Collective motion of squirmers in confined environments

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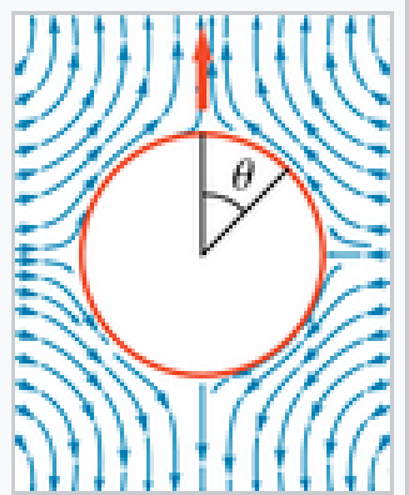
What is a squirmer ?

- Introduced by James Lighthill in 1952 [4]
- Extended by John Blake in 1971 [4]
- Model for simulating cilia by imposing boundary conditions on a spherical rigid microswimmer :
    - Tangential time-independant velocity at the boundary, propelling the squirmers.
    - In particular, we fix the propulsion type β and velocity B_1.

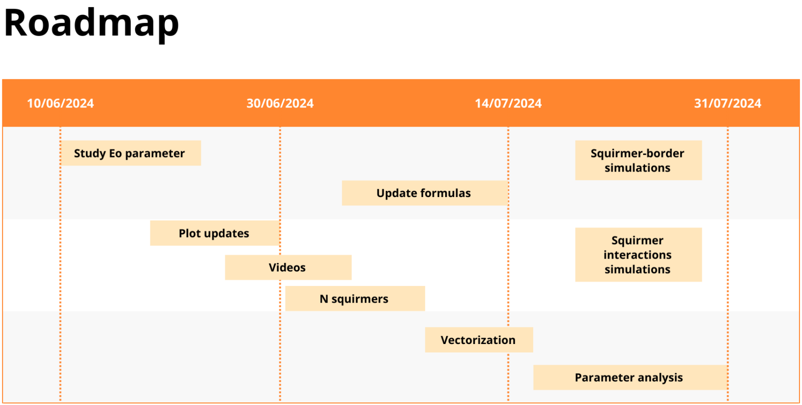


[4]

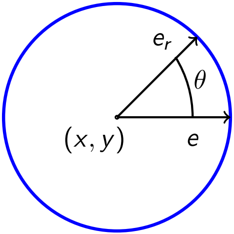
Objectives

- Rewrite the expressions for forces and torques from reference:[1] so that they fit within our framework.
- Investigate the impact of the β parameter on the interaction
  - between two squirmers.
  - between a squirmer and a wall.
- Update and vectorize the code to simulate the interactions between a large number of squirmers.
- Examine the impact of numerical parameters on the collective behavior of the squirmers.

Roadmap


Roadmap
10/06/2024
30/06/2024
14/07/2024
31/07/2024
Study Eo parameter
Squirmer-border simulations
Update formulas
Plot updates
Squirmer interactions simulations
Videos
N squirmers
Vectorization
Parameter analysis

Squirmer model



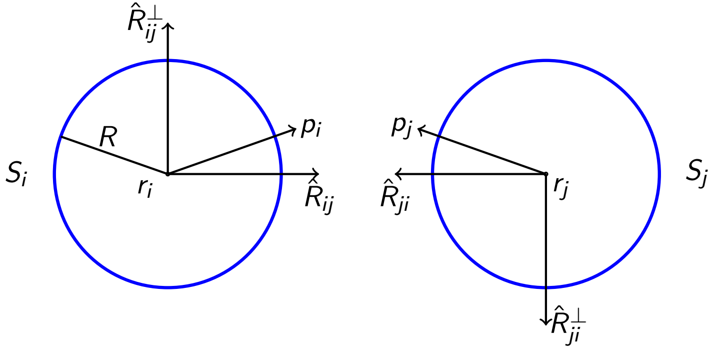
- The velocity u in polar coordinates [2] :

$$\begin{cases} u_r(R,\theta) &= 0 \\ u_\theta(R,\theta) &= B_1(\sin(\theta) + \beta\sin(\theta)\cos(\theta)),\, B_1 = \frac{3}{2}v_0 \end{cases}$$

with $\beta = \frac{B_2}{B_1}$: $\begin{cases} \beta = 0 : \text{neutral swimmer} \\ \beta < 0 : \text{pusher} \\ \beta > 0 : \text{puller} \end{cases}$

- In cartesian coordinates : $u_r = B_1(1 + \beta(e \cdot e_r))[(e \cdot e_r)e_r - e]$

Dynamics of two interacting squirmers



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

The evolution of the mass center

The second law of Newton[6]:

$$m\vec{a} = \sum_i \vec{F}_i.$$

The force of viscosity on a small sphere moving through a viscous fluid is given by the Stokes-Einstein relation[7]:

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

We consider the squirmers propulsion in absence of inertia. One has:

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

Thus:

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

Dynamics of two interacting squirmers

The evolution of the mass center

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

We have :

- v_0 the particle velocity,
- $p_i = (\cos(\theta_i), \sin(\theta_i))^T$ orientation,
- $F_{i(j) \to k}$, the lubrification force applied on the k^{th} squirmer, generated by the i^{th} squirmer in presence of the j^{th} one [1],
- $F^w_{k \to i}$, the lubrification force exerted on the i^{th} squirmer due to the presence of the k^{th} wall[1],
- V_{ij} and V_i the Weeks-Chandler-Andersen potential,
- D the translational diffusivity,
- η_i are independent noises.

Dynamics of two interacting squirmers

Steric force

The steric forces are defined by:

- $$\nabla_{r_{ij}} V_{ij} = \begin{pmatrix} -\frac{E_s}{2R^2\pi\mu}\frac{D_x}{r_{ij}}\left[\frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7}\right] \\ -\frac{E_s}{2R^2\pi\mu}\frac{D_y}{r_{ij}}\left[\frac{2(2R)^{13}}{(r_{ij})^{13}} - \frac{(2R)^7}{(r_{ij})^7}\right] \end{pmatrix}$$
- $$\nabla_{r_i} V_i = \begin{pmatrix} -\frac{E_s(X_{box}-X)}{\pi\mu R^2|r-r_i|}\left[2\left(\frac{R}{|r-r_i|}\right)^{13} - \left(\frac{R}{|r-r_i|}\right)^7\right] \\ -\frac{E_s(Y_{box}-Y)}{\pi\mu R^2|r-r_i|}\left[2\left(\frac{R}{|r-r_i|}\right)^{13} - \left(\frac{R}{|r-r_i|}\right)^7\right] \end{pmatrix}$$
- if $|r_i - r_j| < 2^{\frac{7}{6}}R$, we add $\nabla_{r_{ij}} V_{ij}$
- if $|B - r_i| < 2^{\frac{1}{6}}R$, we add $\nabla_{r_i} V_i$

Dynamics of two interacting squirmers

Lubrification force

- The tangential lubrification force acting on the two spheres :

$$\boxed{F^{y}_{i(j)\to i} = -\frac{9}{16} v_0 \left[(p_i \hat{R}_{ij})(1 + \beta p_i \hat{R}_{ij}) - \frac{1}{2}\beta (p_i \hat{R}^{\perp}_{ij})^2 \right] (ln\epsilon + O(1))}$$

- The normal lubrification force acting on the two spheres :

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

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

$$\boxed{F^{y}_{w\to i} = -\frac{9}{4} v_0 \left[(p_i \hat{R}_{ij})(1 + \beta p_i \hat{R}_{ij}) - \frac{1}{2}\beta (p_i \hat{R}^{\perp}_{ij})^2 \right] (ln\epsilon + O(1))}$$

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

Dynamics of two interacting squirmers

The evolution of the orientation

$\phi = 8\pi\mu r^3$ the rotation flow around a sphere[7]:

$$\frac{d\theta_i}{dt} = \frac{1}{\phi} \sum F[6].$$

The evolution of the rotation of one squirmer is then given by:

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

- $\Gamma_{i(j) \to k}$ 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 η^i.

- The torques acting on the squirmer i :

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

- The torques acting on the squirmer j :

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

- The torques produced by the walls on the squirmer i:

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

- if $|r_i - r_j| < 3R$, we add $F_{i(j)\to i}$ and $\Gamma_{i(j)\to i}$ to the i^{th} squirmer, and $F_{i(j)\to j}$ and $\Gamma_{i(j)\to j}$ to the j^{th}
- if $|B - r_i| < 2R$, we add $F^w_{k\to i}$ and $\Gamma^w_{k\to i}$

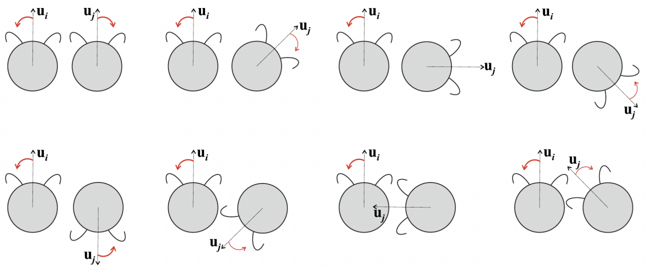
Implementation in Python

- Two classes, `Squirmer` and `Interactingsquirmers`.
- The function `loop_time()` implements a first-order Euler scheme for time integration.
- The code is vectorized.

Numerical Experiments

Interaction between two squirmers

Results from previous study [3]



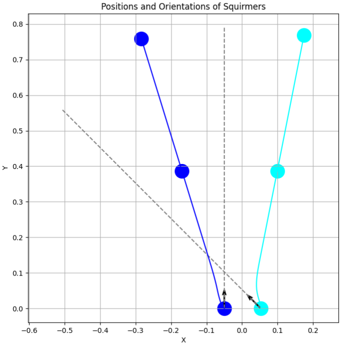
Numerical Experiments

Simulation of two interacting squirmers

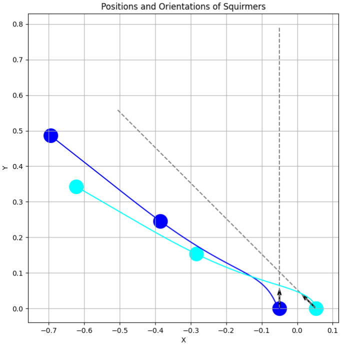
$$\theta_2 = \frac{3\pi}{4}$$

As β decreases, the right squirmer gets pushed away from the left one.

As β increases, the right squirmer gets pulled toward the left one.



$\beta = -1.5$

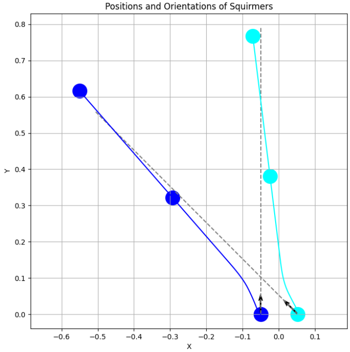


$\beta = 1.5$

Numerical Experiments

Simulation of two interacting squirmers

Result consistent with [3].



$$\beta = 0$$

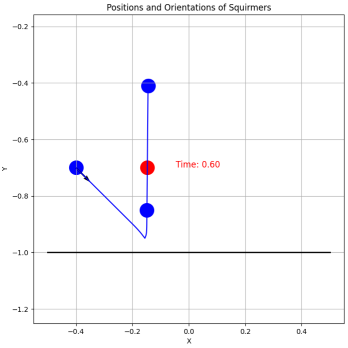
Numerical Experiments

Simulation of squirmer-border interaction

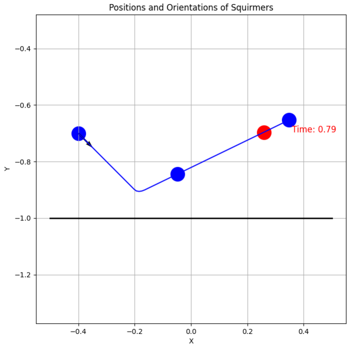
$$\theta = -\frac{\pi}{4}$$

As β decreases, the squirmer gets pulled toward the border.

As β increases, the squirmer gets pushed away from the border.



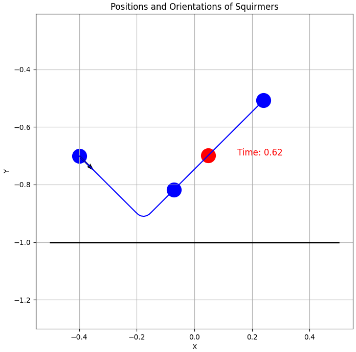
$\beta = -1.5$



$\beta = 1.5$

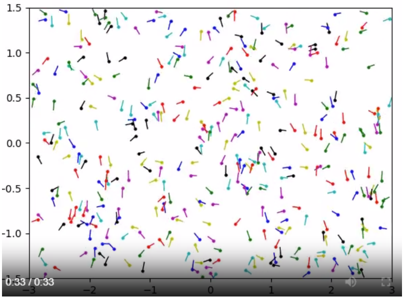
Numerical Experiments

Simulation of squirmer-border interaction



$$\beta = 0$$

N squirmers



375 squirmers in a box

375 squirmers in a channel

Simulation of 375 squirmers by varying the D parameter

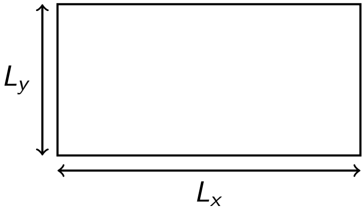
Polar order parameter v_a given by[5]:

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

with p_i the orientation of the i-th squirmer. And ρ is given by:

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

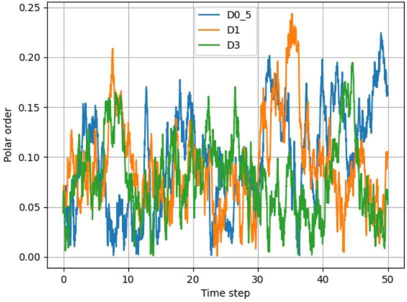
Two sizes of channel are used: Ch_1 with dimensions $L_y = 3$ and $L_x = 6$ and Ch_2 with dimensions $L_y = 2$ and $L_x = 4$.



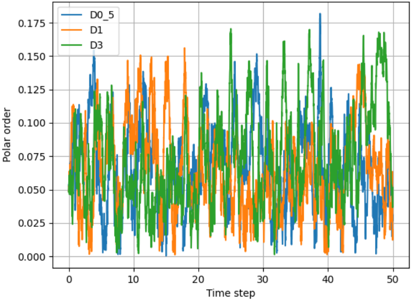
Simulation of 375 squirmers by varying the D parameter

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

More interactions and no collective behavior.



$\beta = 1.5$

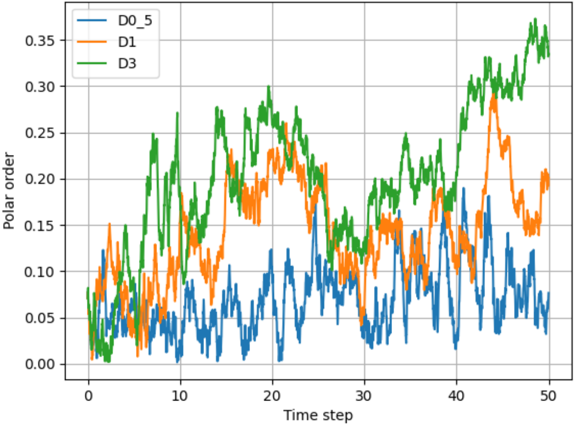


$\beta = -1.5$

Simulation of 375 squirmers by varying the D parameter

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

Collective behavior observed for $D = 3$.



$\beta = 0$

- Not always the same results as reference:[3]
- Varying β value affect the system's dynamics
- Smaller channel size enhances interactions
- No collective behavior observed for $\beta \neq 0$
- Collective behavior emerges for $\beta = 0$ and Ch_2

Conclusion and perspectives

Perspectives

- Longer simulations
- Higher particle densities
- Propensity of squirmers to form clusters over time
- Control the collective behavior of squirmers using β

References

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