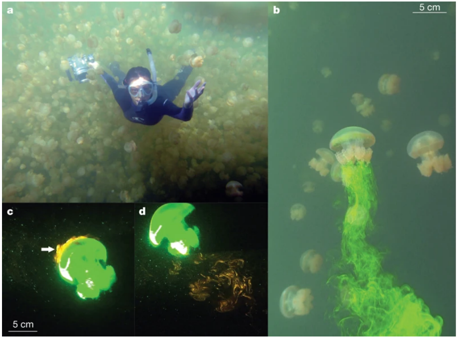
Stirring by microswimmers and their interaction with boundaries

Jean-Luc Thiffeault

6 November 2024

Biomixing: Stirring by swimming organisms

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



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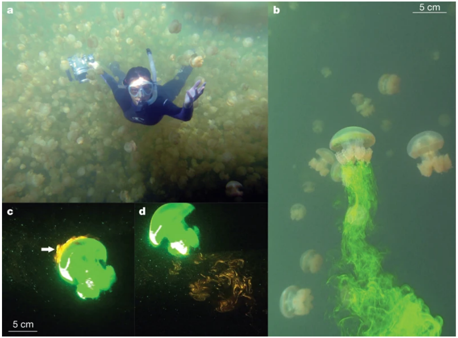

There was quite a stir at the time about biomixing and its possible role in the ocean.

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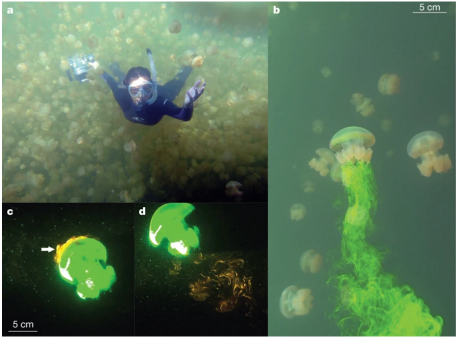

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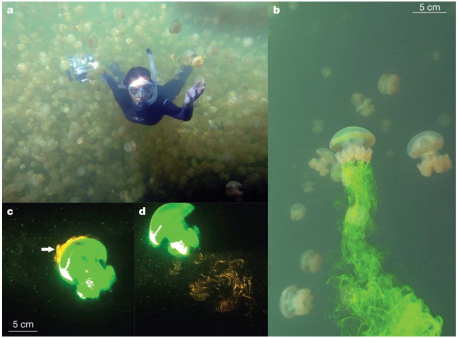

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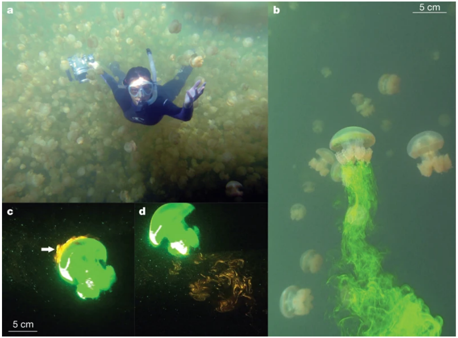

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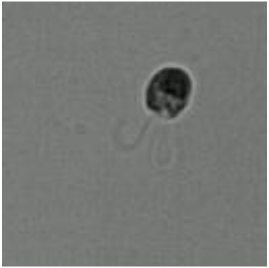
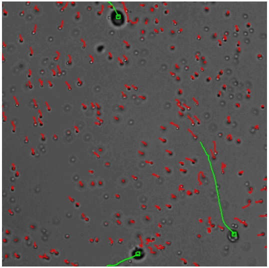
Still could have important local impact, and is more relevant for micro-organisms.

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:

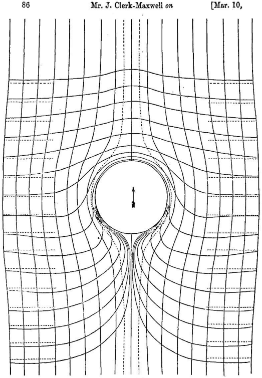


Fig. 1.
Fluid flowing past a fixed cylinder.

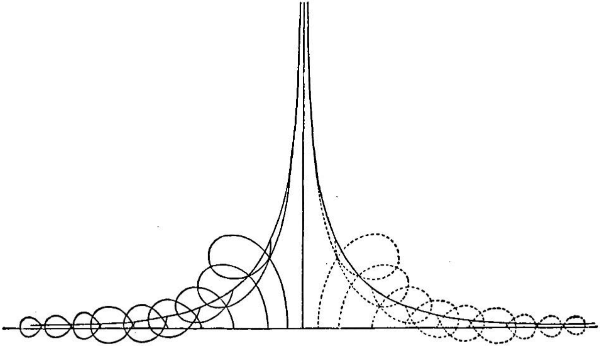
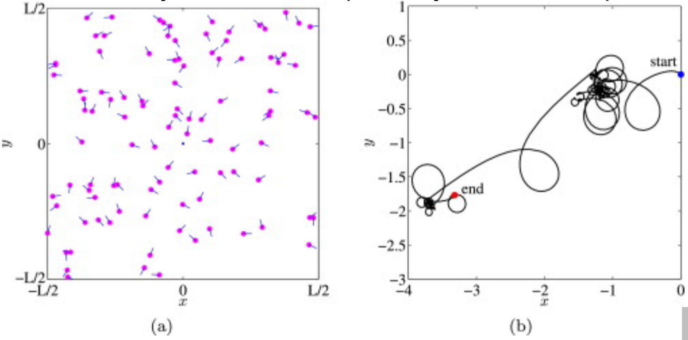


Fig. 2.
Paths of particles of the fluid when a cylinder moves through it.

Maxwell(1869); play video Darwin(1953)

A "gas" of swimmers

Dilute theorey: swimmers repeatedly "kick" fluid particles.



play video

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

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- Care must be taken when going to the infinite-volume limit.

Mean-squared displacement

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$$\left\langle \left(R_\lambda^N\right)^2 \right\rangle = n \int_V \Delta_\lambda^2(\eta)\, dV_\eta$$

with

- $n = N/V$ the number density of swimmers
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- Δ_λ the fluid displacement (drift)
- η the initial fluid position

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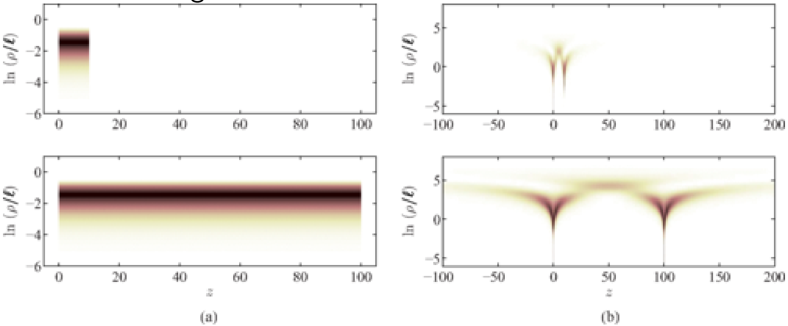
Crucial point:

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' $\Delta_\lambda(\eta) = \lambda^{-1}\Delta(\eta/\lambda)$(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:

$$\boxed{p_{X_\lambda}(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} exp(-n\Gamma_\lambda(k))e^{-ikx}dk}$$

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

The rate function is

$$\Gamma_\lambda(k) := \int_V (1 - sinc(k\Delta_\lambda(\eta)))dV_\eta$$

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:

$$\Psi(\rho, z) = \frac{1}{2}\rho^2 U \left\{ -1 + \frac{l^3}{(\rho^2 + z^2)^{3/2}} + \frac{3}{2}\frac{\beta l^2 z}{(\rho^2 + z^2)^{3/2}} \left(\frac{l^2}{\rho^2 + z^2} - 1 \right) \right\}$$

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

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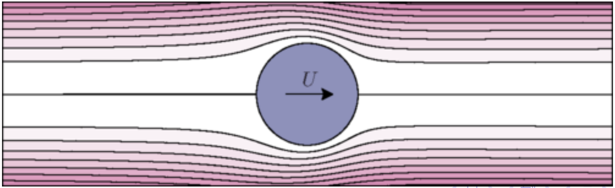
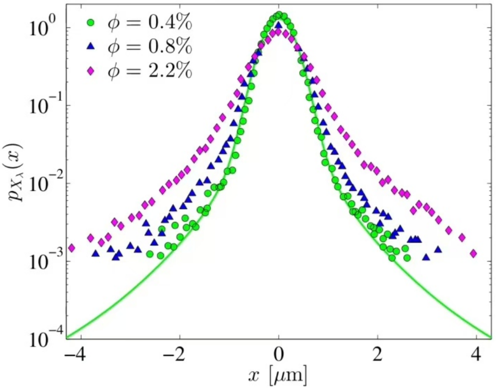
See for example Lighthill(1952); Blake(1971); Ishikawa *et al.* (2006); Ishikawa & Pedley(2007); Drescher *et al.*(2009)
We use the textcolorpurplestresslet strength $\beta = 0.5$, which is close to a treadmiller:

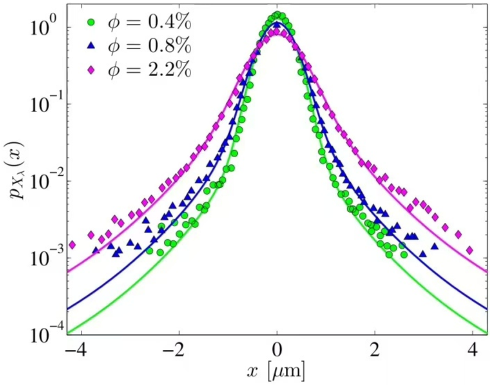


Comparing to Leptos *et al.*



Fit the stresslet strength $\beta = 0.5$ to one curve.

Comparing to Leptos *et al.*

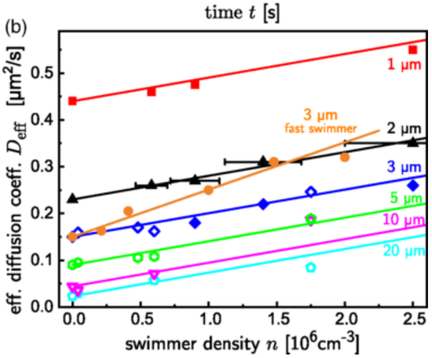


Leptos, K. C., Guasto, J. S., Gollub, J. P., Pesci, A. I. & Goldstein, R. E.(2009) *Phys. Rev. Lett.* **103**, 198103.;
Thiffeault, J.-L. (2015) *Phys. Rev. E*, **92**, 023023

More recent experiments of Ortlieb *et al.*(2019)

Formula for the effective diffusivity from Thiffeault (2015):

$$D_{eff} = D_0 + (0.266 + \tfrac{3}{4}\pi\beta)Unl^4$$

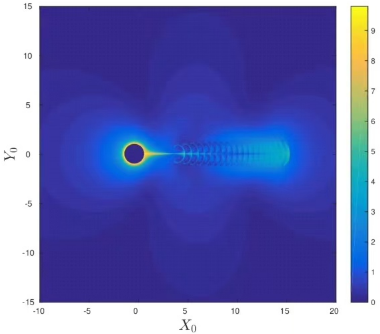


There experiments are longer and they can see convergence to a Gaussian form, at the rate predicted by the dilute theory.

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

Unsteady swimmer

Sphere-flagellum time-dependent swimmer [Peter Mueller]



play video

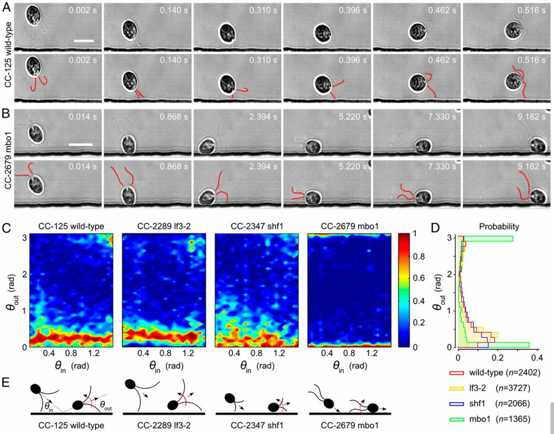
Map of displacement Δ_λ as a function of initial fluid particle position (X_0, Y_0).

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., Spagnoile, S. E., & Thiffeault, J.-L. (2019) *Phys. Rev. Fluids*, **4**(4), 044501

Microswimmer scattering off a surface



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

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

Microswimmer scattering off a surface

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
- Spagnoile, S. E., Moreno-Flores, G. R., Bartolo, D., & Lauga, E. (2015). *Soft Matter,* **11**, 3396-3411
- Ezhilan, B. & Saintillan, D. (2015). *J. Fluid Mech.* **777**, 482-522
- Ezhilan, B., Alonso-Matilla, R., & Saintillan, D. (2015). *J. Fluid Mech.* **781**, R4
- 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

$$
\begin{aligned}
dX &= U dt + \sqrt{2D_X}\, dW_1 \\
dY &= \sqrt{2D_Y}\, dW_2 \\
d\theta &= \sqrt{2D_\theta}\, dW_3
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$$

in its own rotating reference frame

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in its own rotating reference frame

In terms of absolute x and y coordinates, this becomes

$$\begin{aligned} dx &= (U dt + \sqrt{2D_X}\, dW_1)\cos\theta - \sin\theta\sqrt{2D_Y}\, dW_2 \\ dy &= (U dt + \sqrt{2D_X}\, dW_1)\sin\theta + \cos\theta\sqrt{2D_Y}\, dW_2 \\ d\theta &= \sqrt{2D_\theta}\, dW_3 \end{aligned}$$

Fokker-Planck equation

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

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

where the drift vector and diffusion tensor are respectively

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

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

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

Boundary condition

For any fixed volume V we have

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

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

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

$$\mathbf{f} \cdot \mathbf{n} = 0, \quad on \quad \partial V_{refl}$$

where $\mathbf{n}$ 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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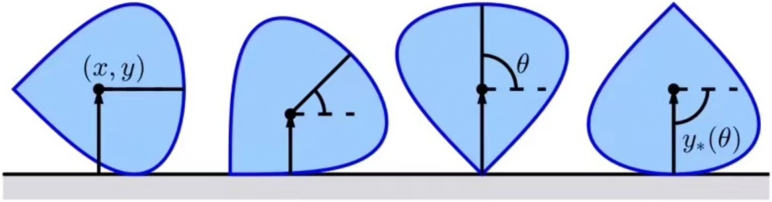
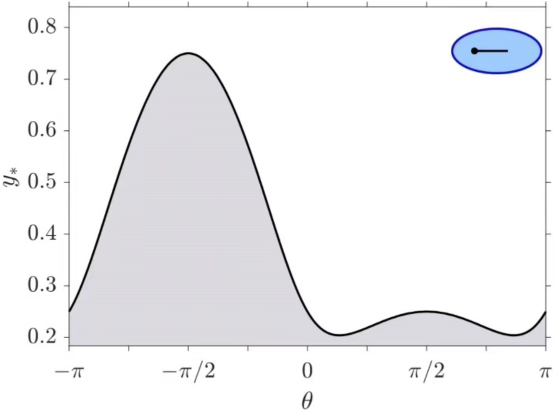
Convex swimmer touching a horizontal wall at $y = 0$:



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.

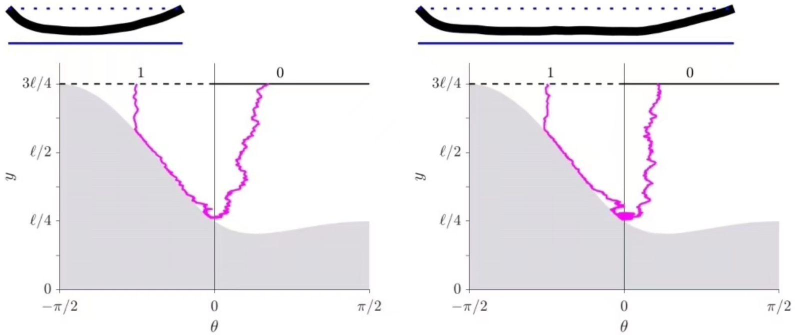
Wall distance function $y_*(\theta)$: off-center ellipse



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

Configuration space and drift in $\theta - y$ plane

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



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

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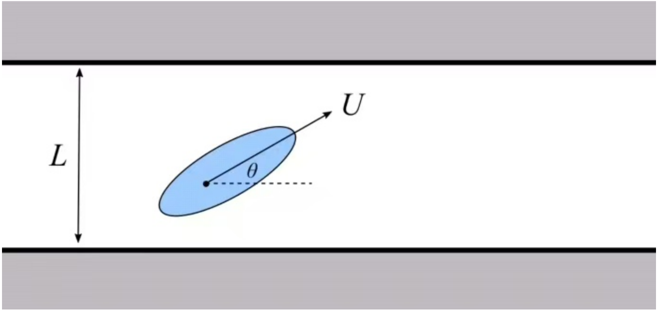
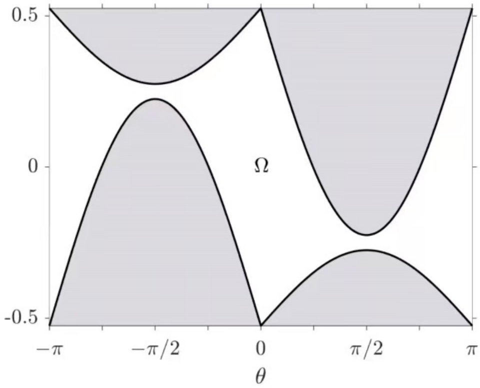
A Microswimmer in a Channel

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 $l = 1$ 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 $p(\theta, y, t) = P(\theta, T)e^{\sigma(\theta)y}$

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

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

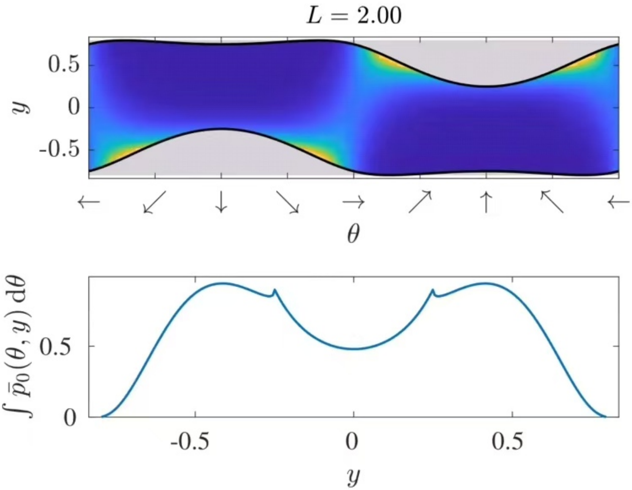
The natural invariant density for the swimmer satisfies

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

which can be solved semi-analytically for some simple shapes.

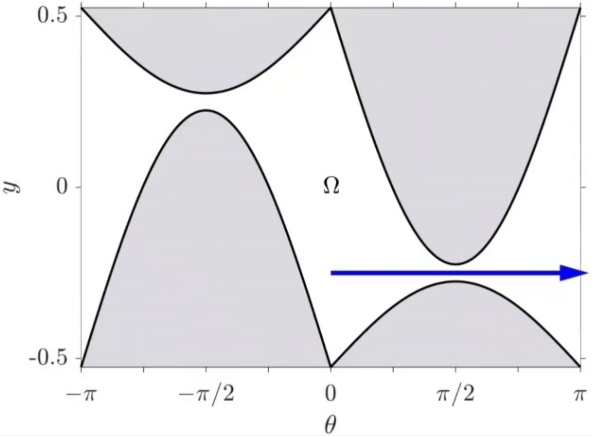
For an asymmetric swimmer, the invariant density has a net rotational drift even at equilibrium.

Invariant density examples



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

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

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

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

For the needle swimmer,

$$\tau_{rev} \approx \frac{\pi}{2\beta D_\theta} e^\beta, \qquad \beta = Ul/4D_Y$$

From this we can get an effective diffusivity

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

Conclusions

- Transport and mixing of, and caused by, microswimmers is 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