Stochastic Fluctuations in Suspensions of Swimming Microorganisms

Peter R. Kramer
Dept. Mathematical Sciences

Yuzhou Qian, Patrick Underhill
Dept. Biological and Chemical Engineering

Rensselaer Polytechnic Institute

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Swimming Microorganisms (Microswimmers)

Key distinction from swimming macroorganisms:

- low Reynolds number: motion stops when force stops (Archimedean dynamics)
- stochastic components apparent
  - Brownian motion, run-and-tumble dynamics, molecular motor noise

Typical coarse-grained description of microswimmers is through their time-averaged force dipole δ

- signed measure of force exerted multiplied by displacement of forces

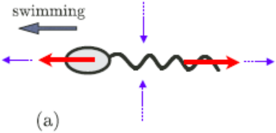
Review

- E. Lauga and R. E. Goldstein, "Dance of the microswimmers," *Physics Today* **65** (9), 30–35 (2012).

Pushers and Pullers

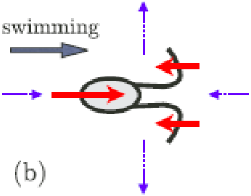
Pushers ($\delta < 0$)

- Most bacteria



Pullers ($\delta > 0$)

- Algal cell (*Chlamy.*)



Images from Lauga and Powers, *Rep. Prog. Phys.* 2009

Observations in Experiments and Simulations

Suspensions of pullers tend to appear statistically isotropic, with short-range orientational correlations.

Suspensions of pushers tend to exhibit patterned motion, with long-range orientational correlations with slow decay

Fluid velocities for pushers (left) vs. pullers (right)

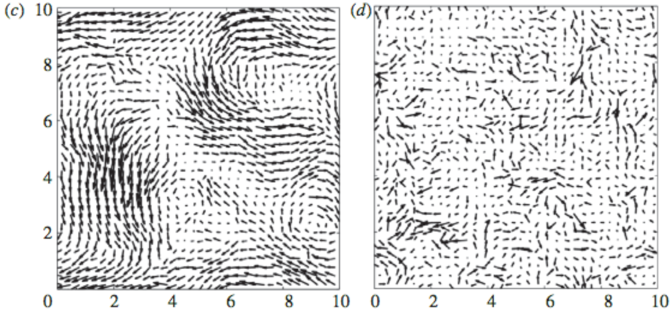


Image from Saintillan and Shelley *Roy Soc Interface* 2012

Point-Dipole Models with Hydrodynamic Interaction

Each swimmer (indexed by i) characterized by position $\mathbf{X}^{(i)} \in \Omega$ in d-dimensional spatial domain Ω, and orientation $\mathbf{N}^{(i)} \in S^{d-1}$.

$$\begin{aligned}
\mathrm{d}\mathbf{X}^{(i)}(t) &= V\mathbf{N}^{(i)}(t)\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}\mathbf{W}_x^{(i)}(t) \\
&\quad + \delta \sum_{j\neq i} \mathsf{K}^{\mathsf{X}}(\mathbf{X}^{(i)}(t) - \mathbf{X}^{(j)}(t)) \cdot \mathsf{M}(\mathbf{N}^{(j)}(t))\,\mathrm{d}t, \\
\mathrm{d}\mathbf{N}^{(i)}(t) &= \sqrt{2D_r}\mathsf{P}(\mathbf{N}^{(i)}(t)) \cdot \mathrm{d}\mathbf{W}_n^{(i)}(t) \\
&\quad + \delta \sum_{j\neq i} \mathsf{P}(\mathbf{N}^{(i)}(t)) \cdot \mathsf{K}^{\mathsf{N}}(\mathbf{X}^{(i)}(t) - \mathbf{X}^{(j)}(t)) \cdot \mathsf{M}(\mathbf{N}^{(j)}(t))\,\mathrm{d}t,
\end{aligned}$$

- V is speed of a swimmer,
- $D(D_r)$ is translation (rotational) diffusivity of swimmer
- $\mathsf{K}^{\mathsf{X}}(\mathbf{x}) \sim |\mathbf{x}|^{1-d}$, $\mathsf{K}^{\mathsf{N}} \sim \boldsymbol{\nabla}\mathsf{K}^{\mathsf{X}}(\mathbf{x}) \sim |\mathbf{x}|^{-d}$ for $|\mathbf{x}| \to \infty$ are hydrodynamic interaction tensors (gradients of Oseen)
- $\mathsf{M}(\mathbf{n}) = \left(\frac{1}{d}\mathsf{I} - \mathbf{n}\otimes\mathbf{n}\right)$, $\mathsf{P}(\mathbf{n}) = (\mathsf{I} - \mathbf{n}\otimes\mathbf{n})$
- $\{\mathbf{W}_x^{(i)}(t), \mathbf{W}_n^{(i)}(t)\}$ are independent d-dimensional Wiener processes ($\langle \mathrm{d}\mathbf{W}(t) \otimes \mathrm{d}\mathbf{W}(t')\rangle = \delta(t-t')\mathsf{I}\,\mathrm{d}t\,\mathrm{d}t'$)

Some Approaches Toward Explaining Suspension Behavior

Complex hydrodynamics (review by Marchetti et al, *Rev. Mod. Phys.* 2013)

Mean field kinetic theories based on point-dipole models (Saintillan and Shelley 2008)

- Nonlinear Fokker-Planck equation for the phase space density $\psi(\mathbf{x}, \mathbf{n}, t)$ of microswimmer variables

Abstracted lattice models, for which more detailed computations possible.

- Thompson, Tailleur, Cates, Blythe 2011

(Deterministic) Mean Field Kinetic Theory

$$\frac{\partial \psi(\mathbf{x},\mathbf{n},t)}{\partial t} = -\boldsymbol{\nabla}_x \cdot (V\mathbf{n}\psi) + D\boldsymbol{\nabla}_x^2\psi + D_r\boldsymbol{\nabla}_n^2\psi - \boldsymbol{\nabla}_x \cdot (\mathbf{U}(\psi)\psi) - \boldsymbol{\nabla}_n \cdot (\mathbf{A}(\psi)\psi)$$

with linear operators:

$$\mathbf{U}(\psi) = \delta \int \mathrm{d}\mathbf{x}' \int \mathrm{d}\mathbf{n}' \mathsf{K}^{\mathsf{X}}(\mathbf{x}-\mathbf{x}') \left(\mathbf{n}'\otimes\mathbf{n}' - \frac{1}{d}\mathsf{I}\right)\psi(\mathbf{x}',\mathbf{n}',t)$$

$$\mathbf{A}(\psi) = (\mathsf{I} - \mathbf{n}\otimes\mathbf{n})\cdot\boldsymbol{\nabla}\mathbf{U}(\psi)\cdot\mathbf{n}.$$

Linear stability analysis about statistically uniform, isotropic state $\psi =$ constant:

- Always linearly stable for pullers ($\delta > 0$)
- Linear instability for pushers ($\delta < 0$) with sufficiently small rotational diffusivity D_r

Limitations of (Deterministic) Mean Field Kinetic Theory

Practical limitations:

- approximates micro swimmers as densely, continuously distributed fields rather than discrete entities
- When stable, statistically stationary state completely trivial, with no flow
- More broadly, finite number of microswimmers and their correlations produce statistical fluctuations that impact upon fluid properties such as enhanced viscosity and mixing

Stochastic Mean Field Kinetic Theory Derivation

Mesoscopic theory which adds stochastic noise from finite number effects

- analogous to a central limit theorem description, whereas deterministic continuum equations arise from law of large numbers
- formally valid when the number of micro swimmers in any spatial region of interest can be treated as large but not infinite

Systematic derivation of noise terms

- Physical principles (not quite fluctuation-dissipation relation)
  - Dean 1996 for diffusion equation
  - Tailleur and Cates 2008, Solon, Cates, Tailleur 2015 adapt for other microswimming models (without hydrodynamic interaction but other physics)
- direct formal mathematical derivation via Itô's lemma in weak form to empirical measure

Lau and Lubensky 2007, 2009 study stochastic version of related fluctuating hydrodynamic equations

Stochastic Mean Field Kinetic Theory

$$
\begin{aligned}
\mathrm{d}\psi(\mathbf{x},\mathbf{n},t) = &-\boldsymbol{\nabla}_x \cdot (V\mathbf{n}\psi)\,\mathrm{d}t + D\boldsymbol{\nabla}_x^2\psi\,\mathrm{d}t + D_r\boldsymbol{\nabla}_n^2\psi\,\mathrm{d}t \\
&- \boldsymbol{\nabla}_x \cdot (\mathbf{U}(\psi)\psi)\,\mathrm{d}t - \boldsymbol{\nabla}_n \cdot (\mathbf{A}(\psi)\psi)\,\mathrm{d}t \\
&+ \boldsymbol{\nabla}_x \cdot \left(\sqrt{2D\psi}\,\mathrm{d}B(\mathbf{x},\mathbf{n},t)\right) \\
&+ \boldsymbol{\nabla}_n \cdot \left(\sqrt{2D_r\psi}\,(\mathsf{I} - \mathbf{n}\otimes\mathbf{n})\,\mathrm{d}\tilde{B}(\mathbf{x},\mathbf{n},t)\right)
\end{aligned}
$$

where $B(\mathbf{x},\mathbf{n},t)$ and $\tilde{B}(\mathbf{x},\mathbf{n},t)$ are cylindrical Brownian motions:

- Gaussian random processes
- mean zero
- correlation function:

$$
\langle \mathrm{d}B(\mathbf{x},\mathbf{n},t)\mathrm{d}B(\mathbf{x}',\mathbf{n}',t')\rangle = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}')\delta(\mathbf{n}-\mathbf{n}')\,\mathrm{d}t\,\mathrm{d}t'
$$

Note $\mathrm{d}B$ and $\mathrm{d}\tilde{B}$ are not quite space-time white noise.

Numerical Discretization of Noise Term

Naive discretization of cylindrical Brownian motion: $\Delta B(\mathbf{x}, \mathbf{n}, t)$

- independent, identically distributed over each space-time volume
- mean zero Gaussian random variables
- variance
$$\langle (\Delta B(\mathbf{x}, \mathbf{n}, t))^2 \rangle = \frac{\Delta t}{(\Delta x)^d (\Delta n)^{d-1}}$$
where d is the number of spatial dimensions.

Noise is very rough in the spatial variables!

- Discretization won't converge in any typical sense
- Mathematical theory for continuum limit may not be well-posed

Physical Meaning of Noise Term

Nonetheless, this rough noise is physically correct.

- particle densities measured over finite (phase space) volume V will have random fluctuations $\sim V^{-1/2}$
- physical continuum theories aren't intended to apply literally as $\Delta x \downarrow 0$, $\Delta n \downarrow 0$
  - rather for $\ell \ll \Delta x \ll L$ where ℓ is atomic length scale, L is macroscopic length scale
- Noise is not converging on the physical spatial mesh under refinement, but does converge when projected onto any fixed spatial (i.e. spectral) mode

This is common situation for mesoscopic SPDEs, and the source of the difficulty in giving mathematical meaning to physically correct equations (and one reason to have given M. Hairer a Fields medal).

Physical Discretization of Noise

One lesson from previous work with stochastic immersed boundary (SIB) method (with Paul Atzberger and Charles Peskin):

- Numerical approximations can be made physically meaningful
- This approach will cause the noise and dissipation to be consistently discretized
- Important for good properties of stationary state

Following this SIB work, we formulate approximating semi discrete models for the stochastic mean field theory for micro swimmers on a regular spatial lattice with spacing Δx and Δn.

- Represent velocity and diffusion by continuous-time random walk hopping rates
- Time remains continuous in model formulation; discretized only in numerical implementation

Stochastic Advection-Diffusion on Lattice

Ideas are the same as for a simple stochastic advection-diffusion equation in one spatial dimension:

$$\begin{aligned} \mathrm{d}\rho(x,t) = &\left[-\partial_x \left(v(x)\rho(x,t)\right) + D\partial_x^2\rho(x,t)\right]\,\mathrm{d}t \\ &+ \partial_x \left(\sqrt{2D\rho(x,t)}\,\mathrm{d}B(x,t)\right) \end{aligned}$$

Discretize space into intervals $\left\{\left[\left(j-\frac{1}{2}\right)\Delta x, \left(j+\frac{1}{2}\right)\Delta x\right)\right\}_j$

- N_j represents the number of particles in $\left[\left(j-\frac{1}{2}\right)\Delta x, \left(j+\frac{1}{2}\right)\Delta x\right)$.
- Think of the particles as living on the lattice of the center points $\{x_j = j\Delta x\}_j$.
- Discretize velocity $v_j \equiv v(x_j)$

Stochastic Dynamics on Lattice

Dynamics governed by continuous-time Markov chain (random walk):

- Rate $r_- = -\frac{v_j}{2\Delta x} + \frac{D}{(\Delta x)^2}$ to hop left: $x_j \to x_{j-1}$
- Rate $r_+ = \frac{v_j}{2\Delta x} + \frac{D}{(\Delta x)^2}$ to hop right: $x_j \to x_{j+1}$
- Probability for process to occur over time interval Δt:
  - rate $\times \Delta t + o(\Delta t)$
- Rates must be positive, so need cell Péclet number $\mathrm{Pec}_j = \frac{|v_j|\Delta x}{D} \leq 2$

Numerical SPDE Representation

With Gaussian approximation for noise terms,

$$\rho_j(t+\Delta t) - \rho_j(t) = \frac{v_{j-1}\rho_{j-1} - v_{j+1}\rho_{j+1}}{2\Delta x}\Delta t + \frac{D(\rho_{j-1} - 2\rho_j + \rho_{j+1})}{(\Delta x)^2}\Delta t + \frac{\tilde{F}_{j-1} - \tilde{F}_j}{\Delta x}\Delta t$$

Deterministic terms appear with central difference discretization

- cell Péclet number $\mathrm{Pec}_j = \frac{|v_j|\Delta x}{D}$ restricted to $\mathrm{Pec}_j < 2$ for stability
  - also for discrete model to be meaningful
- undesirable because micro swimming is believed to be advection-dominated, so this forces small Δx

Linearized Fluctuation Analysis

When statistically isotropic state $\psi = \psi_0$ is linearly stable, linearize based on small parameter proportional to density

$$\begin{aligned} \mathrm{d}\psi(\mathbf{x},\mathbf{n},t) = &-\boldsymbol{\nabla}_x \cdot (V\mathbf{n}\psi)\,\mathrm{d}t + D\boldsymbol{\nabla}_x^2\psi\,\mathrm{d}t + D_r\boldsymbol{\nabla}_n^2\psi\,\mathrm{d}t \\ &- \boldsymbol{\nabla}_n \cdot (\mathbf{A}(\psi))\psi_0\,\mathrm{d}t \\ &\quad + \boldsymbol{\nabla}_x \cdot \left(\sqrt{2D\psi_0}\,\mathrm{d}B(\mathbf{x},\mathbf{n},t)\right) \\ &\quad + \boldsymbol{\nabla}_n \cdot \left(\sqrt{2D_r\psi_0}\,(\mathsf{I} - \mathbf{n}\otimes\mathbf{n})\,\mathrm{d}\tilde{B}(\mathbf{x},\mathbf{n},t)\right) \end{aligned}$$

Analyze by expansion in Fourier modes (in $\mathbf{x}$) and circular/spherical modes (in $\mathbf{n}$)

- yields formally infinite-dimensional O-U equations
- Statistics by numerical linear algebra on Galerkin projections
- Asymptotic analysis for low wavenumber $|\mathrm{k}| \leq D_r/V$

Numerical Results for $d = 2$ Spatial Dimensions

Modal representation is then simple Fourier expansion w.r.t. $\mathbf{x}$ and $\mathbf{n} = (\cos\theta, \sin\theta)$:

$$\psi(\mathbf{x}, \mathbf{n}, t) = \sum_{\mathrm{k}\in\mathbb{R}^2} \sum_{m=-\infty}^{\infty} \mathrm{e}^{2\pi i \mathrm{k}\cdot\mathbf{x}/L} \mathrm{e}^{im\theta} \hat{\psi}_{\mathrm{k},m}(t)$$

where L is the size of the (periodic) spatial domain.
Results presented in nondimensional form

- equivalent to scaling so mean phase space density, dynamic viscosity, and swimmer speed $= 1$
- reported fluctuations to be multiplied by small linearization parameter $\epsilon = \sqrt{1/\bar{N}}$, where $\bar{N}$ is the average number of swimmers in unit nondimensional reference area
- Nondimensional period domain length in computations $= 50$

Statistical Descriptors of Physical Fields

We will examine two basic properties of various (vector or scalar) random physical fields $\mathrm{F}(\mathbf{x})$ obtained by operations on $\psi(\mathbf{x},\mathbf{n},t)$:

- Root-mean-square amplitude

$$A(\mathrm{F}) \equiv \langle|\mathrm{F}(\mathbf{x})|^2\rangle^{1/2} = \left(\sum_{\mathrm{k}\in\mathbb{R}^2}\langle|\hat{\mathrm{F}}(\mathrm{k})|^2\rangle\right)^{1/2}.$$

- Correlation length (statistical representation of pattern size)

$$\ell_{\mathrm{c}}(\mathrm{F}) \equiv \sqrt{\frac{\int_{\mathbb{R}^2}|\,\mathsf{Tr}\,\mathsf{C}_{\mathrm{F}}(\mathbf{x})|\,\mathrm{d}\mathbf{x}}{A(\mathrm{F})^2}}$$

where the correlation function is defined:

$$\mathsf{C}_{\mathrm{F}}(\mathbf{x}) \equiv \langle\mathrm{F}(\mathbf{x}'+\mathbf{x})\otimes\mathrm{F}(\mathbf{x}')\rangle = \sum_{\mathrm{k}\in\mathbb{R}^2}\mathrm{e}^{2\pi\mathrm{i}\mathrm{k}\cdot\mathbf{x}}\langle\hat{\mathrm{F}}(\mathrm{k})\otimes\hat{\mathrm{F}}^*(\mathrm{k})\rangle$$

$\langle\cdot\rangle$ denotes statistical average, and t is suppressed since we always compute in statistically stationary state.

Statistical Properties of Concentration

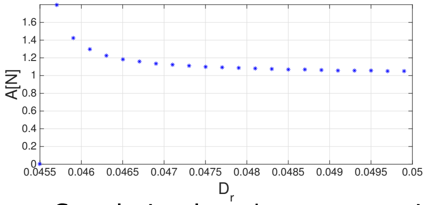
Concentration field $\rho(\mathbf{x}, t) \equiv \int_{S^1} \psi(\mathbf{x}, \mathbf{n}, t)\, \mathrm{d}\mathbf{n}$:

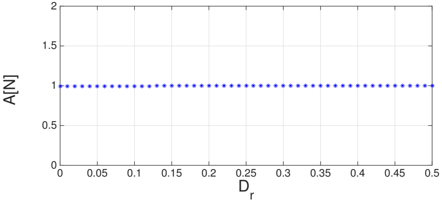
- No interesting structure for either pushers or pullers
  - $O(\left(\frac{|\mathrm{k}|V}{D_r}\right)^4)$ perturbation in asymptotic analysis
- Essentially delta-correlated, as for independent swimmers
- Nontrivial effects certainly seen at higher concentration, due to near-field interactions (Furukawa, Marenduzzo, Cates 2014)
  - beyond point dipole approximations

Statistical Properties of Orientation

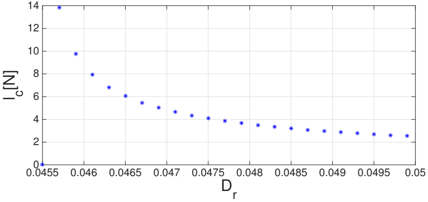
Orientation field $\mathrm{N}(\mathbf{x},t) \equiv \int_{S^1} \mathbf{n}\psi(\mathbf{x},\mathbf{n},t)\,\mathrm{d}\mathbf{n}$:

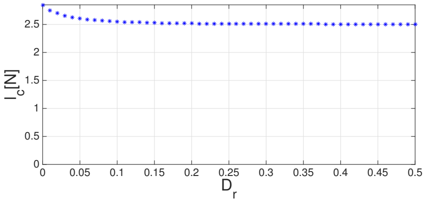
Root-mean-square amplitude w.r.t. rotational diffusivity





Correlation length w.r.t. rotational diffusivity





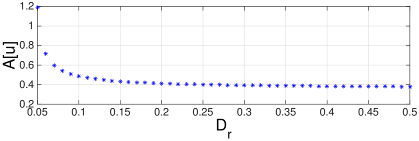
Pushers (unstable for $D_r < 0.045$)

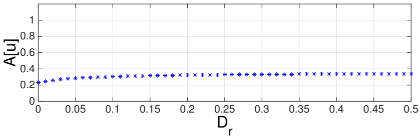
Pullers

Statistical Properties of Fluid Velocity

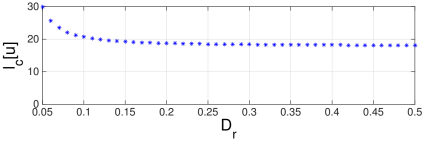
Fluid velocity field
$\mathrm{u}(\mathbf{x},t) \equiv \delta \int_{S^1} \int_{\mathbb{R}^2} \mathsf{K}^{\mathsf{X}}(\mathbf{x}-\mathbf{x}') \cdot \mathsf{M}(\mathbf{n}')\psi(\mathbf{x}',\mathbf{n}',t)\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{n}'$:

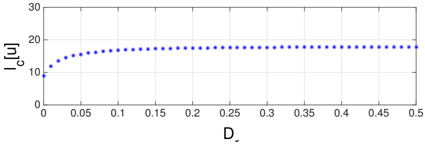
Root-mean-square amplitude w.r.t. rotational diffusivity





Correlation length w.r.t. rotational diffusivity





Pushers (unstable for $D_r < 0.045$) Pullers

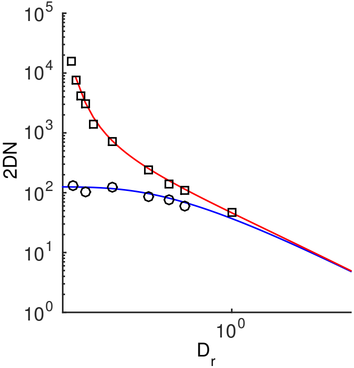
(Velocity correlation length $= 15.5$ for non-interacting swimmers; domain length $= 50$)

Enhancement of Tracer Diffusivity

At low Kubo number (Ku)

$$D \approx \frac{1}{4} \int_0^\infty \langle\langle \mathrm{u}(\mathbf{x}, t') \cdot \mathrm{u}(\mathbf{x}, t' + t) \rangle \, \mathrm{d}t$$

Linearized analysis (lines) vs. finite-difference simulations (symbols) at $\mathrm{Ku} \sim 10^{-5}$



pushers, pullers

Conclusions

- Rational noise model to represent fluctuations about idealized continuum limit
- Computation of fluid/microswimmer statistics in linearly stable regime, where deterministic theory is uninformative

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