Stirring by microswimmers and their interaction with boundaries

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Biomixing: Stirring by swimming organisms

Katija & Dabiri (2009) looked at transport by jellyfish:

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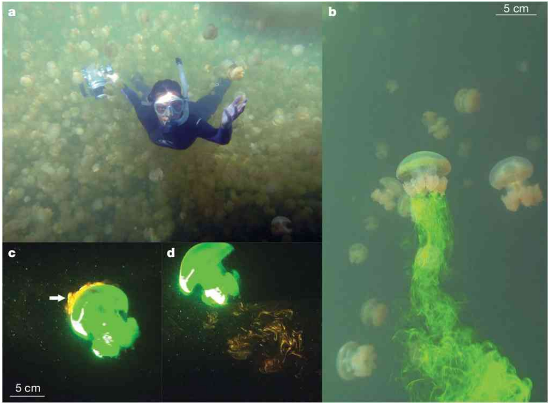


There was quite a stir at the time about biomixing and its possible role in the ocean.

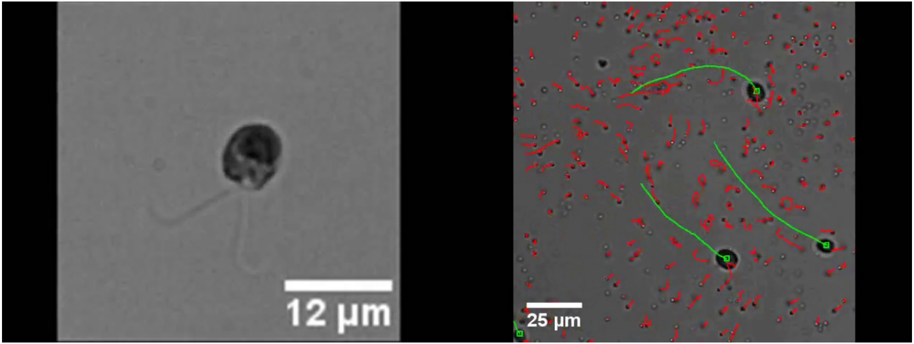
The idea goes back to Walter Munk in the 60s, who dismissed it. Revived by Bill Dewar and others in the 00s.

Since then the consensus is that the effect is negligible, in large part due to stratification (Visser, 2007; Wagner *et al.*, 2014).

Still could have important local impact, and is more relevant for micro-organisms.

Lab experiments

Around the same time precise experiments were being made, most notably in the Gollub and the Goldstein groups:



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Guasto, J. S., Johnson, K. A., & Gollub, J. P. (2010). *Phys. Rev. Lett.* **105**, 168102

Leptos, K. C., Guasto, J. S., Gollub, J. P., Pesci, A. I., & Goldstein, R. E. (2009). *Phys. Rev. Lett.* **103**, 198103

Displacement by a moving body

Use drift trajectories to model mixing induced by swimmers:

86 Mr. J. Clerk-Maxwell *on* [Mar. 10,

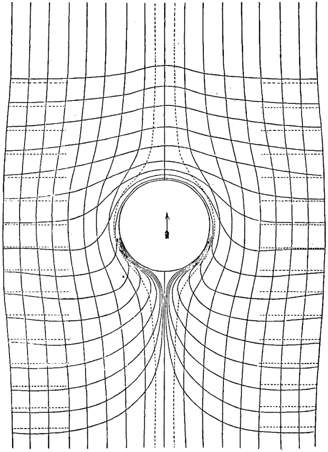

FIG. 1.
Fluid flowing past a fixed cylinder.

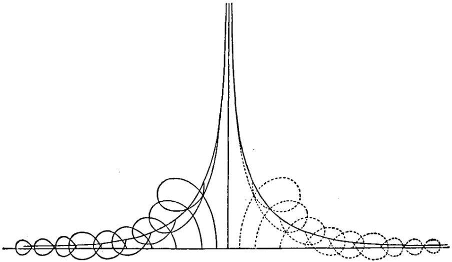

FIG. 2.
Paths of particles of the fluid when a cylinder moves through it.

Maxwell (1869); Darwin (1953)

A ‘gas’ of swimmers

Dilute theory: swimmers repeatedly ‘kick’ fluid particles.

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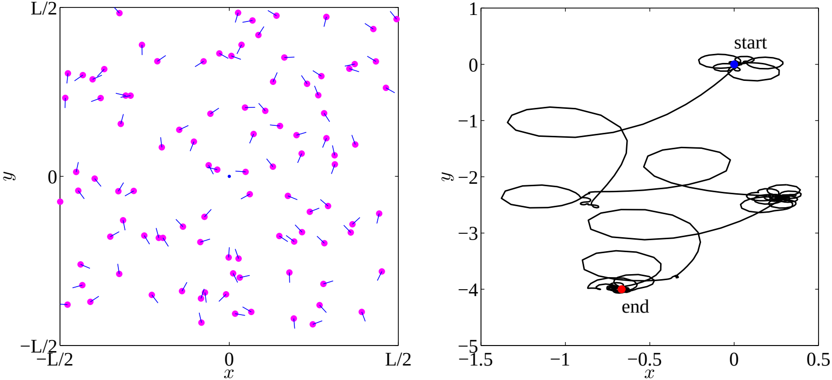


Thiffeault, J.-L. & Childress, S. (2010). *Phys. Lett. A*, **374**, 3487–3490
Lin, Z., Thiffeault, J.-L., & Childress, S. (2011). *J. Fluid Mech.* **669**, 167–177

Strategy: The probability density of displacements

- Find the distribution of displacements for a single swimmer.
- The sum of displacements for many swimmers is the convolution of single-swimmer displacements.
- In Fourier space (characteristic function), the convolution is a simple product, but we must then take an inverse transform.
- Usually this inverse transform is approximated using the Central Limit Theorem, but here we must evaluate it explicitly because of the short times involved.
- Care must be taken when going to the infinite-volume limit.

Mean-squared displacement

R_λ^N is the random particle displacement due to N swimmers;
The mean-squared-displacement is

$$\langle (R_\lambda^N)^2 \rangle = n \int_V \Delta_\lambda^2(\boldsymbol{\eta})\, \mathrm{d}V_{\boldsymbol{\eta}}$$

with

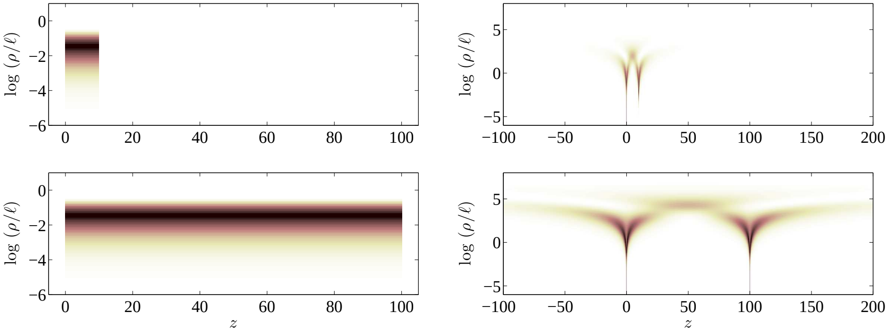
- $n = N/V$ the number density of swimmers
- λ the path length of swimming
- Δ_λ the fluid displacement (drift)
- $\boldsymbol{\eta}$ the initial fluid particle position

Crucial point:

If the integral grows linearly in λ, then the particle motion is diffusive.

Two ways to get diffusive behavior

Plot of the integrand:



Left: support grows linearly with λ (typical of near-field). Thiffeault & Childress (2010)

Right: ‘uncanny scaling’ $\Delta_\lambda(\boldsymbol{\eta}) = \lambda^{-1} D(\boldsymbol{\eta}/\lambda)$ (typical of far-field stresslet). Lin *et al.* (2011); Pushkin & Yeomans (2013)

The distribution of displacements

We can go further with this model and find an expression for the full probability density, in the form of an inverse Fourier transform:

$$\boxed{p_{X_\lambda}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left(-n\,\Gamma_\lambda(k)\right) \mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}k}$$

The limit taken is effectively a continuous convolution of individual distributions.
The rate function is

$$\Gamma_\lambda(k) := \int_V \left(1 - \operatorname{sinc}(k\Delta_\lambda(\boldsymbol{\eta}))\right) \mathrm{d}V_{\boldsymbol{\eta}}\,.$$

Thiffeault, J.-L. (2015). *Phys. Rev. E,* **92**, 023023

A model swimmer

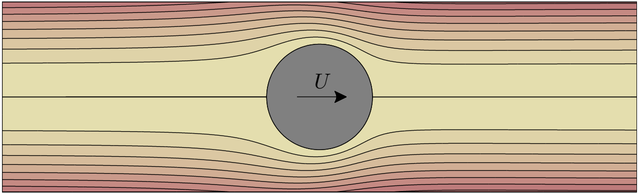
This is as far as we can go without introducing a model swimmer.

We take a squirmer, with axisymmetric streamfunction:

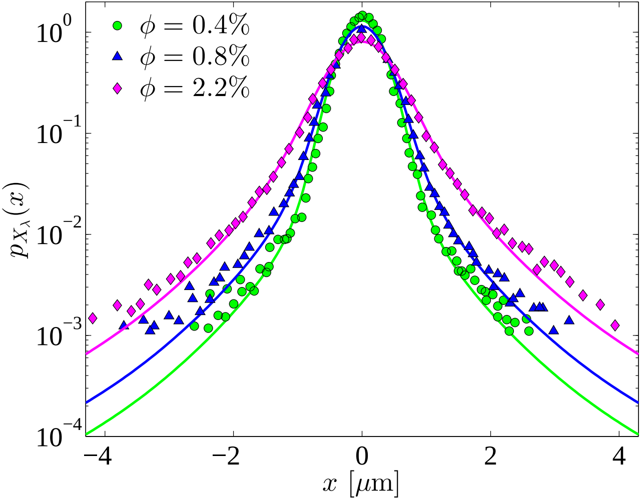
$$\Psi_{\mathsf{sf}}(\rho, z) = \tfrac{1}{2}\rho^2\, U \left\{ -1 + \frac{\ell^3}{(\rho^2 + z^2)^{3/2}} + \tfrac{3}{2} \frac{\beta \ell^2 z}{(\rho^2 + z^2)^{3/2}} \left(\frac{\ell^2}{\rho^2 + z^2} - 1 \right) \right\}$$

See for example Lighthill (1952); Blake (1971); Ishikawa *et al.* (2006); Ishikawa & Pedley (2007); Drescher *et al.* (2009)

We use the stresslet strength $\beta = 0.5$, which is close to a treadmiller:



Comparing to Leptos *et al.*

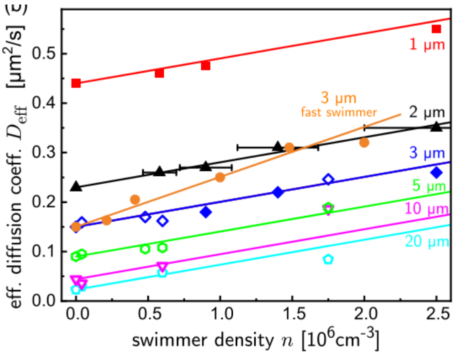


Leptos, K. C., Guasto, J. S., Gollub, J. P., Pesci, A. I., & Goldstein, R. E. (2009). *Phys. Rev. Lett.* **103**, 198103; Thiffeault, J.-L. (2015). *Phys. Rev. E,* **92**, 023023

Recent experiments of Ortlieb *et al.* (2019)

Formula for the effective diffusivity from Thiffeault (2015):

$$D_{\text{eff}} = D_0 + \left(0.266 + \tfrac{3}{4}\pi\beta\right) U\, n\, \ell^4$$

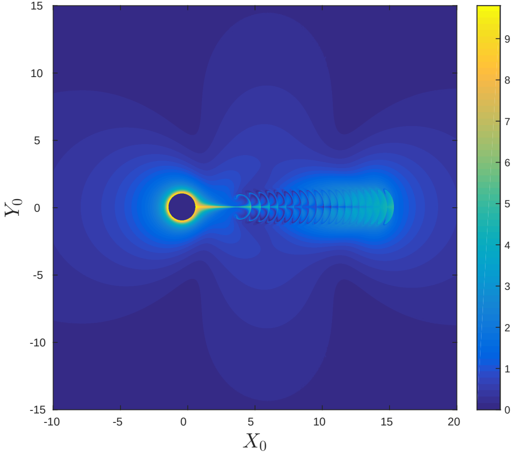


Their experiments are longer and they can see convergence to a Gaussian form, at the rate predicted by the dilute theory.

Ortlieb, L., Rafaï, S., Peyla, P., Wagner, C., & John, T. (2019). *Phys. Rev. Lett.* **122**, 148101

Unsteady swimmer

Sphere-flagellum time-dependent swimmer [Peter Mueller] play movie



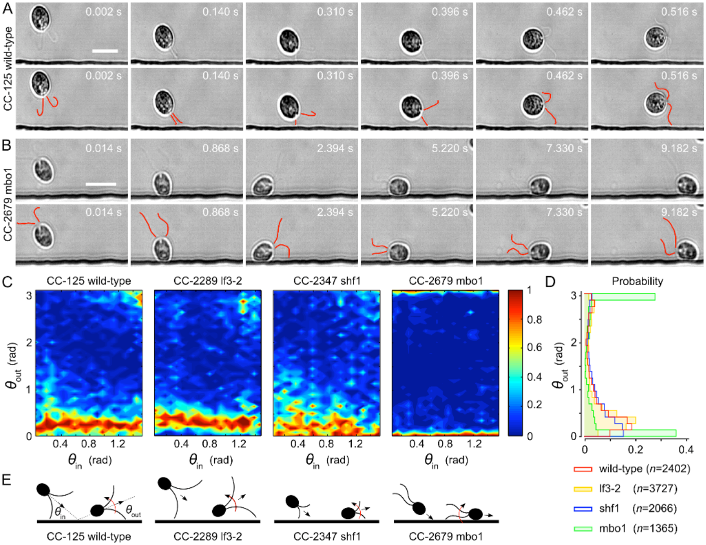
Map of displacement Δ_λ as a function of initial fluid particle position (X_0, Y_0).

Notice the largest displacements are near the swimmer's body, because of the no-slip boundary condition.

Mueller, P. & Thiffeault, J.-L. (2017). *Phys. Rev. Fluids,* **2** (1), 013103

Morrel, T. A., Spagnolie, S. E., & Thiffeault, J.-L. (2019). *Phys. Rev. Fluids,* **4** (4), 044501

Microswimmer scattering off a surface



Kantsler, V., Dunkel, J., Polin, M., & Goldstein, R. E. (2013). *Proc. Natl. Acad. Sci. USA*, **110** (4), 1187–1192

play movie

Microswimmer scattering off a surface

- Large literature focusing on both steric and hydrodynamic interactions.
- Not always clear which one dominates.
- Here: focus on modeling steric interactions only, in particular the role of a microswimmer's shape.
- Joint work with Hongfei Chen

  Chen, H. & Thiffeault, J.-L. (2020). `http://arxiv.org/abs/2006.07714`

See also

- Nitsche, J. M. & Brenner, H. (1990). *J. Colloid Interface Sci.* **138**, 21–41
- Contino, M., Lushi, E., Tuval, I., Kantsler, V., & Polin, M. (2015). *Phys. Rev. Lett.* **115** (25), 258102
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- Elgeti, J. & Gompper, G. (2015). *Europhys. Lett.* **109**, 58003
- Lushi, E., Kantsler, V., & Goldstein, R. E. (2017). *Phys. Rev. E,* **96** (2), 023102

Active Brownian particles

Microswimmers and active particles are often modeled as Brownian particles with a propulsion, using an SDE such as

$$\begin{aligned}
\mathrm{d}X &= U\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1 \\
\mathrm{d}Y &= \sqrt{2D_Y}\,\mathrm{d}W_2 \\
\mathrm{d}\theta &= \sqrt{2D_\theta}\,\mathrm{d}W_3
\end{aligned}$$

in its own rotating reference frame.

In terms of absolute x and y coordinates, this becomes

$$\begin{aligned}
\mathrm{d}x &= \left(U\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1\right)\cos\theta - \sin\theta\,\sqrt{2D_Y}\,\mathrm{d}W_2 \\
\mathrm{d}y &= \left(U\,\mathrm{d}t + \sqrt{2D_X}\,\mathrm{d}W_1\right)\sin\theta + \cos\theta\,\sqrt{2D_Y}\,\mathrm{d}W_2 \\
\mathrm{d}\theta &= \sqrt{2D_\theta}\,\mathrm{d}W_3\,.
\end{aligned}$$

Fokker–Planck equation

Fokker–Planck equation for the probability density $p(x, y, \theta, t)$:

$$\partial_t p = -\nabla \cdot (\boldsymbol{u}\, p - \nabla \cdot \mathbb{D}\, p) + \partial_\theta^2 (D_\theta\, p)$$

where the drift vector and diffusion tensor are respectively

$$\boldsymbol{u} = \begin{pmatrix} U \cos\theta \\ U \sin\theta \end{pmatrix}$$

$$\mathbb{D} = \begin{pmatrix} D_X \cos^2\theta + D_Y \sin^2\theta & \frac{1}{2}(D_X - D_Y)\sin 2\theta \\ \frac{1}{2}(D_X - D_Y)\sin 2\theta & D_X \sin^2\theta + D_Y \cos^2\theta \end{pmatrix}.$$

Note that $\nabla := \hat{\boldsymbol{x}}\, \partial_x + \hat{\boldsymbol{y}}\, \partial_y$ (no θ).

Boundary condition

For any fixed volume V we have

$$\partial_t \int_V p \,\mathrm{d}V = -\int_V \big(\nabla \cdot (\boldsymbol{u}\, p - \nabla \cdot (\mathbb{D}\, p)) - \partial_\theta^2 (D_\theta\, p)\big)\,\mathrm{d}V$$
$$= -\int_{\partial V} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{S}$$

where ∂V is the boundary of V, and the flux vector is

$$\boldsymbol{f} = \boldsymbol{u}\, p - \nabla \cdot (\mathbb{D}\, p) - \hat{\boldsymbol{\theta}}\, \partial_\theta (D_\theta\, p).$$

Thus, on the reflecting (impermeable) parts of the boundary we require the no-flux condition

$$\boldsymbol{f} \cdot \boldsymbol{n} = 0, \quad \text{on} \quad \partial V_{\mathsf{refl}}$$

where $\boldsymbol{n}$ is normal to the boundary.

Swimmer touching a wall at $y = 0$

Denote by $y_*(\theta)$ the vertical coordinate of a swimmer with orientation θ when it touches the wall.

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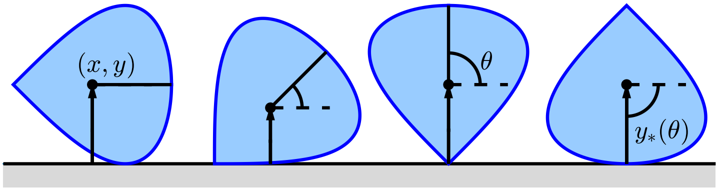
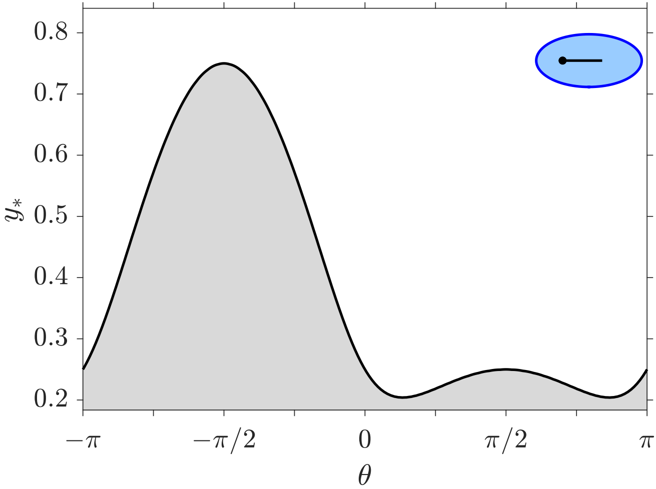
Convex swimmer touching a horizontal wall at $y = 0$:



We call $y_*(\theta)$ the wall distance function. The swimmer's y coordinate must satisfy $y \geq y_*(\theta)$, otherwise the swimmer is inside the wall.

Wall distance function $y_*(\theta)$: off-center ellipse



$$y_*(\theta) = \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta} - \tfrac{1}{2} a \sin \theta$$

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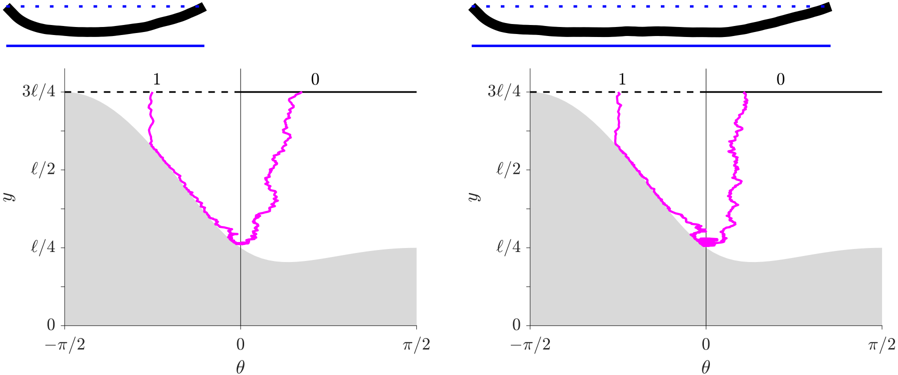
Configuration space and drift in θ–y plane

Drift is $U \sin\theta\, \hat{\boldsymbol{y}}$; no-flux condition forces swimmer to align with the wall.



Once the particle crosses $\theta = 0$ (parallel to wall), it is pushed upward by the drift.

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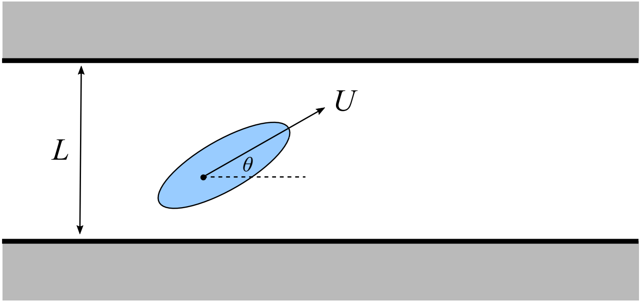
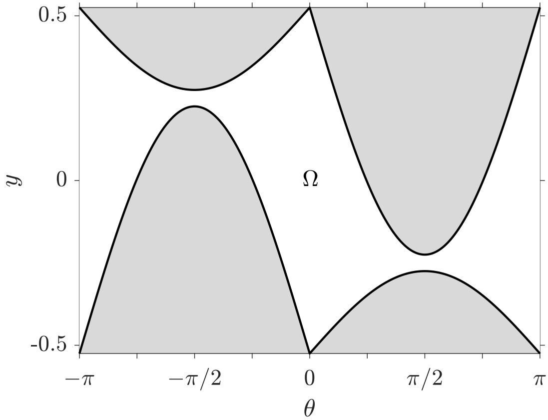
A Microswimmer in a Channel

For example, one application of this configuration space formalism is to the transport of microswimmers in a narrow channel:



A swimmer will turn around once in a while, effectively undergoing a 1D random walk. What is the effective horizontal diffusion coefficient?

Channel configuration space



Configuration space for the needle in of length $\ell = 1$ in a channel of width $L = 1.05$. (x not shown.)

A point in this space specifies the position and orientation of the swimmer.

Reduced equation

The Fokker–Planck equation is challenging to solve because of the complicated boundary shape.

Tractable limit $D_\theta \ll 1$ (small rotational diffusivity)

Get a (1+1)D PDE for $p(\theta, y, t) = P(\theta, T)\,\mathrm{e}^{\sigma(\theta) y}$

$$\boxed{\partial_T P + \partial_\theta(\mu(\theta)\,P - \partial_\theta P) = 0} \qquad T := D_\theta\, t$$

The shape of the swimmer enters through drift $\mu(\theta)$.

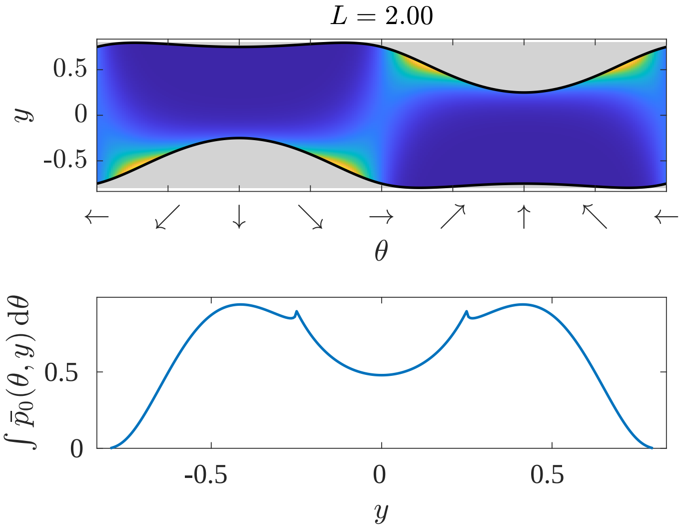
The natural invariant density for the swimmer satisfies

$$\partial_\theta(\mu(\theta)\,\mathcal{P} - \partial_\theta \mathcal{P}) = 0.$$

which can be solved semianalytically for some simple shapes.

For an asymmetric swimmer, the invariant density has a net rotational drift even at equilibrium.

Invariant density examples



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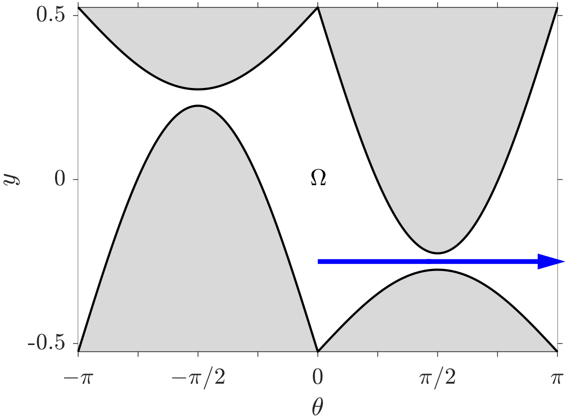
Reversal

Whenever the swimmer goes through one of the bottlenecks below, this corresponds to a reversal of swimming direction.



Mean Reversal Time

The mean reversal time τ_{rev} is

$$\boxed{\tau_{\text{rev}} = \frac{1}{4D_\theta}\int_0^\pi \frac{\mathrm{d}\vartheta}{\mathcal{P}(\vartheta)}}$$

where $\mathcal{P}(\theta)$ is the marginal invariant probability density for the swimmer.

Intuitively, small $\mathcal{P}$ corresponds to "bottlenecks" that dominate the reversal time.

For the needle swimmer,

$$\tau_{\text{rev}} \approx \frac{\pi}{2\beta D_\theta}\,\mathrm{e}^{\beta}, \qquad \beta = U\ell/4D_Y.$$

From this we get an effective diffusivity

$$\boxed{D_{\textsf{eff}} \approx \tfrac{1}{2}\tau_{\text{rev}}\,U^2}$$

Conclusions

- Transport and mixing of, and caused by, microswimmers is a fertile area of study.
- The interaction of microswimmers with boundaries is a huge topic, and I apologize for not doing justice to the literature today, for lack of time.
- Our focus is on modeling interactions using the rich concept of configuration space, involving all the degrees of freedom of the swimmer constrained by boundaries.
- Steric interactions are part of the boundary conditions rather than modeled as a potential.
- Can add lots of effects to F–P equation:
  - hydrodynamics
  - interaction forces
  - deformable body and flagella
  - 3D

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