Stochastic Dynamics of Confined Microswimmers

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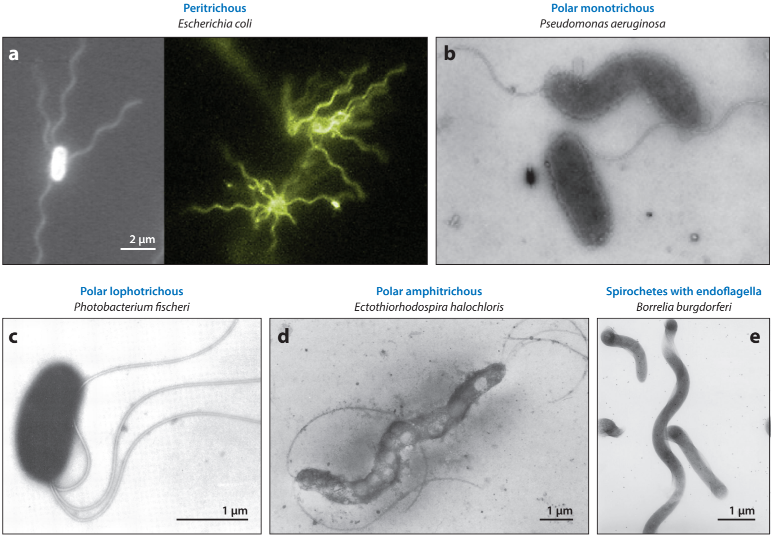
Biological Microswimmers



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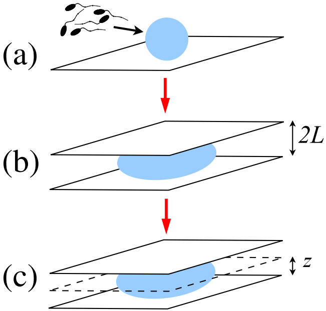
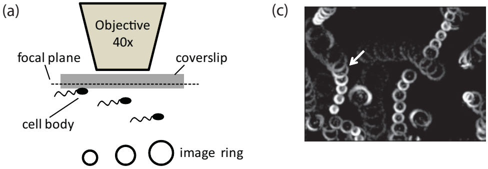
[1] [Lauga, Ann. Rev. Fluid Mech., (2016)] and bibliography therein

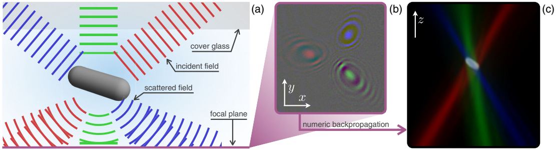
Experimental Settings and Observation protocols



Adapted from [Berke et al., Phys. Rev. Lett. (2008)].

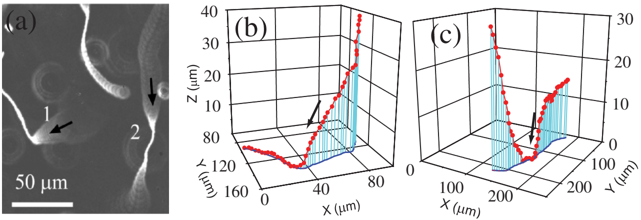


[Li et al., Phys. Rev. (2011)]



[Bianchi et al., Phys. Rev. X (2017)]

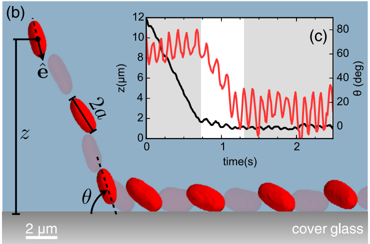
Observed Trajectories



(a): Image rings:
$r \propto$ dist. to focal plane

(b,c) Trajectory.

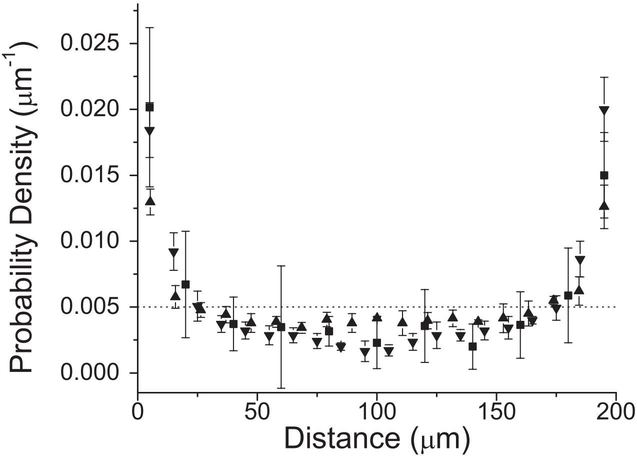
[Li & Tang, Phys. Rev. Lett. (2009)]



[Bianchi et al., Phys. Rev. X (2017)]

$$\begin{cases} z & \text{height} \\ \theta & \text{angle w.r.t. to horiz. plane} \end{cases}$$

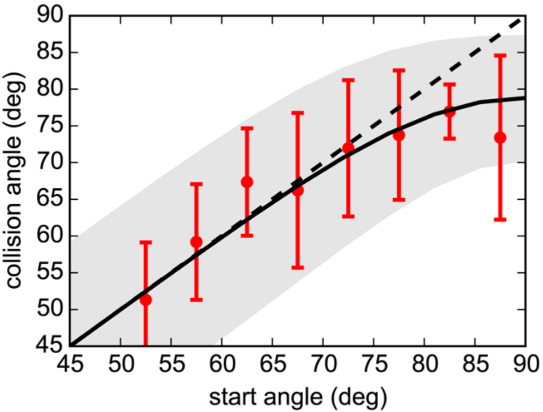
Experimental Data – Stationary Density Distributions



(*)

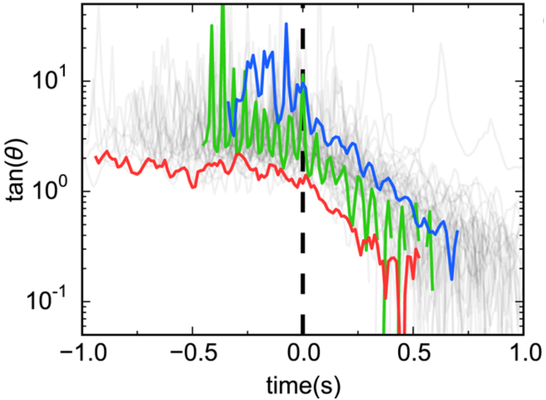
- *Bull spermatozoa* (squares) [Rotschild, Nature (1963)]
- *E. coli* (down triangles) [Berke et al., Phys. Rev. Lett. (2008)]
- *C.crescentus* (up triangles) [Li & Tang, Phys. Rev. Lett. (2009)](*)

Experimental Data – Impact Angle Distribution



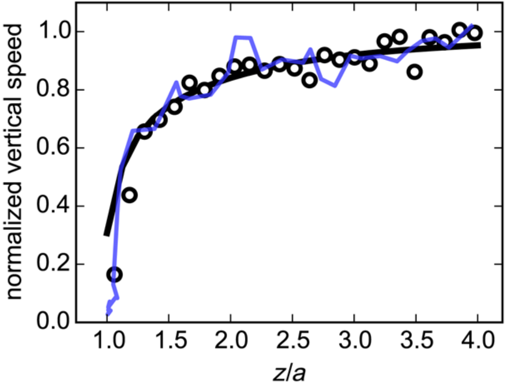
First impact angle as function of launch angle.
[Bianchi et al., Phys. Rev. X (2017)]

Experimental Data – Post-Collision Angle Evolution



[Bianchi et al., Phys. Rev. X (2017)]

Experimental Data – Normalized Vertical Speed



- a: half-length of microswimmer
- z: dist. from boundary.

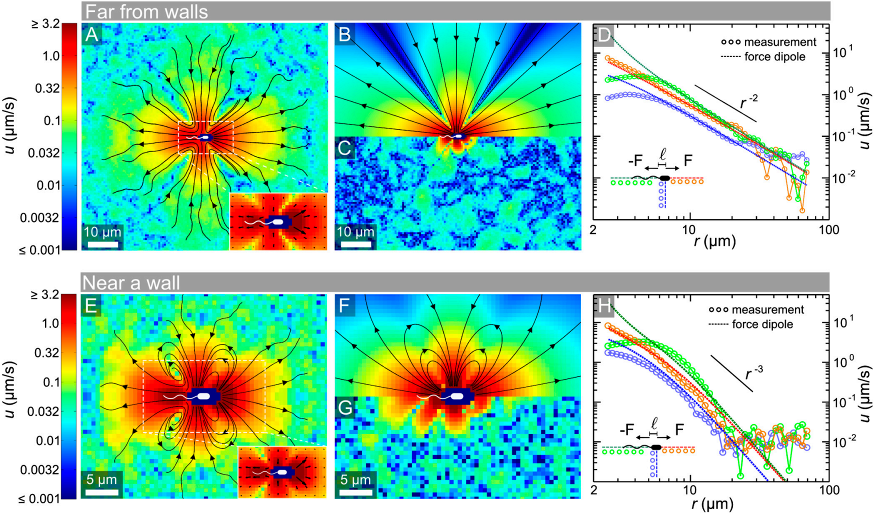
[Bianchi et al., Phys. Rev. X (2017)]

Description and explanation?

- Hydrodynamic models:
  - Swimmer generates fluid velocity field u,
  - Swimmer is affected by u.

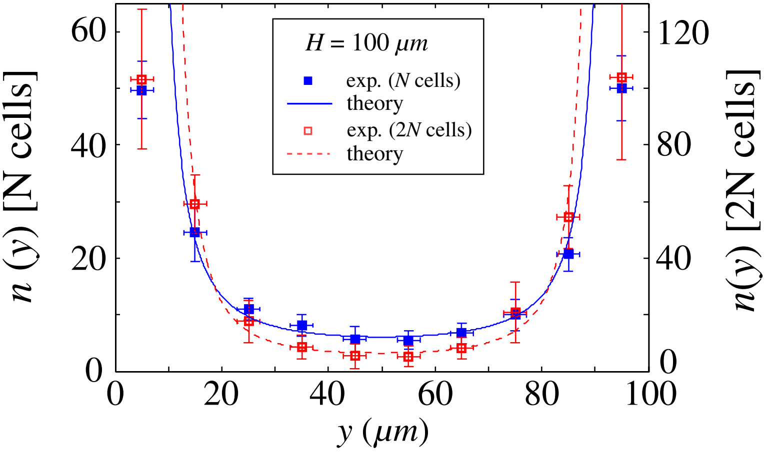
- Free swim + contact models:
  - Free swim + white noise (angular and/or positional)
  - Reorientation at boundary contact.

Hydrodynamic models – velocity field



[Drescher, Dunkel, Cisneros, Ganguly, Goldstein, PNAS (2011)]

Hydrodynamic model – predictions



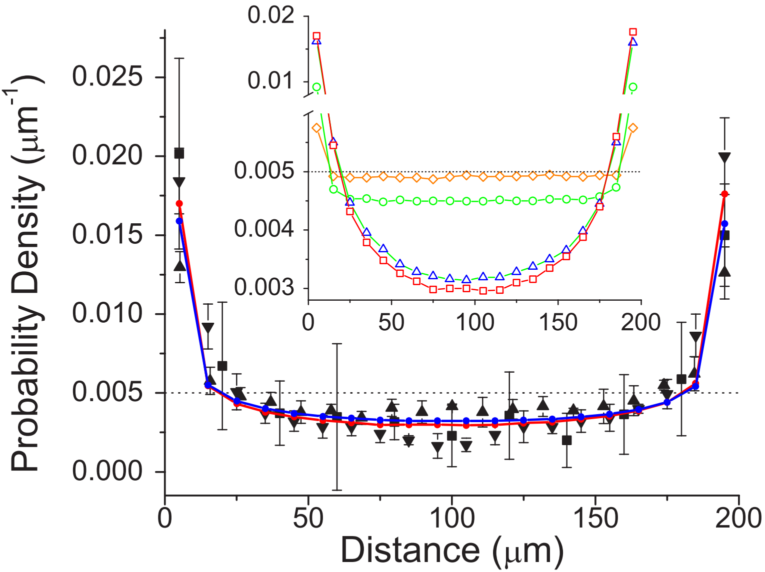
[Berke et al., Phys. Rev. Lett. (2008)]

Contact models

Dance with me!

[Li & Tang, Phys. Rev. Lett. (2009)]
[Li et al., Phys. Rev. (2011)]

Contact model – predictions

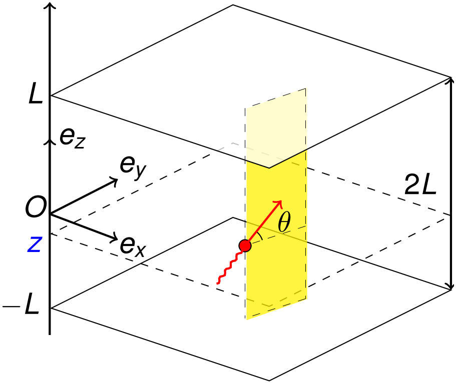


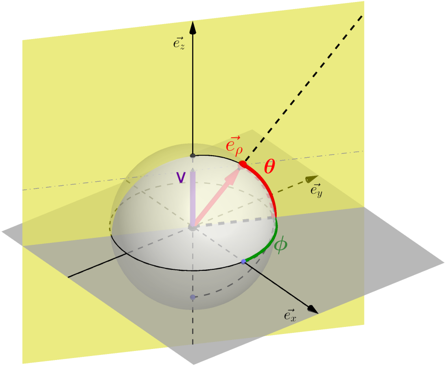
[Li & Tang, Phys. Rev. Lett. (2009)]

Broad Objectives

- Provide framework able to integrate both types of interactions: hydrodynamic and contact
- "Inverse problem": from terminal distributions, deduce "force terms"

3D model and projection





$z \in [-L, L]$ vertical position.

$\theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ angle w.r.t. horiz.

$v = \sin\theta$ norm^{ed} vert. speed.

Free Motion phase ($\mathcal{FM}$)

Swimmer does not touch boundaries.

$$\begin{cases} \dot{z} = Cv, & z \in (-L, L) \\ v = \sin\theta, & \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \\ \dot{\theta} = \dot{w}, & \end{cases} \tag{1}$$

C: constant swimming speed in ($\mathcal{FM}$)

w: reflected Brownian motion (RBM) in $[-\frac{\pi}{2}, \frac{\pi}{2}]$ starting at $\omega_0 = \theta_0$.

($\mathcal{FM}$) lasts while $|z| < L$.

Boundary Contact phase ($\mathcal{BC}$)

Swimmer remains in contact with a boundary.

$$\begin{cases} \dot{z} = 0, & z \in \{-L, L\} \\ v = \sin\theta, & \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \\ \dot{\theta} = \dot{w}, & \end{cases} \tag{2}$$

w: reflected Brownian motion (RMB) in $[-\frac{\pi}{2}, \frac{\pi}{2}]$ starting at $\omega_0 = \theta_0$.

($\mathcal{BC}$) lasts until $v > 0$ for $x = -L$ (resp. $x < 0$ for $x = L$).

Then, a new ($\mathcal{FM}$) begins.

Model in (x, v)

During $(\mathcal{FM})$ and $(\mathcal{BC})$:

$$\begin{cases} v = sin(\theta) \\ \dot{\theta} = \dot{w} \end{cases} \tag{3}$$

The solution v of the SDE above is trajectorially equal to that of

$$\dot{v} = -\frac{1}{2}v + \sqrt{1 - v^2}\,\dot{w}, \tag{4}$$

with w RBM, and equal in law to that of:

$$\dot{v} = -\frac{1}{2}v + \sqrt{1 - v^2}\,\dot{W}, \tag{5}$$

where W is a Brownian motion.

Model in (x, v)

Let $\bar{\mathcal{D}} = \mathcal{D} \cup \mathcal{D}_\pm$, with:

$$\begin{cases} \mathcal{D} = (-L, L) \times [-1, 1], \\ \mathcal{D}_+ = \{L\} \times [-1, 1], \\ \mathcal{D}_- = \{-L\} \times [-1, 1]. \end{cases}$$

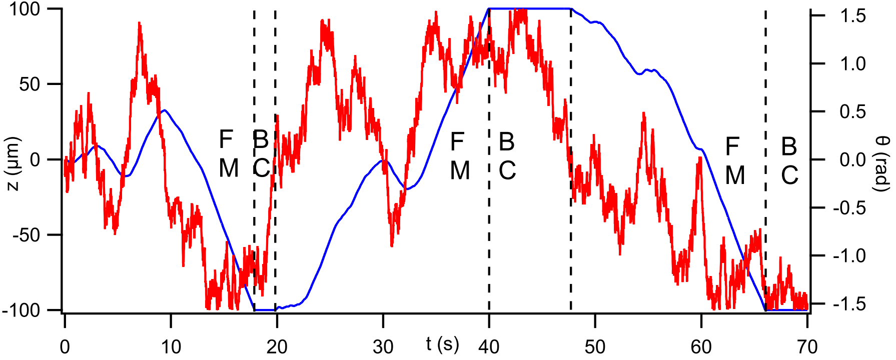
SDE for the full motion:

$$\begin{cases} \dot{z} = \begin{cases} Cv, & \text{in } \mathcal{D} \\ 0, & \text{on } \mathcal{D}_\pm \end{cases} \\ \dot{v} = -\frac{1}{2}v + \sqrt{1 - v^2}\,\dot{W}, & \text{in } \bar{\mathcal{D}} \\ z(0) = z_0; \quad v(0) = v_0. \end{cases} \tag{6}$$

Agent-Based Simulations

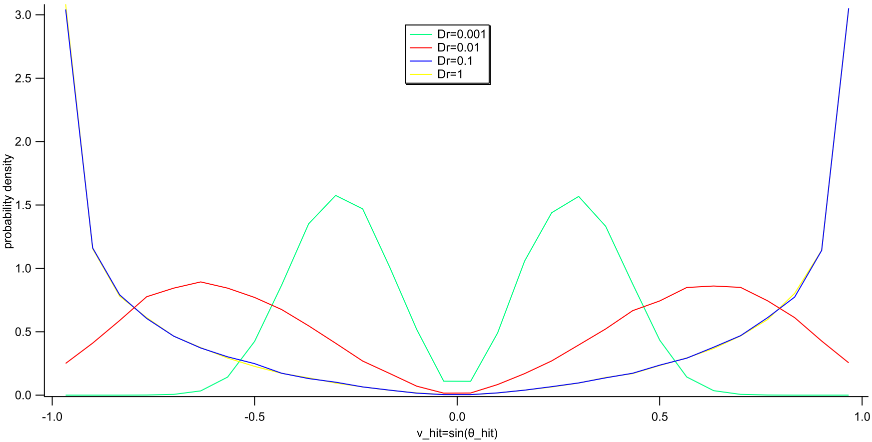
- C++ code
- $(\mathcal{FM})$ and $(\mathcal{BC})$ phases.
- Projection on $\bar{\mathcal{D}}$ to avoid $|z| > L$ and $|v| > 1$.
- White noise implemented by Gaussian random variable increments during time step dt.
- Parameters chosen to match literature on *E. coli*.

Simulation Results – Position and Angle Tracking



sample of simulated trajectory

Simulation Results – Angle of First Impact



First impact angles for different diffusion coefficients – rough simulation

Model in (x, v) — Reorientation "force" term

Let $\bar{\mathcal{D}} = \mathcal{D} \cup \mathcal{D}_{\pm}$, with:

$$\begin{cases} \mathcal{D} = (-L, L) \times [-1, 1], \\ \mathcal{D}_{+} = \{L\} \times [-1, 1], \\ \mathcal{D}_{-} = \{-L\} \times [-1, 1]. \end{cases}$$

SDE for the full motion:

$$\begin{cases} \dot{z} = \begin{cases} Cv, & \text{in } \mathcal{D} \\ 0, & \text{on } \mathcal{D}_{\pm} \end{cases} \\ \dot{v} = -\frac{1}{2} v + \sqrt{1 - v^2}\ \dot{W} + F(z, v)\ , \qquad \text{in } \bar{\mathcal{D}} \\ z(0) = z_0; \quad v(0) = z_0. \end{cases} \tag{7}$$

SVI – motivation

See blackboard

SVI

$(z(t), v(t)) \in [-L, L] \times [-1, 1]$ unique solution of SVI:

$$\begin{cases} \dot{V}_t = -\frac{1}{2} V_t + \sqrt{1 - V_t^2}\, \dot{W}_t, \\ (\dot{Z}_t - V_t) \cdot (\xi - Z_t) \geq 0, \forall |\xi| \leq L, |Z_t| \leq L, \end{cases} \tag{8}$$

(X, V) time-homogeneous Markov process
on compact state space $\bar{\mathcal{D}} = [-L, L] \times [-1, 1]$.
Hence, admits invariant measure ν.

[A. Bensoussan, J-L. Lions. Contrôle impulsionnel et inéquations quasi variationnelles. Dunod, Paris 1982.]

Semi-group and infinitesimal generator

Definition (semi-group w.r.t stochastic process)

$\forall (z, v) \in \bar{\mathcal{D}},\ \phi \in \mathcal{C}(\bar{\mathcal{D}}; \mathbb{R}), t \geq 0,$

$$P_t\phi(z, v) \triangleq \mathbb{E}\left(\phi(Z_t, V_t) | (Z_0, V_0) = (z, v)\right). \tag{9}$$

The infinitesimal generator can be computed by Itô's Lemma:

$$\lim_{t\to 0} \frac{1}{t}(P_t\phi(z, v) - \phi(z, v)) = A\phi(z, v)\mathbf{1}_{\{|z|<L\}} + B_{\pm}\phi(z, v)\mathbf{1}_{\{z=\pm L\}},$$

$$\text{where} \begin{cases} A \triangleq \dfrac{1 - v^2}{2} \dfrac{\partial^2}{\partial v^2} - v\dfrac{\partial}{\partial v} + v\dfrac{\partial}{\partial z} \\ B_{\pm} \triangleq \dfrac{1 - v^2}{2} \dfrac{\partial^2}{\partial v^2} - v\dfrac{\partial}{\partial v} \pm \min(0, \pm v)\dfrac{\partial}{\partial z}. \end{cases}$$

Transition Probability

$\mu(z, v, t; \xi, \eta, s)$: proba measure of state (ξ, η) at time s provided initial state at time t is (z, v).

$\mu(z, v, t; \xi, \eta, s)$ does not have a density w.r.t. Lebesgue measure!

$$
\mu(z, v, t; \xi, \eta, s) \begin{array}{l} \nearrow p(z, v, t; L, \eta, s) \\ \rightarrow p(z, v, t; \xi, \eta, s) \quad (-L < \xi < L) \\ \searrow p(z, v, t; -L, \eta, s) \end{array}
$$

Kolmogorov Backward Equation

$\forall u(z,v,t) \in C_z^1 C_y^2 C_t^1$, if u satisfies:

$$\begin{cases} \dfrac{\partial u}{\partial t} + Au = 0 \quad in \quad \mathcal{D}, \\ \dfrac{\partial u}{\partial t} + B_{\pm} u = 0 \quad in \quad \mathcal{D}_{\pm}, \end{cases} \tag{10}$$

with terminal condition $\lim_{t \to s} u(z,v,t) = f(z,v)$,
Then $u(z,v,t)$ has the following probabilistic interpretation

$$\begin{aligned} u(z,v,t) = & \int_{\mathcal{D}} p(z,v,t;\xi,\eta,s) f(\xi,\eta) \mathrm{d}\xi \mathrm{d}\eta \\ & + \int_{-1}^{1} p(z,v,t;-L,\eta,s) f(-L,\eta) \mathrm{d}\eta \\ & + \int_{-1}^{1} p(z,v,t;L,\eta,s) f(L,\eta) \mathrm{d}\eta. \end{aligned} \tag{11}$$

Stochastic Control – Motivation

- Two models with different zones of validity.
- Interactions between microswimmers are unaccounted for.

$\Longrightarrow$ Modelling issues for an *a priori* F.

- Terminal data available – density distribution, impact angle, etc.
- Ability to target terminal distributions by choosing $F(x, v)$.
- Optimal choice of F?
  Fleming log transform: $J(x, v, t) = -\ln u(x, v, t)$ can be seen as the $\arg\min$ of a control problem – see:

[Delarue and Menozzi (2010)], [Fleming and Soner (2006), Ch.6].

Doob h-Transform – (1)

We begin in $(\Omega, \mathcal{F}, \mathbb{P})$.

- Condition for $v = v_* \in [0, 1]$ at first boundary hit time.
- Minimize L^2 norm functional.

Let $h(z, v) = p(z, v, 0; \pm L, \pm v_*, \tau_L)$: transition proba. to be at $(\pm L, \pm v_*)$ at first hit time of $|x| = L$, provided start at (z, v) at $t = 0$.

$$\begin{cases} Ah = 0, & \text{in } \mathcal{D}; \\ h(L, v) = \frac{1}{2}\delta_{v_\star}(v), & \text{for } v > 0; \\ h(-L, -v) = \frac{1}{2}\delta_{-v_\star}(v), & \text{for } v < 0. \end{cases}$$

Recall: $A = \frac{1-v^2}{2}\frac{\partial^2}{\partial v^2} - v\frac{\partial}{\partial v} + v\frac{\partial}{\partial z}$.

Doob h-Transform – (2)

- $X_t := h(Z_t, V_t)$ is a martingale.
- Define change of measure: for any R.V. Y,
$$\mathbb{E}_{\mathbb{Q}_t}[Y] = \mathbb{E}_{\mathbb{P}}[YX_t],$$
where $X_t = \frac{\mathrm{d}\mathbb{Q}_t}{\mathrm{d}\mathbb{P}}$.
- Itô's lemma yields:
$$X_t = \exp\left(\int_0^t \frac{\partial_z h(Z_s, V_s)}{h(Z_s, V_s)} \,\mathrm{d}W_s - \frac{1}{2}\int_0^t \left(\frac{\partial_z h(Z_s, V_s)}{h(Z_s, V_s)}\right)^2 \mathrm{d}s\right)$$
- $$\tilde{W}_t = W_t - \int_0^t \frac{\partial_z h(Z_s, V_s)}{h(Z_s, V_s)} \,\mathrm{d}s$$
is a $\mathbb{Q}$-Brownian Motion thanks to Girsanov's theorem – see [Karatzas - Shreve (1991), Ch.3.5]

Doob h-Transform – (2)

Under the new proba $\mathbb{Q}$ (conditioned for first impact at $v = v_*$),

$$\begin{cases} \dot{z} = \begin{cases} Cv, & \text{in } \mathcal{D} \\ 0, & \text{on } \mathcal{D}_\pm \end{cases} \\ \dot{v} = -\frac{1}{2}v + \sqrt{1-v^2}\ \dot{\tilde{W}} + F_h(z,v)\ , & \text{in } \bar{\mathcal{D}} \\ z(0) = z_0; \quad v(0) = v_0. \end{cases} \tag{12}$$

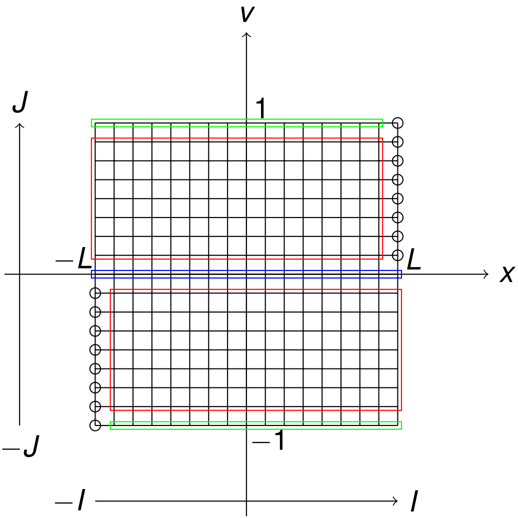
with:

$$F_h(z,v) = \partial_z \ln h(z,v). \tag{13}$$

Stochastic Dynamics of Confined Microswimmers

Mesh for discretization

Finite difference method is chosen to solve for $h(x, v)$.



$\partial_{vv} h$: central difference

v<0:

$$\partial_v h \approx \frac{h_{i,j+1} - h_{i,j}}{dv}$$

$$\partial_x h \approx \frac{h_{i,j} - h_{i-1,j}}{dx}$$

v>0:

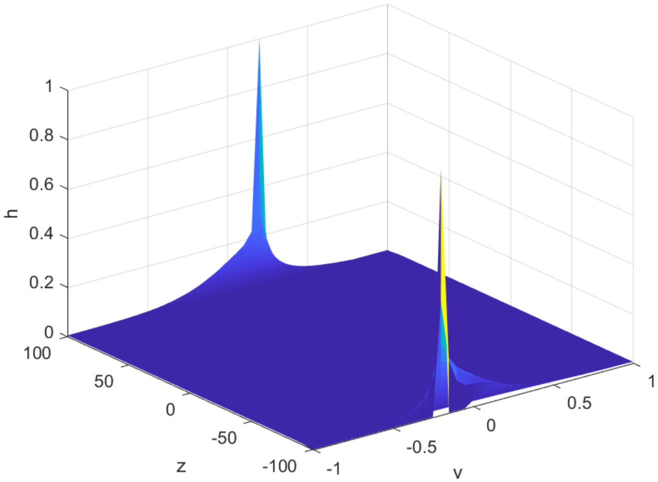
$$\partial_v h \approx \frac{h_{i,j} - h_{i,j-1}}{dv}$$

$$\partial_x h \approx \frac{h_{i+1,j} - h_{i,j}}{dx}$$

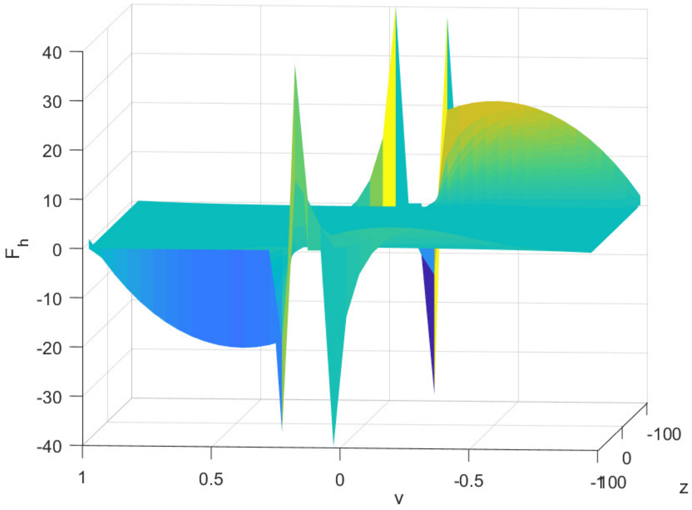
Advantage of scheme

1. “Implicit” scheme: unconditionally stable;
2. Maximum Principle for discretized equation;

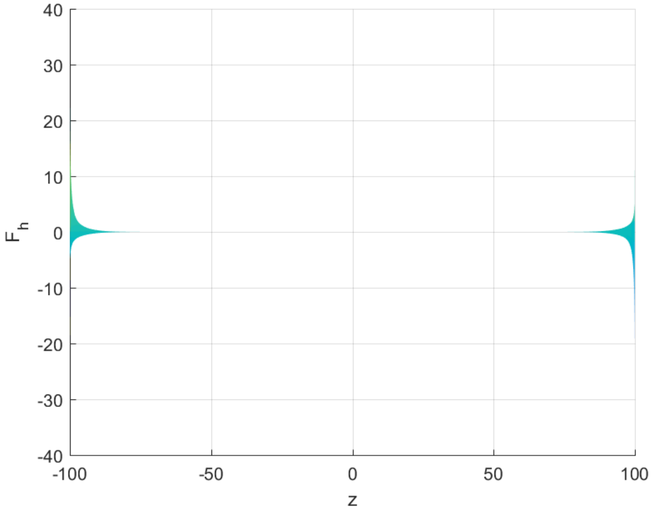
Numerical image of $h(x, v)$



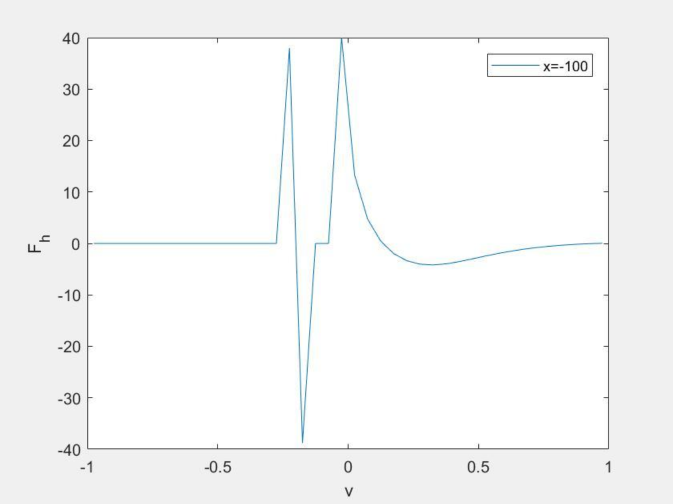
Numerical image of $F_h(x, v)$ (1)



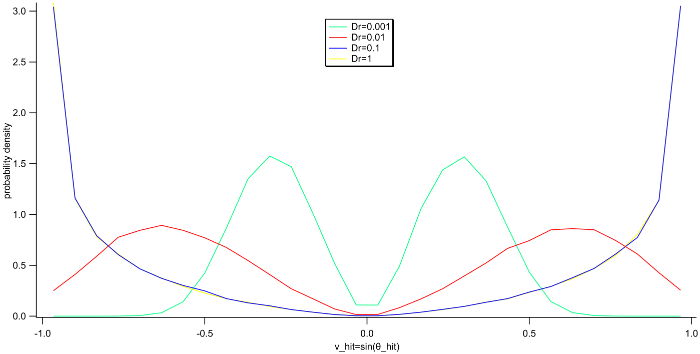
Numerical image of $F_h(x, v)$ (2)



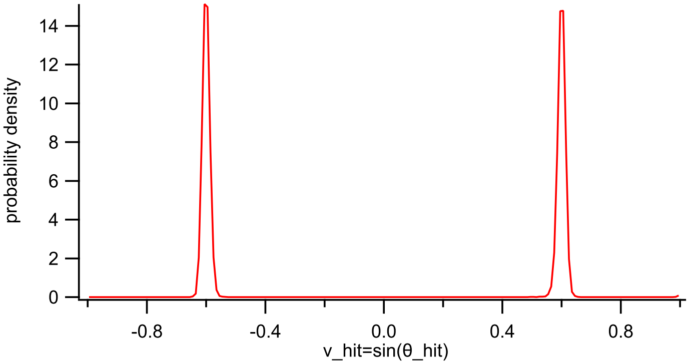
Numerical image of $F_h(x, v)$ (3)



Impact angles for $F = 0$



Impact angles for $F_h(x, v)$



Fit error order of magnitude: 10^{-2}.

We can target an impact angle distribution.

Take-home message

Existing modeling framework:

Model	Experimental data
Microswimmers in confinement	vertical position Z_t
hydrodynamic forces and torques	normalized vertical speed V_t
reorientation force due to contact	angle θ – impact angle θ_0
	density distributions.

Our framework:

- Description of both swimming and contact with SVI.
- Recovery of "optimal" reorientation forces thanks to Doob h-Transform.

Work in progress

- Define *i.i.d.* repeating pattern ("long cycles") to describe data spanning many $(\mathcal{FM})$ and $(\mathcal{BC})$ phases [done for a toy model]. [Bensoussan, Mertz, Yam, C. R. Math. (2012)]
- Couple with Doob h-Transform or other stochastic control tools to deduce "optimal" force from steady state data.
- Replace Rotational Brownian motion by Run and Tumble.

Thank you for your attention!