Lost in configuration space

Microswimmers and active particles often interest
with boundaries.

\begin{align*}
\text{hydrodynamic} \\
\text{stochastic (contact)}
\end{align*}

Hydrodynamic is well-understood.

Particle feels its "image" in the boundary.
Use Stokes flow, for most part \times image system.

Steric is trickier: lots of ad-hoc models, experimentally
motivated & validated.

\Rightarrow \text{reflect?} \Rightarrow \text{or use a}
\text{confining potential}

\Rightarrow \text{oop!}

Flagella & shape play crucial roles.

Is there a "mathematically sound" way of modeling
steric interactions? Can we include effect of shape
of swimmer?
A model: elliptical swimmer (2D)

Center is at \( x = (x, y) \)

\[ \text{CONFIGURATION } (x, y, \theta). \]

What happens when we make contact with a planar wall?

\[ \theta = 0 \]
\[ y_x = a \]
\[ \theta = \frac{\pi}{2} \]

Closest approach \( y_x(\theta) \) depends on angle.

The range of allowable \( (x, y, \theta) \) is called configuration space

\[ \text{ellipse: } y_x(\theta) = a^2 \sin^2 \theta + b^2 \cos^2 \theta \]

\( a \) point is an allowable configuration

\( x \) is unconstrained (not shown)
Add some dynamics:

\[ \mathbf{U} = U \cos \theta, \sin \theta \]

constant speed of swimming

Trajectory A: moves down, encounters wall "constraint" keeps it from entirely but still free downward drift.

The swimmer must rotate to horizontal.

Depends on shape! \( \theta \rightarrow " \text{prole}" \)

B: \( \theta \rightarrow \text{oops, stuck!} \)

Some shapes have strange landscape.
So what's the mathematical model?  

\[ \text{ABP} \ (\text{Active Brownian Particle}) \]

\[ dX = \bar{U} \, dt + \sqrt{2D_x} \, dW_x \]

\[ d\theta = \Omega \, dt + \sqrt{2D_\theta} \, dW_\theta \]

\( W_i(t) \) are Brownian motion.  \( \frac{1}{\text{time}} \) rotational diffusion

Lab frame:  

\[ dx = \bar{U} \cos \theta \, dt + \sqrt{2D_x} \, dW_x \]

\[ dy = \bar{U} \sin \theta \, dt + \sqrt{2D_y} \, dW_y \]

"Smother" than Brownian motion.

Persistence length \( \frac{U}{D_\theta} \).

(like some simple polymer models)

Because of boundaries, better to solve for probability density

\[ p(x,y,\theta,t) \rightarrow \text{Fokker-Planck eqn} \]

\[ (\text{Smoluchowski}) \]

\[ \partial_t p + \nabla \cdot (\bar{U} p) + \partial_\theta (-\omega p) \]

\[ = D \nabla^2 p + D_\theta \partial_\theta^2 p \]
Flux form: \[ \frac{\partial p}{\partial t} + \nabla \cdot f = 0 \quad f = \nabla p + \rho \theta \hat{p} \]

in \( \Omega \) (domain) \[- D \nabla p - D_r \theta \rho \hat{p} \theta \]

Now we can impose a natural flux preserv, BC:

\[ f \cdot \hat{n} = 0 \] on \( \partial \Omega \) (boundary)

This is so that \[ \frac{d}{dt} \int_{\Omega} p \, dV = - \int_{\partial \Omega} f \cdot ds = 0 \]

This gives the effect described before:

With noise, typical traj.:

\[ \text{"sleep" at } \theta = 0 \]

sleep until random fill

take it any
With this technology, we can complicate the domain.

Channel: \[\begin{array}{c}
\text{Swimmer bounces} \\
\text{around between two} \\
\text{parallel plane wells.}
\end{array}\]

Configuration space:

In the small Dr. limit, we derived a "reduced equation" that allows us to derive quantities such as the invariant density of swimmers. They tend to cluster at wells but not always depending on shape. Hydrodynamic interactions are also important but can be easily included. \[\text{(Chen \& Thiffeault, JFM, 2021)}\]

Can also define configuration space for multiple particles. Each point in that space is the location and orientation of all particles. Very complex! Topology not well understood.

\[\text{(Volume of configuration space related to phase transition)}\]
Swimmer in a lattice:

First consider a fixed orientation. We can imagine the lattice is moving around the swimmer.

Configuration space reproduces the shape of swimmer.

We can already answer some interesting questions: a non-swimming particle will diffuse through a lattice of pores following exactly the same equation as heat conduction in a perforated domain, a problem solved by Rayleigh using a reflection method.

\[
D_{	ext{eff}} = \frac{D}{1 + \phi} \\
\phi = \text{volume fraction of swimmer} \\
(\text{small})
\]

for a circular particle.
This was for fixed orientation. If the angle changes randomly, need to include $\theta$:

![Diagram]

$\theta = \pi$ \hspace{1cm} Take the previous picture and twist it in $\theta$

$\theta = 0$ \hspace{1cm} 3D periodic cell in $(x,y,\theta)$

Solve heat equation in $Q$, with a tubular obstacle $\Omega$ that describes shape. $f \cdot n = 0$ on $\partial Q$

Adding a swimming velocity impairs a drift that can create boundary layers along the tubular obstacle.

Rayleigh's theory, or tools from homogenization theory ($U=0$) allow us to compute the transport coefficients in the lattice.

This is ongoing work with Hongfei Chen & Ziheng Zhang.

Some further work: Full 3D, multiparticle, deformable particles and boundaries, computational methods, random environments, run-and-tumble dynamics...