Coarse-grained computations for collective effects in biosuspensions

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Motivation and DOE Relevance

Why bio or bio-inspired materials? Novel properties, e.g. harvest photons from the sun in a solar panel, deliver cargo and mix fluid in microfluidic devices.

Self-organization: Collective swimming of bacteria increases mixing rates of nutrients and oxygen, drastically reduces viscosity of suspensions. Harvest and control the power of microorganism motion needed for development of hybrid biomechanical energy conversion systems.

Objective: Develop computational models that reveal self-organization mechanisms behind collective swimming and guide the design of biomaterials.

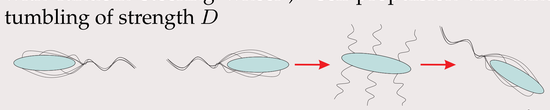
Key challenge: Computationally prohibitive fine scales. Coarse-graining techniques for such systems need to be developed.

1. Dilute Bacterial Suspensions

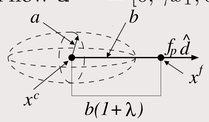
Experiments (Aranson, ANL): suspensions of bacteria may self-organize into collective swimming characterized by (i) increased mixing rate and (ii) drastic reduction of effective viscosity (E.V.)

Objective: Propose differential equation based models that reveal self-organization mechanisms contributing to collective swimming

Dilute suspension of swimming bacteria (bacteria interact with ambient flow only) with two modes of motion ("motor boat with random steering wheel"): self-propulsion and random tumbling of strength D



Model: Self-propulsion – a point force, $f_p\mathbf{d}\delta(\mathbf{x}-\mathbf{x}^f)$, f_p-magnitude, $\mathbf{d}\in\mathcal{S}^2$ -orientation vector, λ effective length of flagellum. Bacterium modeled as a prolate spheroid in an infinite Stokesian fluid with background flow $\mathbf{u}^{BG}=[0,\gamma x_1,0]$.



Results: Asymptotic formula in the limit $B\to 0$ (almost spherical particles). E.V. obtained by averaging bulk stress over all orientations

$$\hat{\eta}=\eta+\phi\left[\frac{5}{2}\eta-\frac{f_pD}{(36D^2+\gamma^2)}B+\mathcal{O}(B^2)\right]+\mathcal{O}(\phi^2). \quad (1)$$

$B\sim$ Bretherton const. 0/1 sphere/needle, D: magnitude of rot. diffusion, ϕ: concentr., γ: BG flow

Red: active addition to Einstein's formula [1]. Mechanisms for decrease: self-propulsion $f_p>0$, elongation $B>0$, and tumbling $D>0$

2. Semidilute: Add Interactions

Semi-dilute suspensions - the velocity field acting on each particle is sum of flows produced by all other particles $\mathbf{u}(\mathbf{x}^i)=\sum_{j\neq i}\mathbf{u}^j(\mathbf{x}^i)$ [2].

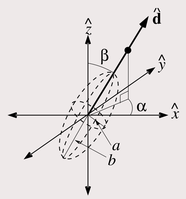
Model: Bacterium modeled as point force dipole (verified experimentally *K. Drescher et al.*) with size and shape.

Size: Point dipoles close to each other cause artificial divergence. Introduce excluded volume constraints, via truncated L-J potential. Soft collisions: When particles are close the repulsive portion of the L-J potential slows each particle and pushes them apart.

Shape: Shape parameter B enters the model via (3) (Jeffery equations: (3) with no interactions).

The magnitude of the dipole moment $|U_0|=|F||h|$ and shape B remain constant as $h\to 0$

(a) E. Coli - Food Poison Journal



(b) Model of bacterium

Equations of Motion of N bacteria:

$$\dot{\mathbf{x}}^i=V_0\mathbf{d}^i+\sum_{j\neq i}\mathbf{u}^j(\mathbf{x}^i)+\sum_{j\neq i}\mathbf{L}^j(\mathbf{x}^i)+\mathbf{v}^{BG} \quad (2)$$

$$\dot{\mathbf{d}}^i=-\mathbf{d}^i\times[\omega^{BG}+\sum_{j\neq i}\omega^j(\mathbf{x}^i)] \quad (3)$$

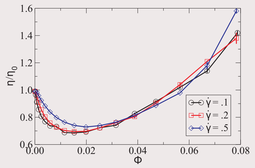
$$+\mathbf{d}^i\times B\mathbf{d}^i\times[E^{BG}+\sum_{j\neq i}E^j(\mathbf{x}^i)]\cdot\mathbf{d}^i$$

$V_0\sim U_0/\eta$: swim speed, $\mathbf{v}^{BG},\omega^{BG},E^{BG}$: velocity, vorticity, rate of strain of BG flow

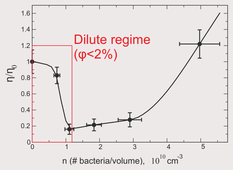
$\mathbf{u}^j(\mathbf{x}^i):=\hat{\mathbf{u}}(\mathbf{x}^i-\mathbf{x}^j,\mathbf{d}^j)$: flow on the ith bacterium due to the jth - $\hat{\mathbf{u}}$: solution to a single bacterium problem with Lees-Edwards boundary conditions.
$\mathbf{L}^j(\mathbf{x}^i):=\mathbf{L}\left(\mathbf{x}^i-\mathbf{x}^j\right)$: velocity due to Lennard-Jones interactions.
$\omega^j(\mathbf{x}^i):=\nabla\times\mathbf{u}^j(\mathbf{x}^i)$: vorticity due to flow from jth bacterium
$E^j(\mathbf{x}^i):=\frac{1}{2}\left(\nabla\mathbf{u}^j(\mathbf{x}^i)+\nabla[\mathbf{u}^j(\mathbf{x}^i)]^T\right)$: rate of strain due to jth

2. Semidilute: Numerical Results

Simulations (GPU):



Experiment (Aranson):



Captures dilute trend of a sharp decrease in viscosity with increasing concentration.

Qualitatively matches experimental results through full range of concentrations ($\Phi\leq 8\%$). When density is large see increase in viscosity not captured by **any** previous analytical results.

Previous simulations only capture a much smaller number of bacteria: this approach 100,000+.

2. Semidilute: Kinetic Theory

Mean field approximation: Using Law of Large Numbers: Sums of interaction terms in (2)-(3) replaced by ensemble average (expectation) w.r.t. $P(\mathbf{x},\mathbf{d})$

$P(\mathbf{x},\mathbf{d})$, the probability distribution for a bacterium to be at position $\mathbf{x}$ with orientation $\mathbf{d}$, satisfies Liouville's equation:

$$\partial_tP(\mathbf{x},\mathbf{d})=-\nabla_{\mathbf{x}}\cdot(\dot{\mathbf{x}}P(\mathbf{x},\mathbf{d}))-\nabla_{\mathbf{d}}\cdot(\dot{\mathbf{d}}P(\mathbf{x},\mathbf{d})) \quad (4)$$

Introduce angular distribution $\mathbf{d}=\mathbf{d}(\alpha,\beta)$:

$$P_d(\mathbf{d}):=\frac{1}{\rho L^3}\int P(\mathbf{x},\mathbf{d})d\mathbf{x}. \quad (5)$$

$\rho=N/L^3$: number density

For steady state ($t\to\infty$) obtain explicit asymptotic solution of (4) as $B\to 0$ ($B=0/1$: sphere/needle)

$$\boxed{P_d(\alpha,\beta)\approx\frac{1}{4\pi}-\frac{3B}{8\pi(1+\xi^2)}\sin^2(\beta)\left[\cos(2\alpha)+\xi\sin(2\alpha)\right]}$$

$\xi=\frac{16\pi^2BU_0\rho\epsilon}{25\dot{\gamma}}$, U_0: dipole strength, ϵ: normalized variance of positional density.

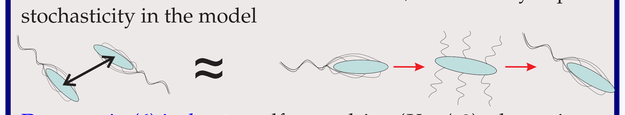
For small concentration ϕ total stress $\sigma^d(\mathbf{d})+\sigma^{LJ}(\mathbf{x})\approx\sigma^d(\mathbf{d})\to$ depends only on orientation and take average w.r.t. $P_d(\mathbf{d})$ to calculate the effective viscosity of a semidilute suspension (with interactions)

$$\boxed{\frac{\hat{\eta}-\eta}{\eta}=\frac{\sigma^d_{xy}}{\gamma}=\frac{-16\pi^2B^2U_0^2\rho\epsilon}{125\dot{\gamma}^2(1+\xi^2)}} \quad (6)$$

η: ambient fluid viscosity, γ: shear rate

Set $D=-\frac{8\pi^2BU_0\rho\epsilon}{25}$ to be the strength of rotational diffusion in a dilute suspension with tumbling [1]. We find the same $P_d\to$ same $\hat{\eta}$.

Hydrodynamic interactions $\approx$ random noise, called *Self-Induced Noise*: interactions introduce randomness, without any explicit stochasticity in the model



Decrease in (6) is due to: self-propulsion ($U_0\neq 0$), elongation ($B\neq 0$), and interactions

3.Current Work:Beyond Mean Field

Objective: Look for critical concentration ϕ_{crit} where collective motion (large scale structures) appears.

Model: Semidilute bacterial suspension of force dipoles in 3D. Approximate (2)-(3) by mean field with fluctuations ξ_x,ξ_d.

$$\dot{\mathbf{x}}^i=V_0\mathbf{d}^i+\langle\mathbf{u}(\mathbf{x}^i)\rangle+\langle\mathbf{L}(\mathbf{x}^i)\rangle+\xi_x(\mathbf{x},\mathbf{d}) \quad (7)$$

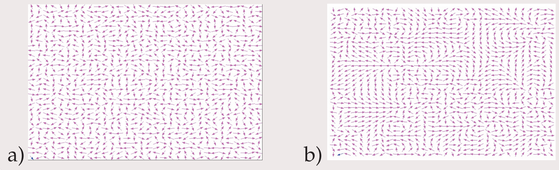
$$\dot{\mathbf{d}}^i=-\mathbf{d}^i\times\langle\omega(\mathbf{x}^i)\rangle-\mathbf{d}^i\times B\mathbf{d}^i\times\langle\mathbf{E}(\mathbf{x}^i)\rangle\cdot\mathbf{d}^i+\xi_d(\mathbf{x},\mathbf{d}) \quad (8)$$

Key features: Collisions included via $\mathbf{L}$ and self-induced noise included via ξ_x,ξ_d.

Goals:

- Numerically solve the equations of motion (2)-(3) on GPUs using periodic boundary conditions in a $2D$ domain.
- Extract dependence of large scale motion as a function of system parameters, e.g. dipole strength, bacterium velocity, concentration.

Velocity field where concentration doubles from a) to b). Large scale structures, e.g. "vortices", arise in b).



3.PDEs,many non-separated scales

PDEs with non-smooth coefficients & many scales: Classical FEM and homogenization do not work.

Extend ideas from classical homogenization with periodic coefficients to design *multiscale shape functions (basis)* that depend on coefficients and capture scales with error estimate (10) ([3]).

Question: Is there an analog of the homogenization approximation for arbitrarily rough coefficients $\sigma=\{\sigma_{ij}(x)\in L^\infty(\Omega)\}$, with many non-separated scales?

$$\begin{cases}-\mathrm{div}(\sigma\nabla u)=g\in L^2(\Omega) & x\in\Omega\\ u=0 & x\in\partial\Omega\end{cases} \quad (9)$$

Current work: Introduce computational mesoscale h. Construct a finite dimensional approximation $\hat{u}_h$ with controlled error in the H^1-norm, bypassing the homogenized PDE (**that does not exists**)

$$\|u-\hat{u}_h\|_{H^1}\leq Ch\|f\|_{L^2}. \quad (10)$$

Next, extend this approach to Stokes eqn in the domain with a *fine-grained* moving boundary that represents swimming bacteria.

Objective: Avoid expensive recomputing of the basis at each time step

Idea: Choose a clever (computationally inexpensive) advection of the basis.

References and Funding

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[1] B. M. Haines, I. S. Aranson, L. Berlyand, D. A. Karpeev. Effective viscosity of bacterial suspensions: A three-dimensional PDE model with stochastic torque *CPAA* (2012)

[2] S. D. Ryan, B. M. Haines, L. Berlyand, F. Ziebert, I. S. Aranson. Viscosity of bacterial suspensions: Hydrodynamic interactions and self-induced noise *PRE* **83** 050904(R) (2011)

[3] L. Berlyand, H. Owhadi. Flux norm approach to finite dimensional homogenization approximations with non-separated scales and high contrast *Arch. Rat. Mech. Anal.* (2010)