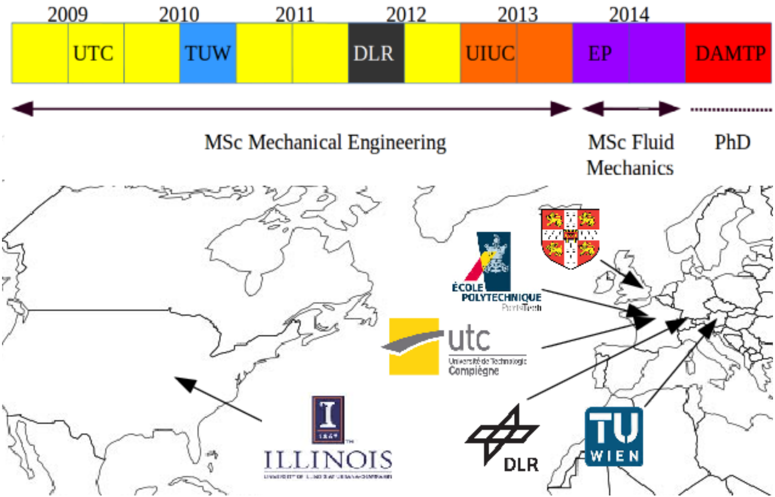
Collective dynamics in confined active suspensions

Adrien Lefauve

DAMTP, University of Cambridge

CUED Fluid Mechanics Seminar
November 14, 2014

About me


2009
2010
2011
2012
2013
2014
UTC
TUW
DLR
UIUC
EP
DAMTP
MSc Mechanical Engineering
MSc Fluid Mechanics
PhD
ÉCOLE POLYTECHNIQUE
utc
Compiègne
ILLINOIS
DLR
TU WIEN

Outline

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

Outline

Biologically active suspensions

Microorganisms self-propelling in a viscous liquid

- collective motion
- large-scale coherent flows

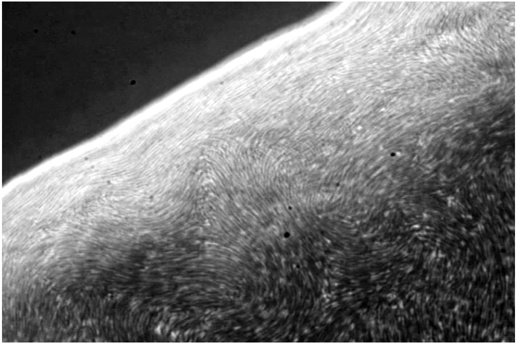


Figure: Bacterial swarming on a surface. Weibel Lab, University of Wisconsin

Motivations

- Applied
  - Efficient low-Re mixing! ($Re = \frac{Ud}{\nu} \sim \frac{10^{-5} \times 10^{-6}}{10^{-6}} = 10^{-5}$)
  - Chemical/pharmaceutical engineering
  - Optimal nutrient mixing in bacterial colonies

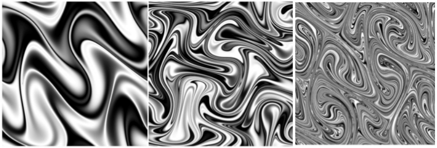


Figure: Mixing Saintillan (2012)

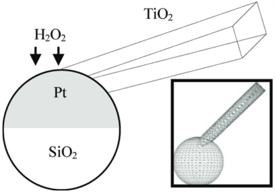


Figure: Artificial nanoswimmer Gibbs et al., *Nano Lett.* (2011)

Motivations

- Fundamental
  - Collective dynamics of active, interacting agents
  - Local, individual interactions $\rightarrow$ large-scale coherent patterns?
  - Self-organisation (condensed matter physics, cell biology)

Hydrodynamic interactions

- A swimmer induces a local disturbance flow

  Dominant far-field term: source dipole ($\sim 1/r^2$ decay)

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

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

with dipole moment $\boldsymbol{\sigma}_j = \sigma[\dot{\mathbf{R}}_j - \mathbf{u}(\mathbf{R}_j)]$

and $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$, $\hat{\mathbf{R}}_{ij} = \mathbf{R}_{ij}/|\mathbf{R}_{ij}|$

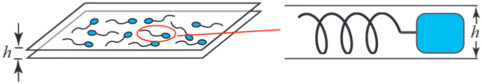


Figure: Rigid 2D confinement Tsang & Kanso, *Phys. Rev. E* (2014)

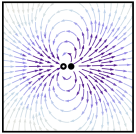


Figure: Source dipole Spagnolie & Lauga, *JFM* (2012)

Hydrodynamic interactions

- Response of individual particle to external flow
    - advection by flow
    - reorientation of fore-aft asymmetric particles with/against flow

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

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

→ 'large-tail' particles (vigorous flagella) align with the flow

→ 'large-head' particles (weak flagella) align against the flow

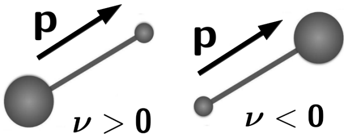


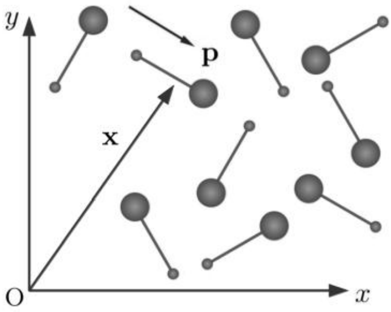
Figure: Large-tail vs large-head dumbbell swimmer

Outline

Continuum description

Probability distribution function $\Psi(\mathbf{x}, \mathbf{p}, t)$ of finding a particle

- at position $\mathbf{x}$
- with orientation $\mathbf{p}$
- at time t



Continuum description

- Conservation of particles $\rightarrow$ continuity equation for Ψ:

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

- Fluxes $\dot{\mathbf{R}}$ and $\dot{\mathbf{p}}$ require fluid velocity $\mathbf{u}(\mathbf{x}, t)$:

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

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

Local phase properties:

- concentration: $c(\mathbf{x}, t) = \int_{\mathbf{p}} \Psi\ \mathrm{d}\mathbf{p}$
- polarization: $\mathbf{P}(\mathbf{x}, t) = 1/c \int_{\mathbf{p}} \mathbf{p}\Psi\ \mathrm{d}\mathbf{p}$

Linear stability analysis

- Uniform, isotropic base state:

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

- Small perturbations:

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

- Linearize continuity for Ψ and uncouple $\mathbf{u}$ (incompressibility)

- 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.

- Natural timescale $\tau = D_R^{-1}$, lengthscale $\ell = \frac{v_s}{2D_R}$, fraction ϕ

- Dimensionless Péclet number : $Pe = \phi \times \nu\ell = \frac{\text{reorientation}}{\text{diffusion}}$

Large-head instability

Large heads are potentially unstable!

- For all $Pe < -1$ if $k = 0$ Brotto *et al.*, *Phys. Rev. Lett.* (2013)
- Finite k: instability only above threshold size $L_c = 2\pi/k_c$
- Unstable mode near the transition:
  travelling waves coupling concentration and polarization

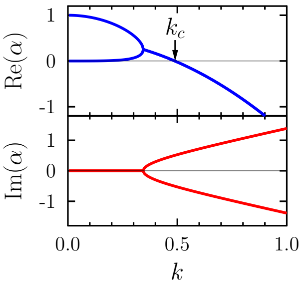
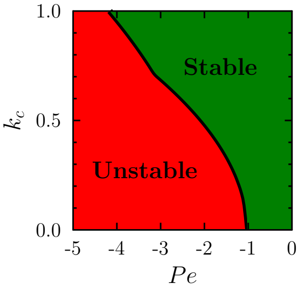


Figure: Growth rate ($Pe = -2$)



Critical size vs Pe

Outline

Discrete particle simulation

- Periodic, 2D domain, N point particles with random $\mathbf{R}_i(0)$, $\mathbf{p}_i(0)$
- RK4 time integration $4N$ ODEs, all coupled by pair interactions

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

where

$$\mathbf{u}(\mathbf{R}_i) = \sum_{j\neq i} \mathbf{u}^d(\mathbf{R}_i|\mathbf{R}_j, \boldsymbol{\sigma}_j) \quad \text{and} \quad \boldsymbol{\sigma}_j = \sigma[\dot{\mathbf{R}}_j - \mathbf{u}(\mathbf{R}_j)]$$

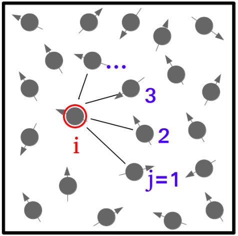


Figure: Pair interactions

Nonlinear dynamics of large-heads

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

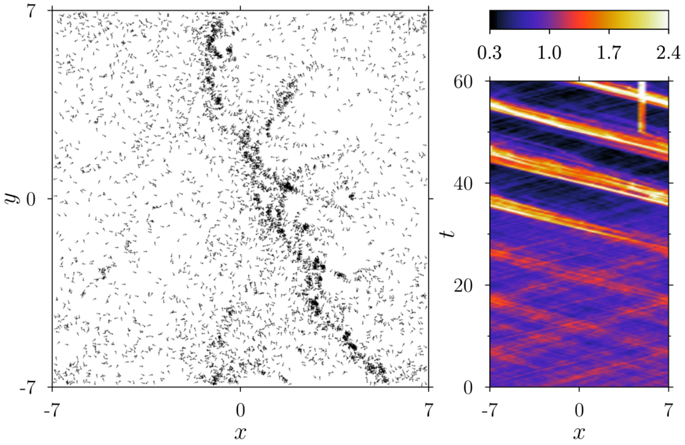
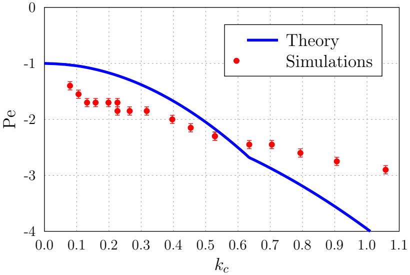


Figure: Snapshot $x - t$ concentration

Nonlinear dynamics of large-heads

- Critical system size:

  qualitative agreement with linear stability



- Long-time dynamics: pattern formation

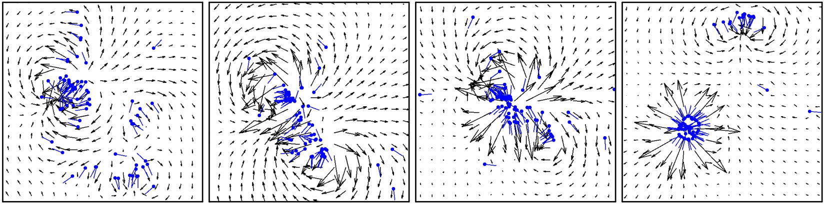
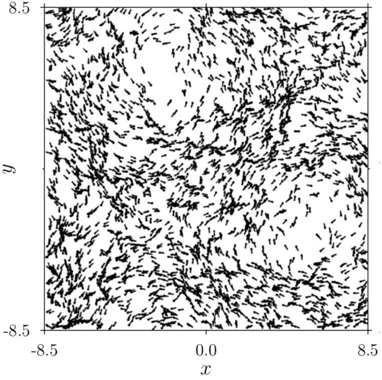


Figure: Flow during formation of a circular cluster

Nonlinear dynamics of large-tails

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

- large scale counter-rotating vortices
- quasi-periodic dynamics



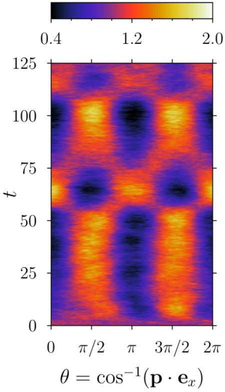
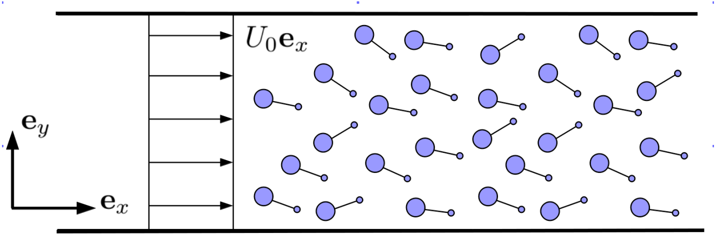


Figure: Particles snapshot Orientations

Stabilizing external flow

Let us superimpose a uniform flow $\mathbf{U}_0 = U_0 \mathbf{e}_x$

- No more isotropic: net polarization $|\mathbf{P}_0|(\xi) > 0$, where $\xi = \frac{\nu U_0}{D_R}$
- A uniform suspension is now stable
- In q1D geometry: assume $\Psi(\mathbf{x}, \theta, t) = c(x, t)\ \Psi_0(\theta)$



Quasi-1D model with external flow

- Equations for Ψ and $\mathbf{u}$ simplify a lot
- Conservation law for $c(x,t)$:

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

- Traffic flow equation!

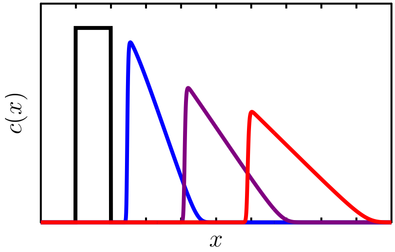


Figure: Persisting shock at tail, development of rarefaction wave at front

Traffic flow of quasi-aligned swimmers

- Traffic jam simulation ($N = 4000$, $\xi = +4$)
- Agreement with traffic flow equation

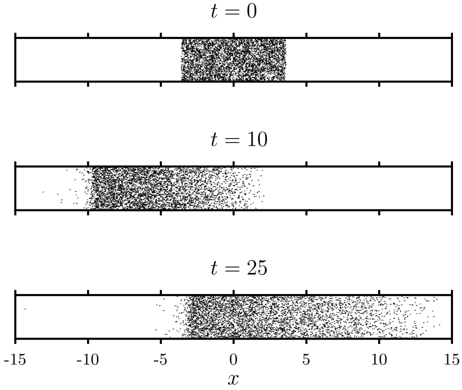
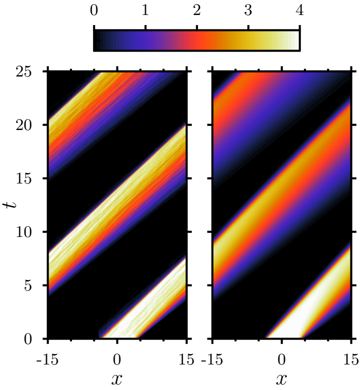


Figure: Snapshots



$x - t$ concentration (simulation vs theory)

Outline

Conclusions

Collective dynamics of confined active suspensions:

- 2D, rigid confinement changes governing equations
  - different flow around swimmer (source dipole)
  - new dynamics: reorientation with/against flow
- Spontaneous emergence of collective motion
  - "large-head" swimmers
    - polarized density waves above a critical system size
    - formation of dense circular clusters
  - "large-tail" swimmers
    - quasi-periodic giant vortices
- Traffic flow behavior in q1D geometry
  - rescaling of single-swimmer dynamics by local concentration

Conclusions

Limitations:

- Theory + particle simulations rely on the dilute assumption
- Role of contact interactions for higher concentration?

Confined suspensions are tractable (2D & linearity of Stokes flow)

$\rightarrow$ well-suited for gaining insight into basic mechanism behind self-organization in more complex systems

Acknowledgements

Work done in Department of Mechanical Science & Engineering at University of Illinois at Urbana-Champaign (USA)

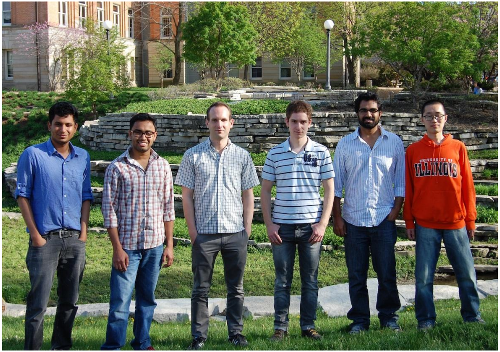


Figure: Dr. David Saintillan's research group

Thank you !