Theory and Simulation of Confined Active Suspensions

Adrien Lefauve & David Saintillan

Mechanical Science and Engineering
University of Illinois at Urbana-Champaign

July 8, 2013

Overview

1. Motivation and governing equations
2. Linear theory
3. Numerical simulations
4. Conclusions

Section 1

Motivation and governing equations

Biologically active suspensions

Self-propelling microorganisms in a viscous fluid $\rightarrow$ collective motion:

- large-scale coherent flows,
- giant density fluctuations
- chaotic fluid mixing...

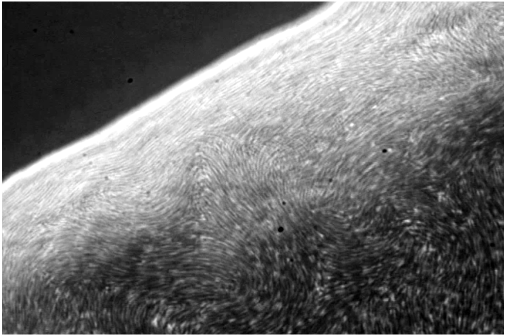


Figure: Bacterial turbulence on a surface. Weibel Lab, University of Wisconsin

Long-ranged hydrodynamic interactions

- Slow decay of low-*Re* disturbance flows
- Far-field dominated by a force dipole singularity in 3D
- Responsible for large-scale alignment and correlated motion

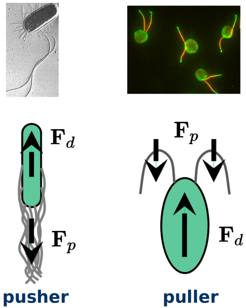


Figure: Force dipoles due to inertialess swimming

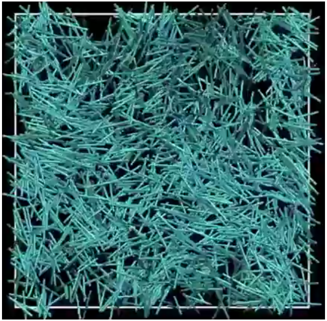


Figure: Pushers simulation. Saintillan & Shelley, *J. R. Soc. Interface* **9**, 571 (2012)

Governing equations under confinement

2D confinement between rigid plates:

- suppresses force dipole $(1/r^3)$ and amplifies source dipole $(1/r^2)$

  Liron & Mochon, *J. Eng. Math.* **10**, 287 (1976)

$$\mathbf{u}^d(\mathbf{R}_i|\mathbf{R}_j,\boldsymbol{\sigma}_j) = \frac{1}{2\pi|\mathbf{R}_{ij}|^2}(2\hat{\mathbf{R}}_{ij}\hat{\mathbf{R}}_{ij} - \mathbf{I})\cdot\boldsymbol{\sigma}_j, \quad \text{where} \quad \boldsymbol{\sigma}_j = \sigma[\dot{\mathbf{R}}_j - \mathbf{u}(\mathbf{R}_j)]$$

- allows reorientation of fore-aft asymmetric particles with the flow

  Brotto *et al.*, *Phys. Rev. Lett.* **110**, 038101 (2013)

$$\begin{aligned} \dot{\mathbf{R}} &= v_s\,\mathbf{p} + \mathbf{u} \\ \dot{\mathbf{p}} &= \nu'\,(\mathbf{I} - \mathbf{pp})\cdot\nabla\mathbf{u}\cdot\mathbf{p} + \nu\,(\mathbf{I} - \mathbf{pp})\cdot\mathbf{u} \end{aligned}$$

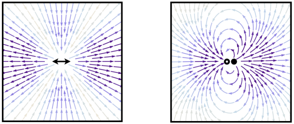


Figure: Force vs mass dipole

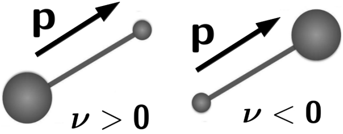


Figure: Large-tail vs large-head

Continuum description

Kinetic model, coupling :

- distribution function $\Psi(\mathbf{x}, \mathbf{p}, t)$ satisfying a continuity equation:

$$\frac{\partial \Psi}{\partial t} = -\nabla_{\mathbf{x}} \cdot (\Psi\, \dot{\mathbf{R}}) - \nabla_{\mathbf{p}} \cdot (\Psi\, \dot{\mathbf{p}}) + D\, \nabla_{\mathbf{x}}^2 \Psi + D_R\, \nabla_{\mathbf{p}}^2 \Psi,$$

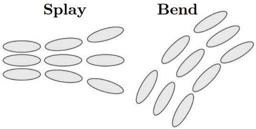
- mean-field fluid velocity $\mathbf{u}(\mathbf{x}, t)$:

$$\mathbf{u}(\mathbf{x}, t) := \int_{\mathbf{p}} \int_{\mathbf{x}'} \Psi(\mathbf{x}', \mathbf{p}, t)\ \mathbf{u}^d(\mathbf{x}|\mathbf{x}', \boldsymbol{\sigma})\ d\mathbf{x}'\ d\mathbf{p}.$$

Saintillan & Shelley, *Phys. Fluids* **20**, 123304 (2008)

Local phase properties:

- concentration: $c(\mathbf{x}, t) = \int_{\mathbf{p}} \Psi\ d\mathbf{p}$
- polarization: $\mathbf{P}(\mathbf{x}, t) = 1/c \int_{\mathbf{p}} \mathbf{p}\Psi\ d\mathbf{p}$
- nematic order: $\mathbf{Q}(\mathbf{x}, t) = 1/c \int_{\mathbf{p}} (\mathbf{pp} - \frac{1}{2}\mathbf{I})\Psi\ d\mathbf{p}$



Section 2

Linear theory

Linear stability analysis

- Uniform, isotropic base state:

$$\Psi_0(\mathbf{x}, t) = \frac{c_0}{2\pi}, \qquad \mathbf{u}_0(\mathbf{x}, t) = \mathbf{0}$$

- Small perturbations:

$$\Psi(\mathbf{x}, \mathbf{p}, t) = \Psi_0 + \varepsilon \Psi'(\mathbf{x}, \mathbf{p}, t), \quad \mathbf{u}(\mathbf{x}, t) = \varepsilon \mathbf{u}'(\mathbf{x}, t) \quad \text{where } |\varepsilon| \ll 1$$

- Linearization of the continuity equation:

$$\frac{\partial \Psi'}{\partial t} = -\nabla_{\mathbf{x}} \Psi' \cdot (v_s \mathbf{p}) + \Psi_0 \Big(\nu \mathbf{u}' \cdot \mathbf{p} - \nabla \cdot \mathbf{u}' \Big) + D \nabla_{\mathbf{x}}^2 \Psi' + D_R \frac{\partial^2 \Psi'}{\partial \theta^2}$$

- Coupling velocity field:

$$\nabla \cdot \mathbf{u} \overset{\text{def}}{=} \int_{\mathbf{p}} \int_{\mathbf{x}'} \Psi(\mathbf{x}', \mathbf{p}, t) \; \nabla \cdot \mathbf{u}^d(\mathbf{x}|\mathbf{x}', \boldsymbol{\sigma}) \; \mathrm{d}\mathbf{x}' \; \mathrm{d}\mathbf{p}$$

at leading order in ε: $\quad \nabla \cdot \mathbf{u}' = -\sigma c_0 v_s \nabla \cdot \mathbf{P}'$

Fourier transform and eigenvalue problem

- Assume plane-wave perturbations: $\Psi'(\mathbf{x}, \mathbf{p}, t) = \tilde{\Psi}(\mathbf{k}, \mathbf{p}) e^{i\mathbf{k}\cdot\mathbf{x}+\alpha t}$
  $\mathbf{k}$ is the wave vector and α the complex growth rate.
- Expand Fourier amplitude $\tilde{\Psi}$ in discrete Fourier modes:

$$\tilde{\Psi}(\theta) = \sum_{n=-\infty}^{+\infty} \tilde{\Psi}_n \exp(in\theta) \quad \text{where} \quad \theta = \cos^{-1}(\hat{\mathbf{k}} \cdot \mathbf{p})$$

- Linearized equation yields an eigenvalue problem for modes $\tilde{\Psi}_n$:

$$\frac{\alpha + k^2 D}{D_R} \begin{bmatrix} \vdots \\ \tilde{\Psi}_{-2} \\ \tilde{\Psi}_{-1} \\ \tilde{\Psi}_0 \\ \tilde{\Psi}_1 \\ \tilde{\Psi}_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \ddots & \ddots & & & & & \\ \ddots & -4 & -ik' & & & & \\ & -ik' & -1-\frac{Pe}{2} & -ik' & -\frac{Pe}{2} & & \\ & & -ik'(1-\sigma c_0) & 0 & -ik'(1-\sigma c_0) & & \\ & & -\frac{Pe}{2} & -ik' & -1-\frac{Pe}{2} & -ik' & \\ & & & & -ik' & -4 & \ddots \\ & & & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \tilde{\Psi}_{-2} \\ \tilde{\Psi}_{-1} \\ \tilde{\Psi}_0 \\ \tilde{\Psi}_1 \\ \tilde{\Psi}_2 \\ \vdots \end{bmatrix}$$

  where $Pe = \nu \frac{\sigma c_0 v_s}{2D_R} = \frac{\text{reorientation}}{\text{diffusion}}$ is a signed Péclet number.

- Non-dimensionalization: timescale D_R^{-1} and lengthscale $\frac{v_s}{2D_R}$

Large-head instability

Generic long-wavelength instability

- Confirmed unstable region $Pe < -1$ for $k = 0$ (Brotto *et al.*)
- Finite k: instability only above threshold size $L_c = 2\pi/k_c$
- Existence of two unstable regimes according to the system size. Near the transition: concentration, polarization and splay waves

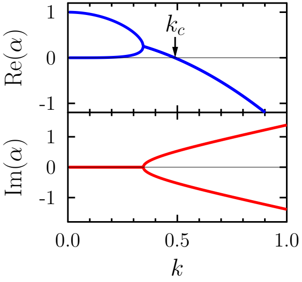
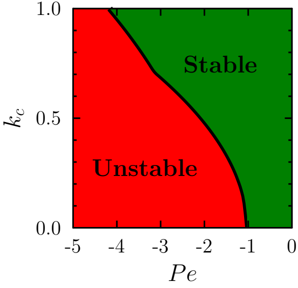


Figure: Growth rate ($Pe = -2$)



Critical size

Stabilizing external flow

Revisit stability with superimposed uniform flow $\mathbf{U}_0$

- Diffusion balance: $\Psi_0(\theta) = A e^{\xi \cos\theta}$, with flow strength $\xi = \frac{\nu U_0}{D_R}$
- Linearized equation includes new advective terms:

$$\frac{\partial \Psi'}{\partial t} = -\nabla\Psi' \cdot (v_s \mathbf{p} + \mathbf{U}_0) + \Psi_0(\nu \mathbf{u}' \cdot \mathbf{p} - \nabla \cdot \mathbf{u}') + D\nabla^2\Psi' + D_R \nabla_p^2 \Psi'$$
$$+ \nu\Big((\mathbf{I} - \mathbf{pp}) \cdot (\nabla_p \Psi' \cdot \mathbf{U}_0 + \nabla_p \Psi_0 \cdot \mathbf{u}') - \Psi' \mathbf{U}_0 \cdot \mathbf{p}\Big)$$

- Incompressibility becomes: $\nabla \cdot \mathbf{u}' = -f v_s \Big(\nabla \cdot \mathbf{P}' + \frac{\nabla c'}{c_0} \cdot \mathbf{P}_0\Big)$

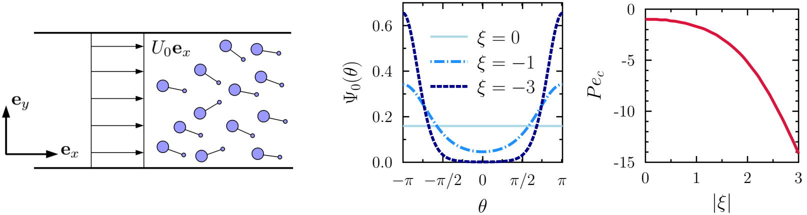


Figure: Polar state Added stability for $k = 0$

Section 3

Numerical simulations

Discrete particle simulation

- Periodic 2D domain of size L
- Random initial positions and orientations (uniform, isotropic)
- RK4 integration of $\dot{\mathbf{R}}_i$, $\dot{\mathbf{p}}_i$, with $\mathbf{u}(\mathbf{R}_i) = \sum_{j \neq i} \mathbf{u}^d(\mathbf{R}_i | \mathbf{R}_j, \boldsymbol{\sigma}_j)$
- Efficient algorithm for interactions due to images

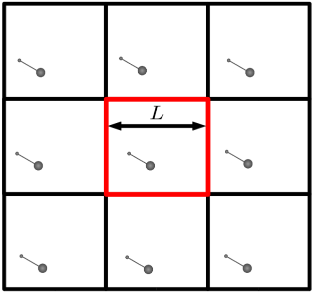


Figure: $N = 1$ particle and its 8 closest periodic images

Nonlinear dynamics of large-heads

Heavily polarized density waves ($N = 5000$ particles, $Pe = -2.2$)

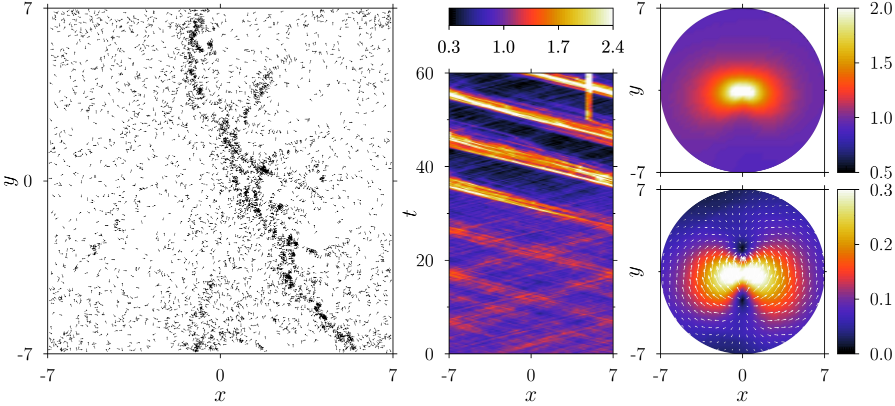
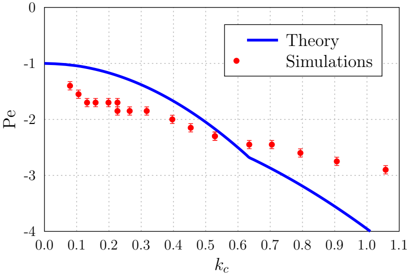


Figure: Snapshot Spatiotemporal x-concentration Pair distributions

Nonlinear dynamics of large-heads

- Critical system size for unstable transition: good agreement with linear stability



- Long-time dynamics: pattern formation

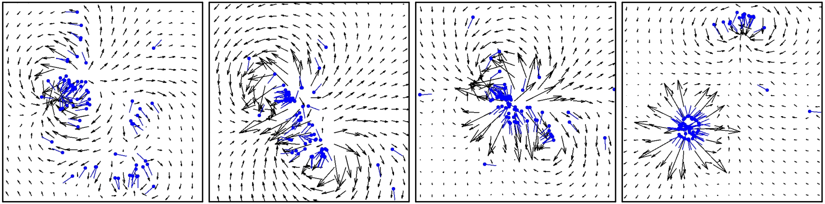


Figure: Flow during formation of a circular cluster

Nonlinear dynamics of large-tails

Nonlinear long-wavelength instability (here $N = 3600$, $Pe = 3.7$)

- large scale splay and bend modes / counter-rotating vortices
- quasi-periodic dynamics

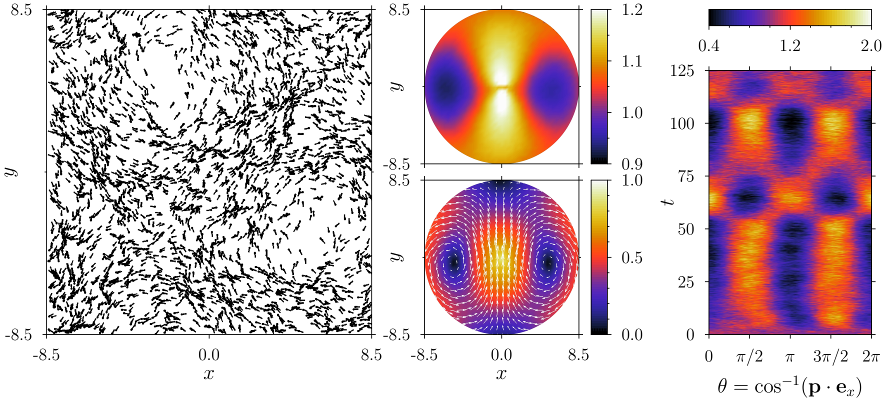


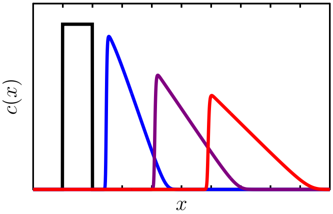
Figure: Particles snapshot Pair distributions Orientations

Quasi-1D model with imposed flow

- Recall: uniform external flow $\rightarrow$ alignment and stabilization
- Derive a q1D kinetic model, assuming:
  - flow $U_0\mathbf{e}_x$ and stable orientation distribution $\Psi_0(\theta) = A\exp(\xi\cos\theta)$
  - 1D: $\Psi(\mathbf{x},\theta,t) = c(x,t)\Psi_0(\theta)$ and $\mathbf{u}(\mathbf{x},t) = u(x,t)\mathbf{e}_x$
- Continuity & velocity $\rightarrow$ conservation law for $c(x,t)$:

$$\frac{\partial c}{\partial t} + \frac{\partial q}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \quad \text{with the flux} \quad q(x) = \Big[U_0 + v_s P_0 \underbrace{\Big(1 - \sigma c(x)\Big)}_{\text{negative coupling}}\Big] c(x).$$

- Traffic flow equation
  - modeling of density waves
  - shock at the tail
  - rarefaction wave at front



Traffic flow of quasi-aligned swimmers

- Traffic jam simulation ($N = 4000$, $\xi = +4$)
- Agreement with q1D kinetic model

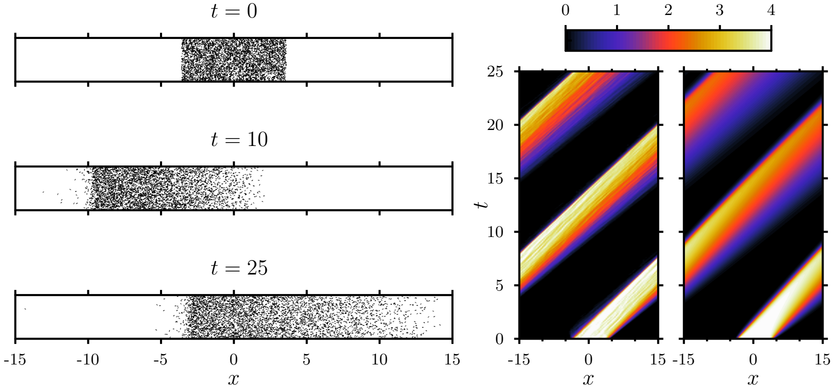


Figure: Snapshots Spatiotemporal x-concentration (simulation vs theory)

Section 4

Conclusions

Hydrodynamic interactions in confined active suspensions:

- spontaneous emergence of collective motion
  - large-head swimmers
    - polarized density waves above a critical system size
    - formation of dense circular patterns
  - large-tail swimmers
    - quasi-periodic nematic modes and vortices
- rescaling of 1D single-swimmer dynamics
  - global traffic flow behavior (simulations & q1D continuous model)

Model relies on the dilute assumption $\rightarrow$ role of steric interactions?

Confined suspensions are tractable:

- analytically: 2D & linearity of Stokes flow
- computationally: "fast" decay of interactions ($1/r^2$ in 2D)

$\rightarrow$ well-suited for broader the study of mechanisms behind collective motion & self-organization in more complex many-body systems

Figure: Bird flocks

Thank you !