D_o} \eta_o^{(i)}$$

We have:

- $\Gamma_{i(j)\to k}$  the torque exerted on the  $k^{th}$  particle by the flow associated to the  $i^{th}$  particle, but perturbed by the presence of the  $j^{th}$  particle,
- $\Gamma^w_{k\to i}$  the torque exerted on the  $i^{th}$  particle by the interactions with the  $k^{th}$  walls,

- $D_o$  the angular diffusivity equal to  $\frac{3D}{4R^2}$ ,
- $\eta_o^{(i)}$  the noises, independent of  $\eta^i$ .

Similarly to the forces, one has  $\phi = 8\pi\mu r^3$  the rotation flow around a sphere[8]:

$$\frac{d\theta_i}{dt} = \frac{1}{\phi} \sum F[7].$$

The torques acting on the squirmer i can be calculated explicitly by [1]:

$$\Gamma_{i(j)\to i} = \frac{16\lambda}{5(\lambda+1)} \mu \pi R^2 p_i \hat{R}_{ij}^{\perp} \sum_n B_n W_n(p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

So:

$$\phi\Gamma_{i(j)\to i} = \frac{8}{5}\mu\pi R^2 p_i \hat{R}_{ij}^{\perp} (B_1 + B_2 p_i \hat{R}_{ij}) (ln\epsilon + O(1)),$$
  
$$= \frac{8}{5}\mu\pi R^2 p_i \hat{R}_{ij}^{\perp} \frac{3}{2} v_0 (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

$$\Gamma_{i(j)\to i} = \frac{3}{10} \frac{v_0}{R} p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

The torques acting on the squirmer j can be calculated explicitly by:

$$\Gamma_{i(j)\to j} = \tfrac{4\lambda^2}{5(\lambda+1)} \mu \pi R^2 p_i \hat{R}_{ij}^\perp \sum_n B_n W_n(p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

So:

$$\phi\Gamma_{i(j)\to j} = \frac{2}{5}\mu\pi R^2 p_i \hat{R}_{ij}^{\perp} (B_1 + B_2 p_i \hat{R}_{ij}) (ln\epsilon + O(1)),$$
  
$$= \frac{2}{5}\mu\pi R^2 p_i \hat{R}_{ij}^{\perp} \frac{3}{2} v_0 (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

$$\Gamma_{i(j)\to j} = \frac{3}{40} \frac{v_0}{R} p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)).$$

One can note that for two squirmers having the same radius r,  $\lambda = 1$  and:

$$\Gamma_{i(j)\to j} = \frac{1}{4}\Gamma_{i(j)\to i}$$

Similarly as for the forces, the torques produced by the walls can be calculated by replacing one of the spheres with one of infinite diameter:

$$\Gamma_{w\to i} = \frac{3}{5} \frac{v_0}{R} p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1))$$

## 7 Implementation

In each file, we have added comments describing the various functions and classes. In this section, we will briefly detail the files to make their reading and the reproducibility of the results easier to achieve.

#### vicsek

#### **Parameters**

- N the number of particles in the system,
- R the range of interaction of the particles,
- L the length of the square,
- v0 the constant velocity of the particles,
- radius the radius of the particles,
- T the time of simulation,
- dt the time step,
- noise the  $\eta$  parameter, used to counteract the alignment of the particles.

The class initializes N particles with random position and orientation within the square. The square has reflective boundary conditions.

#### Methods

- distance(p1, p2) returns the distance between p1 and p2.
- dist\_particles(particle) returns a list which contains the distances between the particle and all other particles of the system.
- how\_many\_in\_square() prints and returns the percentage of particles inside the square. It is used to test if the code contains errors.
- ploar\_order\_parameter() computes and returns  $v_a$  the polar order parameter.
- ref\_border\_x(particle, boundary) and ref\_border\_y(particle, boundary) simulates the reflective borders.
- vector\_x(p1, p2) and vector\_y(p1, p2) return respectively the vector in the x and y direction of the particles.
- average\_orient(particle) returns the average orientation of the particles in a range R of the particle in argument (including itself).
- update\_orient() computes the orientation  $\theta_i(t+\Delta t)$  using average\_orient.

- update\_position() computes the position  $r_i(t + \Delta t)$  using the reflective boundaries if necessary
- loop\_time() uses update\_orientation() and update\_position() for each time iteration.
- plot(ax) plots the square and the particles.

#### simulation

• sim\_vicsek(N) used to simulate the behaviors of N particles in a square with the Vicsek model. loop\_time is used and a graph is made with the positions and orientations of the particles for each step.

#### codemat

This file is the original matlab code that was the base of the study.

#### squirmer

The file contains the Squirmer class which takes the parameters:

- $\bullet$  coordinates x and y,
- orientation,
- radius,
- beta,
- velocity,

of a squirmer and computes B1 and B2.

#### csv\_file

This file contains two functions:

- export\_data\_csv(filename, data) takes a file name and data from loop\_time() (section interactingsquirmers) and exports it.
- read\_csv\_file(filename) takes a file name and returns the data, not currently utilized but may be usefull for future functions.

#### plot

• plot\_sim\_nsquirmers(histories, Nx, Ny, N, a, border, sim\_border, filename, dir) takes histories the liste returned by loop\_time, Nx and Ny the length and width of the rectangle, N the number of squirmers, a the radius of the squirmers, border a boolean which determines if the borders are plotted or not, sim\_border a boolean which is only True when a simulation with a single border and a single squirmer is done, filename and dir the names of the file and directory in which the graph is saved. It then plots the evolution of each squirmer's position over time, a circle is plotted at the initial position, at half of the simulation time and at the end of the simulation, the radius of the circle plotted is proportional to the radius of the squirmers.

This function is used for simulations with a small number of Squirmers and a low simulation time.

- plot\_time(interact, list\_plot, filename, label, dir) takes interact an Interactingsquirmers, list\_plot, the list to plot over time, usually the list of the minimal distance between the squirmers or the liste of the polar parameter, label is a string used for the y-label in the graph and filename and dir is the name of the file and directory in which the graph will be saved.
  - This function is used to plot the minimal distance between squirmers and the polar order parameter over time.
- create\_video\_from\_history(history, Nx, Ny, N, a, filename, dir, fps) takes history the list of loop\_time, Nx and Ny the length and width of the rectangle, N the number of squirmers, a the radius of the squirmers, filename and dir the name of the file and directory in which the video is saved, fps the number of frames per second. This function is used to create videos with a high number of squirmers and a long simulation time.

#### interactingsquirmers

#### **Parameters**

This file implements the Interactingsquirmers class which takes:

- N, the number of squirmers,
- xs, ys and orientations the positions and orientations of the squirmers,
- radius, the radius of the squirmers,
- beta, the  $\beta$  parameter,
- v0, the velocity  $v_0$ ,
- Nx and Ny, the length and width of the rectangle,

- dt, the time step and dt\_out the time step for output,
- T, the final time of simulation,
- Es, the amplitude (intensity) of steric interactions,
- ds, the distance where the steric interactions become significative,
- mu, the viscosity,
- R, the distance which defines if a particle is seen as a neighbour for the clustering order parameter,
- D, the translational diffusivity D,
- n and no the noises associated with the forces and torques,
- border, a boolean which defines if the simulation is made in a box(True) or a channel(False).

#### Methods

This class has many functions:

- is\_in\_rectangle() and check\_squirmers\_rectangle() verify if the squirmers are initially in the rectangle.
- polar\_order\_parameter() returns the polar order parameter  $v_a$ .
- distance\_all() returns (Dx, Dy, dists) the directional vector of  $R_i$  to  $R_i$  and the distance between each squirmer.
- forcesSteric(Dxs, Dys, dists) returns the steric forces (Fs\_x, Fs\_y) computed with the directional vector and the distance calculated with distance\_all().
- forcesLubrification(Dx, Dy, dist, theta) and torquesLubrification(Dx, Dy, dist, theta) returns the lubrification forces and torques.
- compute\_force\_squirmer\_border\_x(self, xs, ys) and compute\_force\_squirmer\_border\_y(self, xs, ys) computes and returns the steric forces between the squirmers and the walls.
- force\_torque\_lubrification\_border\_x(self, xs, theta, border) and force\_torque\_lubrification\_border\_y(self, ys, theta, border) computes and returns the lubrification forces and torques between the squirmers and the walls.
- ref\_border\_x(self, xs, orientation, boundary) and ref\_border\_y(self, xs, orientation, boundary) simulates reflective borders when border is True.

- perio\_border\_x(self, xs, boundary) simulates periodic borders when border is False.
- loop\_time() is the primary function which updates the positions and orientations of each squirmer for each time step dt based on the steric forces and the lubrification forces and torques, then updates four lists, self.vector\_min\_dist for the minimal distance between the squirmers, self.list\_polar for the polar order parameter, self.list\_cluster\_param for the clustering order parameter and history for the positions, orientations, forces and torques at each time step dt\_out. The function then returns history.
- run(choice, N, a, beta, v0, Nx, Ny, dt, dt\_out, T, Es, ds, mu, R, lnEps\_cr, D, n, no, border, filename, border\_plot) is used to run a simulation, it takes the argument choice that can be:
  - 'plot' to plot the graph of the trajectories of the squirmers in the 'graphs' directory, used for a small number of squirmers and a low simulation time.
  - 'video' to create a video of the trajectories of the squirmers in the 'videos' directory, used for a large number of squirmers or a high simulation time,
  - 'Eo\_sim', not used anymore, to test the lubrification torques' intensity,
  - 'border', to simulate the behaviors of a squirmer near a wall, only plot possible,
  - 'sim\_2\_sq', to simulate the behaviors of two squirmers near each other, plot and video possible,
  - 'sim\_D', to simulate the influence of the D parameter on the squirmers' behaviors, only video possible.

#### Reproducibility-run.py

The file run.py is utilized to define the parameters and to choose the simulation to conduct.

To execute the simulations, run the following command:

```
python Code/run.py sim_choice N filename
```

with N the number of squirmers and filename the name of the file in which the resulting graph or video will be stored. sim\_choice can be:

- vicsek to simulate the behaviors of N particles using the Vicsek model.
- video to run a simulation with N squirmers and to store the resulting video
  of the squirmers trajectories and the graphs of the minimum distance
  between squirmers, the polar order parameter and the clustering order
  parameter over time in the videos directory.

- plot to run a simulation with N squirmers and to store the resulting graphs of the squirmers behaviors, the minimum distance between squirmers, the polar order parameter and the clustering order parameter over time in the graphs directory.
- Eo\_sim used at the start of the internship to study the impact of the Eo parameter on the orientations, not used anymore.
- border to run simulations between a squirmer and a wall, four simulations are made per beta in the betas list in the run function in the interactingsquirmers file. The graphs are stored in the graphs/simulations/border/betalabel directory with betalabel the label of beta.
- sim\_2\_sq to simulate the behaviors of two squirmers near each other for five β values. The resulting graphs or videos are stored in the graphs/simualtions/sim\_sq\_sq/labelbeta or the videos/simualtions/sim\_sq\_sq/labelbeta directory.
- sim\_D to simulate the behaviors of N squirmers for different D values, the resulting graphs and videos are stored in the videos/simulations/sim\_D directory.

#### Tests

Two tests are implemented to validate a simulation. The first test is in the loop\_time() of the Interactingsquirmers class. At each time step, we check that the forces verify:

$$F \cdot dt < v_0$$

where F represents the steric or lubrification forces.

The second test is executed upon a push or a pull request. This test performs a simulation with 375 squirmers in a box with reflective borders and test if at any point during the simulation a negative distance has been registered.

# 8 Numerical Experiments

In this section, we will present the results of several numerical experiments. The time integration scheme employed is an explicit Euler method, where the position is updated at each iteration using the previous state.

#### 8.1 Simulation of two interacting squirmers

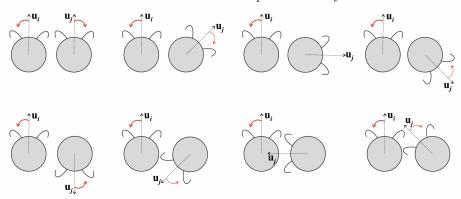
In this section, simulation of two closely positioned squirmers are conducted. The parameters of one squirmer remain fixed throughout all simulations except for its  $\beta$  value, while the initial orientation and  $\beta$  value of the other squirmer are varied. The five  $\beta$  values used are:

$$\beta_0 = 0, \beta_1 = 1.5, \beta_2 = 3, \beta_3 = -1.5, \beta_4 = -3.$$

The left squirmer with a radius of R=0.05 placed at (-R,0), has a velocity of  $v_0=1$ , a translational diffusivity D=0 and an initial orientation of  $\theta_1=\frac{\pi}{2}$  and a  $\beta$  value varying among  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ ,  $\beta_3$  and  $\beta_4$ .

The right squirmer, with the same radius R and velocity  $v_0$ , is placed at  $(\frac{2R}{1.9}, 0)$ . Its orientation  $\theta_2$  varies across the principal orientations of the unit circle and its  $\beta$  value also varies among  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ ,  $\beta_3$  and  $\beta_4$ . We then compare our results to those of a previous study, as shown in the following figure [4].

Behavior observed in a previous study.



A schematic of the encounter between two *Chlamydomonas*.  $u_i$  and  $u_j$  the initial orientational vector and the rotation due to interaction shown in red.

One can execute these simulations by running the command:

python Code/run.py sim\_2\_sq 2 filename

The parameters can be changed in the Code/run.py and Code/interactingsquirmers.py files.

We show the trajectories of the two squirmers as well as their initial orientation.

The grey lines dotted represent the trajectories of the squirmers without any interaction, thus without any force and torque applied on the squirmers. Circles are plotted at the start, middle, and end of the simulation, with their radii proportional to the squirmers' size. The simulation is T=0.8 with a time step  $dt=1e^{-4}$ .

$$\theta_2 = \frac{\pi}{2}$$

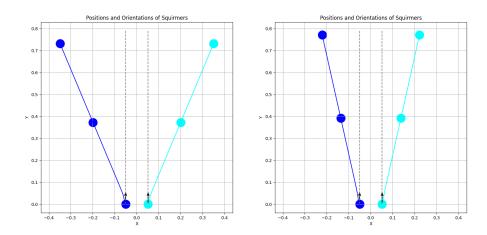


Figure 1:  $\beta = 3$ 

Figure 2:  $\beta = -3$ 

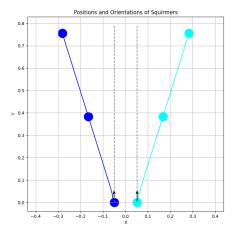


Figure 3:  $\beta = 0$ 

For  $\theta_2 = \frac{\pi}{2}$ , one can observe that their orientation changes due to the lubri-

fication and steric forces which are applied on them. These forces and torques push the squirmers away from each other. and allow avoiding the overlapping of the two particles.

Each squirmer gradually distances itself from the other, consistent with the study [4]. For  $\beta=3$  the squirmers end the simulation at  $x_1=-0.35$  and  $x_2=0.35$ , for  $\beta=-3$  at  $x_1=-0.22$  and  $x_2=0.22$ , for  $\beta=0$  at  $x_1=-0.28$  and  $x_2=0.28$ . It is noteworthy that larger values of  $\beta$  result in stronger forces and torques that push the squirmers further apart when both squirmers have an orientation  $\theta=\frac{\pi}{2}$ .

$$\theta_2 = \frac{3\pi}{4}$$

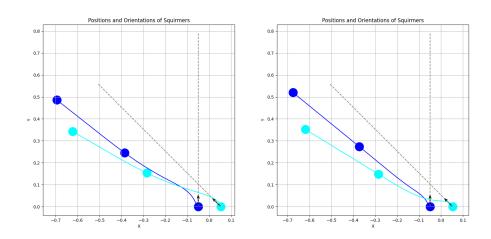
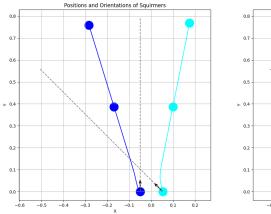


Figure 4:  $\beta = 1.5$ 

Figure 5:  $\beta = 3$ 



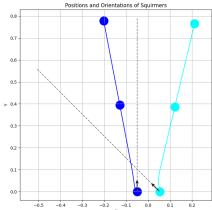


Figure 6:  $\beta = -1.5$ 

Figure 7:  $\beta = -3$ 

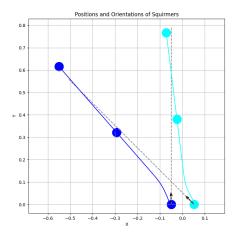


Figure 8:  $\beta = 0$ 

For the case  $\theta_2 = \frac{3\pi}{4}$ , ou results are consistent with the previous study[4] for  $\beta = 0$ . However, for  $\beta > 0$  the right squirmer is attracted to the left one, which does not correspond to the previous study. For  $\beta < 0$  the torques on the right squirmer are larger than those acting on the left one, which also deviates from the previous study.

It is observed that for  $\beta=3$  the forces and torques pull the right squirmer towards the left one more strongly than for  $\beta=1.5$ . Conversely, for  $\beta=-3$  the right squirmer is pushed further away from the left one compared to  $\beta=-1.5$ .

In summary, for  $\theta_2 = \frac{3\pi}{4}$ , as  $\beta$  increases, the right squirmer is more strongly pulled towards the left one. Conversely, as  $\beta$  decreases, the right squirmer is more strongly pushed away from the left one.

$$\theta_2 = \pi$$

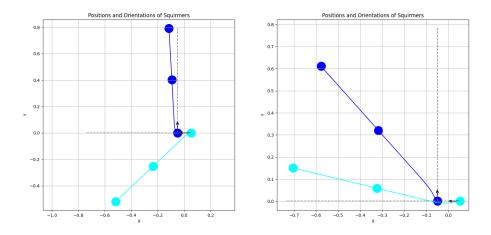


Figure 9:  $\beta = -3$ 

Figure 10:  $\beta = 3$ 

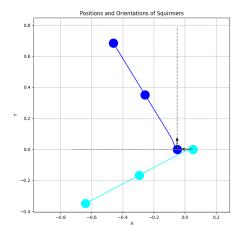


Figure 11:  $\beta = 0$ 

For  $\theta_2 = \pi$ , these results are not consistent with the previous study[4]. Our results show that the right squirmer's position and orientation are altered by the forces and torques for any  $\beta$  while the previous study showed that the right

squirmer's orientation is not supposed to change. Our results appear to be reasonable. The small initial distance between the squirmers, along with the applied forces and torques, causes the right squirmer to change its orientation.

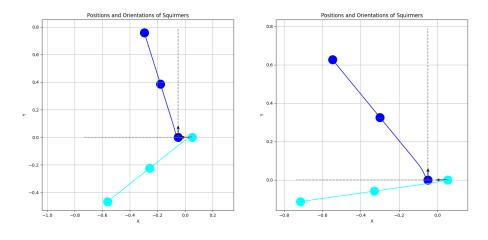


Figure 12:  $\beta = -1.5$ 

Figure 13:  $\beta = 1.5$ 

For  $\beta=-3$ , the orientation at the end of the simulation is less altered compared to  $\beta=-1.5$ . For  $\beta=3$ , the right squirmer ends up behind the left one, whereas for  $\beta=1.5$ , the right squirmer is pushed away. These results indicate that for  $\theta_2=\pi$ , as  $\beta$  increases, the right squirmer is more strongly pulled towards the left one, while as  $\beta$  decreases, the torques acting on the left squirmer also decrease.

$$\theta_2 = -\frac{3\pi}{4}$$

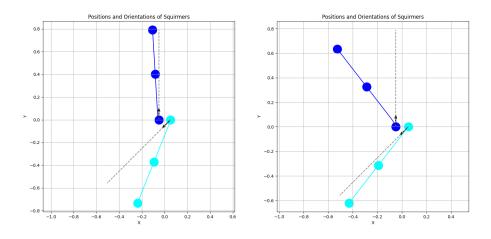


Figure 14:  $\beta = -3$ 

Figure 15:  $\beta = 3$ 

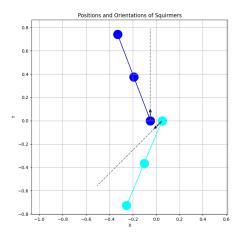


Figure 16:  $\beta = 0$ 

For  $\theta_2=\frac{-3\pi}{4}$ , these results are consistent with the previous study[4] for  $\beta\geq 0$  as the torques acting on the right squirmer are weaker than the ones acting on the left one. On the contrary, for  $\beta<0$  the torques acting on the right squirmer are larger than the ones acting on the left one.

$$\theta_2 = -\frac{\pi}{2}$$

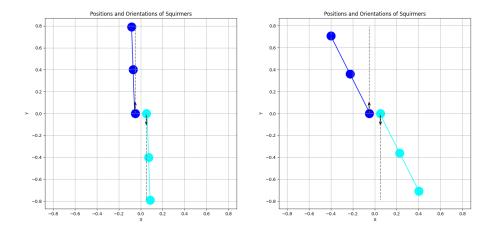


Figure 17:  $\beta = -3$ 

Figure 18:  $\beta = 3$ 

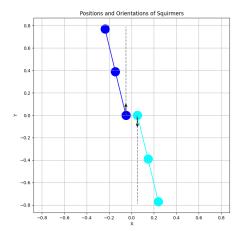


Figure 19:  $\beta = 0$ 

For  $\theta_2 = \frac{-\pi}{2}$ , our results are consistent with the previous study[4] as the torques acting on the right squirmer are equal to those acting on the left squirmer for all values of  $\beta$ .

$$\theta_2 = -\frac{\pi}{4}$$

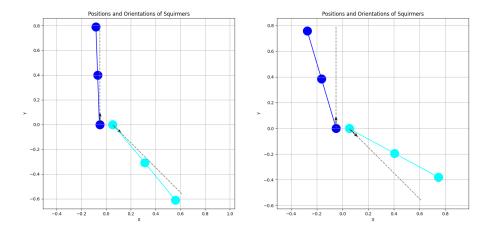


Figure 20:  $\beta = -3$ 

Figure 21:  $\beta = 3$ 

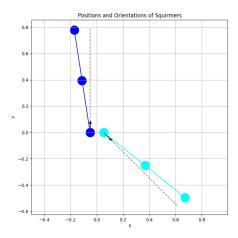


Figure 22:  $\beta = 0$ 

For case  $\theta_2 = \frac{\pi}{4}$ , these results are consistent with the previous study[4] for  $\beta = 0$  as the torques acting on the right squirmer are weaker to those acting on the left squirmer. For  $\beta = 3$  the torques acting on the right squirmer are equal to the those acting on the left squirmer which does not align with the previous study. For  $\beta = -3$  the direction of rotation does not align with the previous study.



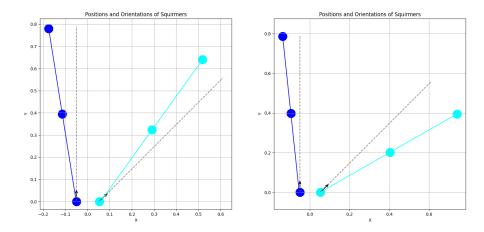


Figure 23:  $\beta = -3$ 

Figure 24:  $\beta = 3$ 

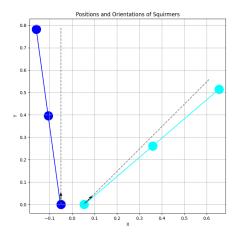


Figure 25:  $\beta = 0$ 

For this last case, these results are consistent with the previous study[4] for  $\beta=0$  as the torques acting on the right squirmer are weaker to those acting on the left squirmer. For  $\beta=3$  the torques acting on the right squirmer are greater to the those acting on the left squirmer, which does not align with the

previous study. For  $\beta=-3$  the direction of rotation does not align with the previous study.

#### 8.2 Simulation of squirmer-border interaction

In this section simulations of a squirmer near a reflective border are conducted. The parameters of the simulations are fixed except for the orientation and  $\beta$  parameter. The squirmer is placed at (x,y)=(-0.4,-0.7), has a radius of R=0.05, a velocity  $v_0=1$ , a translational diffusivity D=0, an initial orientation  $\theta$  varying among  $-\frac{\pi}{6}$ ,  $-\frac{\pi}{4}$ ,  $-\frac{\pi}{3}$  and  $-\frac{\pi}{2}$  and a  $\beta$  value varying among  $\beta_0=0$ ,  $\beta_1=1.5$ ,  $\beta_2=3$ ,  $\beta_3=-1.5$ ,  $\beta_4=-3$ . The border is placed at  $y_b=-1$ , the simulation time is T=0.9 with a time step  $dt=1e^{-4}$ .

One can execute these simulations by running the command:

python Code/run.py border 1 filename

The parameters can be changed in the Code/run.py and Code/interactingsquirmers.py files.

We show the trajectory of the squirmer as well as his initial orientation. A red circle and the corresponding time are marked when the squirmer reaches or exceeds the original height. Circles are plotted at the start, middle, and end of the simulation, with their radii proportional to the squirmer's size.

$$\theta = -\frac{\pi}{6}$$

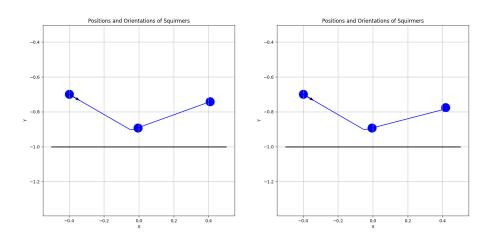


Figure 26:  $\beta = 1.5$ 

Figure 27:  $\beta = 3$ 

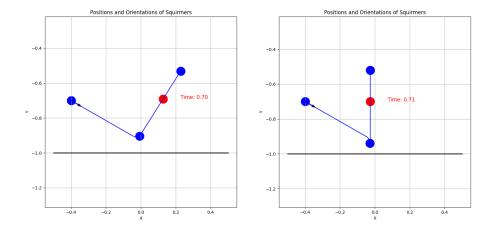


Figure 28:  $\beta = -1.5$ 

Figure 29:  $\beta = -3$ 

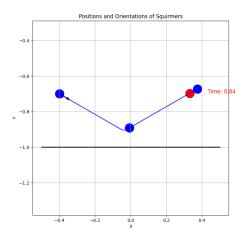


Figure 30:  $\beta = 0$ 

These results show that for  $\theta=-\frac{\pi}{6}$ , as  $\beta$  increases, the squirmer's orientation upon interaction becomes parallel to the border. On the contrary, as  $\beta$  decreases, the squirmer's orientation upon interaction becomes tangential to the border. The fact that the orientation after interaction is tangential does not necessarily mean that the particle reaches the initial height more quickly, as observed when  $\beta=-3$  compared to when  $\beta=-1.5$ .

$$\theta = -\frac{\pi}{4}$$

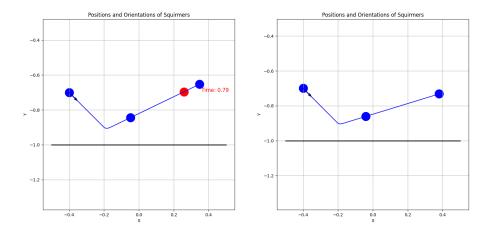


Figure 31:  $\beta = 1.5$ 

Figure 32:  $\beta = 3$ 

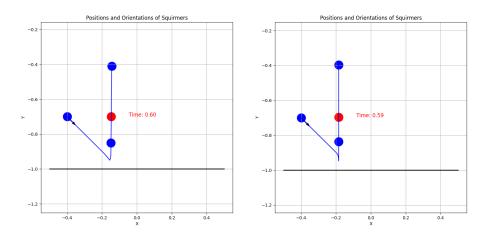


Figure 33:  $\beta = -1.5$ 

Figure 34:  $\beta = -3$ 

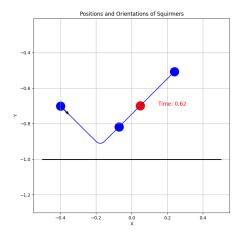


Figure 35:  $\beta = 0$ 

For  $\theta = \frac{-\pi}{4}$  as well as for  $\theta = \frac{-\pi}{3}$  and  $\theta = \frac{-\pi}{2}$ , the same observations are made, as  $\beta$  increases (resp. decreases), the squirmer's orientation upon interaction becomes parallel (resp. tangential) to the border.

One can note that the initial orientation has an impact on the orientation after interaction with the border as for  $\theta = -\frac{\pi}{4}$  and  $\beta = 1.5$ , the squirmer reaches and exceeds the original height during the simulation time. In contrast, for  $\theta = -\frac{\pi}{6}$  and  $\beta = 1.5$ , the squirmer does not reach the initial height.

#### 8.3 $E_0$ parameter

At the beginning of the internship, we studied the effect of the  $E_0$  parameter on the alignment of the squirmers.

One can see the simulations and their resulting graphs in the <code>graphs/Eo\_analysis</code> and <code>videos/Eo\_analysis</code> directories.

The simulation is executed using:

and one modify the Code/run.py file with the parameters one wants to test. Then for each  $E_0$  given in Code/run.py, a simulation is performed and the resulting graphs or videos are stored in the directories graphs or videos.

#### Evolution of the orientation

First we used the expression given in reference: [5]. The torques acting on the squirmer i can be calculated explicitly by:

$$\Gamma_{i(j)\to i} = E_0 p_i \hat{R}_{ij}^{\perp} (1 + \beta p_i \hat{R}_{ij}) (ln\epsilon + O(1)),$$

with  $E_0$  the parameter to test and

$$\Gamma_{j(i)\to i} = \frac{1}{4}\Gamma_{i(j)\to i}.$$

We want to study the effect of  $E_0$  on the alignment of squirmers in an open environment so  $\Gamma_i^W$ , which is the torque exerted by a wall on the squirmer vanishes.

#### **Numerical Experiments**

The simulations are done with two squirmers placed at coordinates  $(x_1, y_1) = (-R, 0)$  and  $(x_2, y_2) = (\frac{2R}{1.5}, 0)$  with radius R = 0.05, velocity  $v_0 = 1$ , viscosity  $\mu = 1$ ,  $\beta$  varying from  $\beta_1 = 0$ ,  $\beta_2 = -7.5$  and  $\beta_3 = 7.5$ , orientation  $\theta_1 = \frac{\pi}{2}$  and  $\theta_2$  varying between the major orientations of the unit circle.

The values for the  $E_0$  parameter are chosen from previous studies[1][5]:

$$E_{0_1} = \frac{3}{10} \frac{v_0}{R}, E_{0_2} = \frac{8}{5} \mu \pi a^2, E_{0_3} = \frac{-3}{2} \frac{v_0}{R}, E_{0_4} = -E_{0_1}, E_{0_5} = -5$$

$$E_{0_6} = \frac{5}{1000}, E_{0_7} = -2, E_{0_8} = -\frac{1}{2}, E_{0_9} = -E_{0_8}$$

We will show the results obtained for  $\theta_2 = \pi$  and  $\beta = 0$ .

$$\beta_1$$
 and  $\theta_2 = \pi$ 

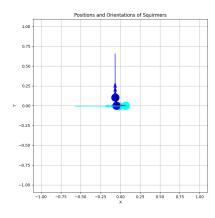


Figure 36:  $E_{0_2} = \frac{8}{5} \mu \pi a^2$ 

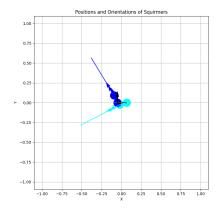
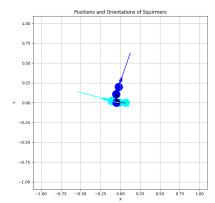


Figure 37:  $E_{0_1} = \frac{3}{10} \frac{v_0}{R}$ 



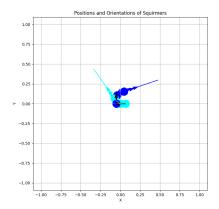


Figure 38:  $E_{0_7} = -2$  Figure 39:  $E_{0_5} = -5$  The arrows show the changes of orientations and a circle is plotted every four times the orientation of a squirmer is affected.

Our results show that as  $E_0$  decreases, the torques acting on the squirmers become stronger, as demonstrated by the example of  $E_0 = -5$ . No value of  $E_0$  could be found that allows the alignment of the squirmers. The alignment of the particles could not be controlled by varying the parameter  $E_0$ . The same conclusion was reached for all other tested values of  $\beta$  and  $\theta$ .

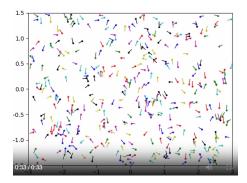
#### 8.4 Simulation of N squirmers

In this section, simulations of 375 squirmers are conducted in a rectangle with dimensions  $L_y=3$  and  $L_x=6$ , over a simulation time of T=10. Two types of boundary conditions are considered: a box with reflective boundaries, and a channel with reflective boundaries in the y-direction and periodic boundaries in the x-direction. The squirmers have a radius of R=0.02, a velocity of  $v_0=1$ , a translational diffusivity of D=0, and  $\beta=0$ . They are randomly positioned within the rectangle, each with a random orientation. The minimum distance between squirmers, as well as the polar order parameter, are plotted at the end of each simulation.

One can do a simulation by running:

#### python Code/run.py video N filename

where N is the number of squirmers, and filename is the name of the output file. The squirmers are represented with their orientations and one can see the videos in the videos directory. The minimal distance and polar order parameter, defined in the following section, are also plotted. Note that in the channel configuration, the minimum distance can appear negative due to the periodic boundaries, which can position one squirmer on top of another.



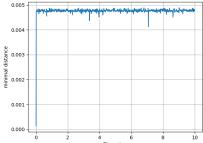


Figure 40: Simulation of squirmers within a box

Figure 41: Minimum distance between squirmers over time

#### 8.5 Study of D parameter

In this section, simulations are conducted with 375 squirmers in a channel, with a simulation time of T=50 and a time step of  $dt=1e^{-4}$ . The squirmers have a radius of R=0.02, a velocity of  $v_0=1$ , a range of  $\beta$  values:  $\beta_0=0, \beta_1=1.5, \beta_2=3, \beta_3=-1.5, \beta_4=-3$  and a translational diffusivity varying among:

$$D_0 = 0.5, D_1 = 1, D_2 = 3.$$

Two different sizes of channel are used:  $Ch_1$  with dimensions  $L_y = 3$  and  $L_x = 6$  and  $Ch_2$  with dimensions  $L_y = 2$  and  $L_x = 4$ . The objective is to examine the impact on the particle density  $\rho$  on collective behavior,  $\rho$  is given by:

$$\rho = \frac{N\pi R^2}{L_x L_y}.$$

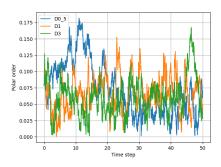
The squirmers are randomly positioned within the channel, each with a random orientation. For simulations with the same  $\beta$  and  $\rho$ , the initial positions and orientations of the squirmers are identical, ensuring that the only varying parameter between two simulations is the diffusivity D.

To analyze the collective behavior of the squirmers, the polar order parameter  $v_a$  is employed:

$$v_a = \frac{1}{N} \left| \sum_{i=1}^N p_i \right|,$$

where  $p_i$  denotes the orientation of the *i*-th squirmer. A value of  $v_a = 1$  indicates that all squirmers are moving in the same direction, while  $v_a \approx 0$  suggests uncorrelated motions.

$$Ch_1(L_x = 6 \ {f and} \ L_y = 4), \ 
ho = 0.026$$



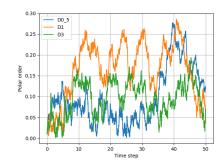
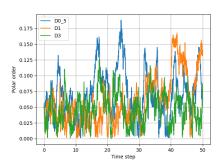


Figure 42:  $\beta = 0$ 

Figure 43:  $\beta = 1.5$ 



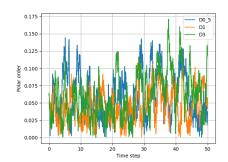


Figure 44:  $\beta = 3$ 

Figure 45:  $\beta = -1.5$ 

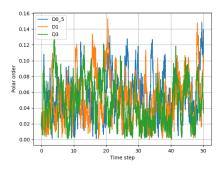
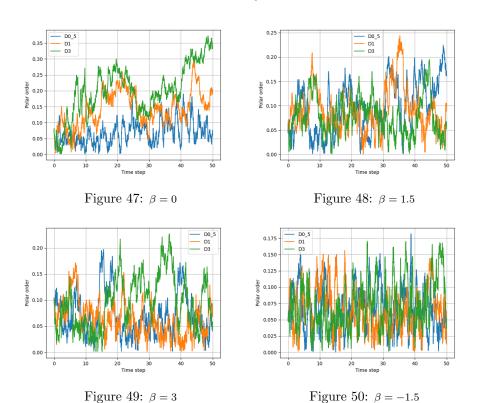


Figure 46:  $\beta = -3$ 

The polar order parameter  $v_a$  is shown over time in blue for D=0.5, in orange for D=1 and in green D=3. The results indicates that for  $Ch_1$ ,

no collective behaviors can be identified, as there is significant variation of  $v_a$  values between consecutive time steps. One can note that for  $\beta < 0$  and  $\beta = 3$ , the fluctuations of  $v_a$  are even more pronounced compared to cases where  $0 < \beta < 3$ . This can be explained by the behavior seen in section Simulation of two interacting squirmers, for  $\beta < 0$ , squirmers tend to repel each other more strongly as  $\beta$  decreases, while squirmers tend to attract each other as  $\beta$  increases.

$$Ch_2(L_x = 4 \text{ and } L_y = 2), \ \rho = 0.059$$



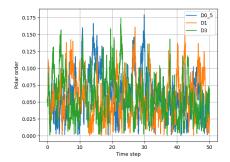


Figure 51:  $\beta = -3$ 

The results for  $Ch_2$  indicates that collective behavior can be identified for  $\beta=0$  and D=3, as  $v_a$  increases over time. A similar trend is observed for D=1 and D=0, although longer simulations are required to confirm this definitively. For  $\beta \neq 0$ , no collective behavior are observed during the simulation. One can see that for  $\beta \leq 0$  in  $Ch_2$ , the divergence of polar order parameter value between time steps is even greater than for  $\beta \leq 0$  in  $Ch_1$ . This can be attributed to the smaller channel size, implying more frequent interactions between squirmers.

# 9 Conclusion and perspectives

We have successfully reformulated the expressions for all forces and torques defined in the studies defined in the studies by Brumley[1] and Lauga[5]. These have been implemented in a Python code to analyze their variations, either between two squirmers, between a squirmer and a border or between a group of squirmers.

Our numerical results have yielded trajectories for specific initial orientations that diverge from those reported by Stark [4].

Our simulations reveal that collective behaviors are largely absent in the  $Ch_1$  channel, with significant variations in  $v_a$  values, particularly for  $\beta < 0$  and  $\beta = 3$ . These variations can be linked to the repulsive and attractive interactions observed for these  $\beta$  values. In the  $Ch_2$  channel, collective behavior emerges for  $\beta = 0$  and higher diffusivity, suggesting that a smaller channel size enhances interactions that promote such behavior. However, for  $\beta \neq 0$ , no collective behavior is observed during the simulation. Additionally, the increasing divergence in polar order parameter values with decreasing  $\beta$  across both channels highlights the influence of  $\beta$  on the system's dynamics.

Having thoroughly examined the interactions between squirmers and their collective behavior, the next phase of our research will focus on longer simulation times, higher particle densities, and exploring the propensity of squirmers to

form clusters over time. Another approach will involve controlling the collective behavior of squirmers using  $\beta$ .

## References

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