Lecture 4: Hydrodynamics of Bacterial Suspensions

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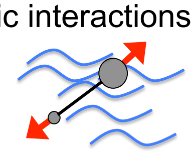
Plan

The methods outlined in the last lecture can be used to derive hydrodynamics for a collection of active particles in a medium with other interactions:

- Short-range interactions due to cluster of motor proteins crosslinking cytoskeletal filaments → relevant to cell cytoskeleton and cytoskeletal extracts
- Fluid-mediated hydrodynamic interactions → relevant to bacterial suspensions.



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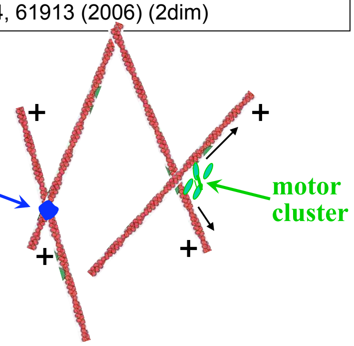
Cytoskeletal filaments & motor proteins

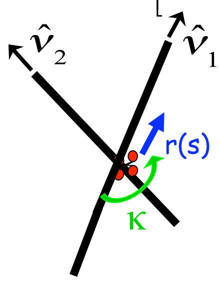
Kruse & Julicher, PRE 67, 51913 (2003) (1dim)
Ahmadi, MCM & Liverpool PRE 74, 61913 (2006) (2dim)

Cytoskeletal filaments (e.g., actin) as polar rods coupled by passive and active crosslinkers



Smoluchowski:

$$\partial_t c(x_1) = \partial_{x_1}\left[D\partial_{x_1} c(x_1) + \int_{x_2} \frac{1}{\zeta}F(12)\, c(x_1)c(x_2)\right]$$



Velocity induced on filament 1 by filament 2 via active crosslinker. Obtained from kinematics of two polar rods crosslinked by an active motor cluster, modeled as a 2-headed rigid object with finite torsional stiffness κ that steps at a rate r(s) along each filament.

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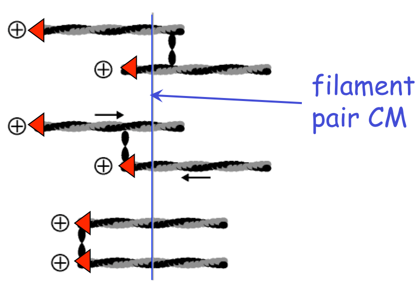
1. Motors drive filament bundling, e.g., 1dim: Kruse & Julicher, PRL 75, 1778 (2000)

$$u(s) = a\frac{dATP}{dt} \sim nm/\mu\sec$$



Mechanism for contractility, effective in both polar and apolar systems. In this model it requires motor stalling at end.

$$\text{bundling "rate": } \alpha \sim \langle s\, u(s)\rangle_{\text{length of filament}}$$

Builds up density inhomogeneities → pattern formation

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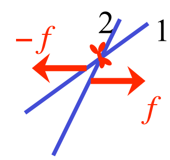
2. Motors yield mass transport

Liverpool & MCM, EPL 69, 846 (2004)

Although a motor-filament pair is a force dipole, i.e., $F_{NET}=0$, the anisotropy of rod diffusion yields $v_{CM}\neq 0$

$$\boxed{\begin{aligned} \zeta_{ij}(\hat{\nu}_1)\mathrm{v}_{1j} &= -f_i \\ \zeta_{ij}(\hat{\nu}_2)\mathrm{v}_{2j} &= f_i \\ \vec{\mathrm{v}}_{CM} = \tfrac{\vec{\mathrm{v}}_1+\vec{\mathrm{v}}_2}{2} &\neq 0 \end{aligned}}$$



$$\zeta_{ij}(\hat{\nu}) = \zeta_{\parallel}\hat{\nu}_i\hat{\nu}_j + \zeta_{\perp}\left(\delta_{ij} - \hat{\nu}_i\hat{\nu}_j\right)$$

active velocity:

$$\mathrm{v}_{CM} \equiv \beta \sim \langle u(s)\rangle_{\text{length of filament}}$$

Self-propulsion as a generic property of all **polar** active units:

- apolar $v_{CM}=0$
- polar $v_{CM}\neq 0$

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Bacterial Suspensions: Outline

- The simplest "swimmer": pullers vs pushers
- Microdynamics of interacting swimmers
- Hydrodynamic interactions
- Instabilities and other results
- Outlook

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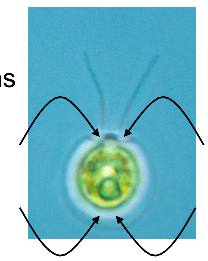
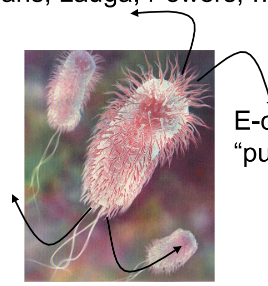
The locomotion of individual organisms is controlled by a cyclic "stroke" (motion of cilia, flagella, …)➔Extensive models of individual swimmers and some progress in understanding pair interaction (Childress, Purcell, Golestanian, Yeomans, Lauga, Powers, …)

Chlamydomonas
"pullers"





E-coli
"pushers"

Our focus: collective behavior on
lengths >> swimmer size & times >> stroke duration :
How do different classes of propulsion mechanisms affect the collective macroscopic physics?

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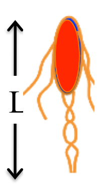
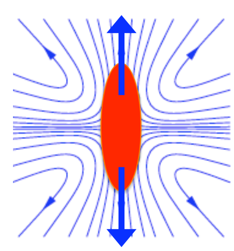
A swimmer as a force dipole



At distances >> L and on times >> duration of one stroke, the forces exerted by swimmer on fluid can be approximated as a static **force dipole**



- No acceleration (Re<<1), net force must vanish
- Approximation is ok because we are interested in collective effects, not in the properties of individual swimmers
- Flow generated by a swimmer is complex and contains all multipoles - these will be generated by hydrodynamic interactions

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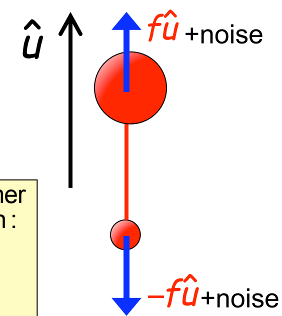
The "simplest swimmer"

- Re<<1 → neglect inertia
- Neutrally buoyant
- Swimmer rides w/ fluid



One swimmer:

$$\partial_t \vec{r}_L = \vec{v}(\vec{r}_L)$$
$$\partial_t \vec{r}_S = \vec{v}(\vec{r}_S)$$

Flow field generated by swimmer is given by the Stokes equation:

$$\vec{\nabla}\cdot\vec{v} = 0$$

$$\eta\nabla^2\vec{v} = \overbrace{f\hat{u}\delta(\vec{r}-\vec{r}_L) - f\hat{u}\delta(\vec{r}-\vec{r}_S)}^{\text{active forces exerted by swimmer on fluid}}$$
+noise

Many swimmers (α=1,…,N)

$$\partial_t \vec{r}_{\alpha L} = \vec{v}(\vec{r}_{\alpha L})$$
$$\partial_t \vec{r}_{\alpha S} = \vec{v}(\vec{r}_{\alpha S})$$

$$\eta\nabla^2\vec{v} = \sum_\alpha \overbrace{\left[f\hat{u}_\alpha\delta(\vec{r}-\vec{r}_{\alpha L}) - f\hat{u}_\alpha\delta(\vec{r}-\vec{r}_{\alpha S})\right]}^{\text{active forces exerted by \textbf{all} swimmers on fluid}}+\text{noise}$$

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Two approaches

a) Solve Stokes eqn. to obtain the flow velocity v.

$$\left.\begin{array}{l}\eta\nabla^2\vec{v} = \vec{F}^{act}\\ \vec{\nabla}\cdot\vec{v} = 0\end{array}\right\} \quad \boxed{v_i(\vec{r}) = \int_{\vec{r}\,'} O_{ij}(\vec{r}-\vec{r}\,')F_j^{act}(\vec{r}\,'),} \quad \underbrace{O_{ij}(\vec{r}) = \frac{1}{8\pi\eta r}\left(\delta_{ij} + \hat{r}_i\hat{r}_j\right)}_{\text{Oseen tensor}}$$

Eliminate v from the eqs of motion for the swimmers → fluid flow is recast as hydrodynamic forces and torques on swimmers. Next, coarse grain the resulting microdynamics of interacting swimmers.

b) Retain the Stokes equation and obtain a hydrodynamic two-fluid model that contains explicitly the flow velocity.

Advantage of (a):
- physical insight on role of hydrodynamic interactions
- crucial role of long-range nature of hydrodynamic forces

Advantage of (b):
- straightforward comparison with phenomenological theory.

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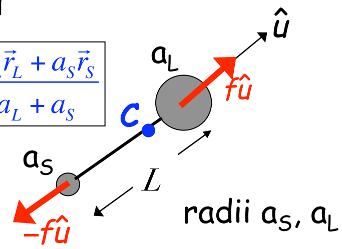
One swimmer

Rigid body dynamics at low Re:
Translation of & rotation about hydrodynamic center C, determined by shape (not mass distribution)

$$\vec{r}_C = \frac{a_L \vec{r}_L + a_S \vec{r}_S}{a_L + a_S}$$



noise

$$\partial_t \hat{u} = \vec{\Gamma}_R(t)$$
$$\partial_t \vec{r}_C = v_0 \hat{u} + \vec{\Gamma}(t)$$

$$v_0 \sim \frac{f(a_S - a_L)}{\xi L}$$

Although NET FORCE=0, SP v_0 is finite if hydrodynamic center C does not coincide with center of force dipole

- Polar (head ≠ tail) $v_0 \neq 0$ → "mover"
- Apolar (head=tail) $v_0=0$ → "shaker"

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Many swimmers

$$\partial_t \vec{r}_{\alpha C} = v_0 \hat{u}_\alpha + \frac{1}{\xi} \sum_{\beta \neq \alpha} \vec{F}_{\alpha\beta} + \vec{\Gamma}_\alpha(t)$$
$$\partial_t \hat{u}_\alpha = \frac{1}{\xi L^2} \sum_{\beta \neq \alpha} \vec{\tau}_{\alpha\beta} + \vec{\Gamma}^R_\alpha(t)$$

Multipole expansion of force distribution about hyd. centers
$\xi = \xi_S + \xi_L = 6\pi\eta(a_S + a_L)$

$$\vec{F}_{12} \simeq \hat{r}_{12} \frac{\alpha}{r_{12}^2}\left[3(\hat{r}_{12}\cdot\hat{u}_2)^2 - 1\right]$$
$$\vec{\tau}_{12} \simeq \hat{u}_1 \times \left[3\hat{r}_{12}\hat{r}_{12} - \vec{\vec{1}}\right]\cdot \hat{u}_2 \left[\frac{\alpha_R}{r_{12}^3}(\hat{u}_1\cdot\hat{u}_2) - \frac{\beta}{r_{12}^5}\right]$$

Polar symmetry
$\beta \sim f(a_L - a_S) \sim v_0$

Nematic symmetry
α, $\alpha_R \sim f(a_L + a_S)$

- Central, dipolar forces, $\sim 1/r^2$
- Sign of α → pusher (tensile) vs puller (contractile)

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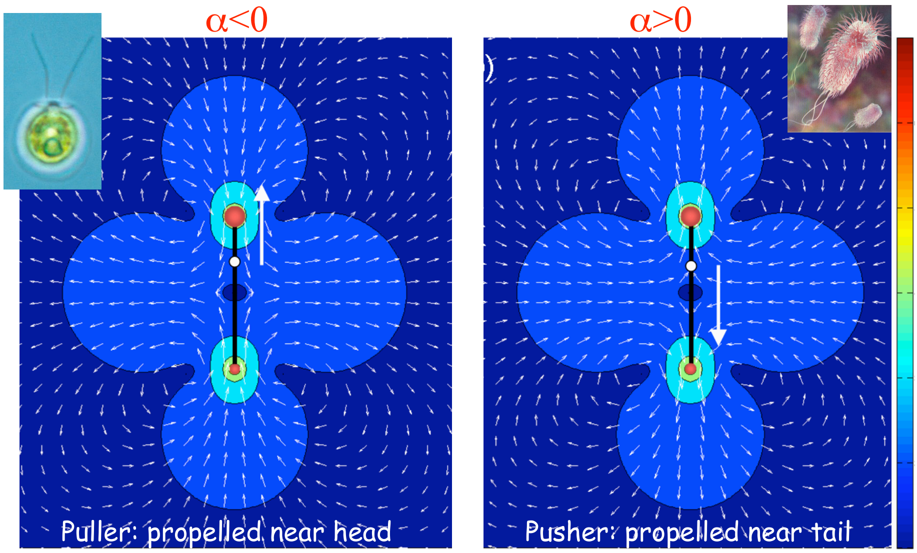

Position of hydrodynamic center wrt mid-point defines puller/pusher character

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From Microdynamics to Hydrodynamics

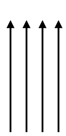
Use standard tools of nonequilibrium statitistical physics to construct dynamical equations for continuum fields on lengths >> L, times >> stroke cycle

$$\partial_t \vec{r}_{\alpha C} = v_0 \hat{\nu}_\alpha + \frac{1}{\zeta}\sum_{\beta\neq\alpha} \vec{F}_{\alpha\beta} + \vec{\Gamma}_\alpha(t)$$
$$\partial_t \hat{\nu}_\alpha = \frac{1}{\zeta L^2}\sum_{\beta\neq\alpha} \vec{\tau}_{\alpha\beta} + \vec{\Gamma}^R_\alpha(t)$$

$$\rho(\vec{r},t) = \left\langle \sum_\alpha \delta(\vec{r}-\vec{r}_{\alpha C}(t)) \right\rangle$$ concentration of swimmers

$$\vec{P}(\vec{r},t) = \frac{1}{\rho(\vec{r},t)}\left\langle \sum_\alpha \hat{\nu}_\alpha \delta(\vec{r}-\vec{r}_{\alpha C}(t)) \right\rangle$$ polar order

$$Q_{ij}(\vec{r},t) = \frac{1}{\rho(\vec{r},t)}\left\langle \sum_\alpha \left(\hat{\nu}_{\alpha i}\hat{\nu}_{\alpha j} - \tfrac{1}{3}\delta_{ij}\right) \delta(\vec{r}-\vec{r}_{\alpha C}(t)) \right\rangle$$ nematic order

Polar order 

Nematic order 

- Dilute suspensions
- Large SP regime $L/r_{12} \ll 1$

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Hydrodynamics of an incompressible active suspension: two equivalent formulations

Flow field appears explicitly → natural formulation of phenomenological models:

$$\partial_t \rho + \vec{u} \cdot \vec{\nabla} \rho = -\vec{\nabla} \cdot \vec{j}$$
$$\partial_t \vec{P} + \vec{F}(\vec{\nabla} \vec{u}) = \text{forces \& torques}$$
$$\partial_t Q_{ij} + F_{ij}(\vec{\nabla} \vec{u}) = \text{forces \& torques}$$
$$\eta \nabla^2 \vec{u} = \text{active stresses}, \qquad \vec{\nabla} \cdot \vec{u} = 0$$

In Stokes regime the flow field u **not** a dynamical variable

Flow field is eliminated at the outset and recast as hydrodynamic interactions among the swimmers

$$\partial_t \rho = -\vec{\nabla} \cdot \vec{J}$$
$$\partial_t \vec{P} = \text{forces \& torques}$$
$$\partial_t Q_{ij} = \text{forces \& torques}$$

Equivalent when u is eliminated on LHS in terms of ρ, P, Q_i

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Hydrodynamics equations for active particles concentration and director field

$$\begin{bmatrix} \rho_{total} = const \\ \vec{\nabla} \cdot \vec{v} = 0 \end{bmatrix}$$

$$\partial_t \rho_p + \vec{\nabla} \cdot \left(\rho_p \left(\vec{\mathrm{v}} + \beta \vec{n} \right) \right) = \vec{\nabla} \cdot D \vec{\nabla} \rho_p$$
$$\left(\partial_t + \left(\vec{\mathrm{v}} + \beta \vec{n} \right) \cdot \vec{\nabla} \right) n_i + \omega_{ij} n_j = \lambda u_{ij} n_j + w \partial_i \rho_p + K \nabla^2 n_i$$
$$\partial_j \sigma_{ij} = 0 \to \eta \nabla^2 \mathrm{v}_i = -\partial_j \left[\alpha\, n_i n_j + \beta \left(\partial_i n_j + \partial_j n_i \right) \right]$$
$$u_{ij} = \tfrac{1}{2} \left(\partial_i \mathrm{v}_j + \partial_j \mathrm{v}_i \right)$$
$$\omega_{ij} = \tfrac{1}{2} \left(\partial_i \mathrm{v}_j - \partial_j \mathrm{v}_i \right)$$

β intrinsic to polar systems
α present in polar and nematic fluids

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Microscopic Derivation

$$\begin{bmatrix} \rho_{total} = const \\ \vec{\nabla} \cdot \vec{v} = 0 \end{bmatrix}$$

We have eliminated the flow velocity from the outset in favor of (long-ranged) hydrodynamic interactions – schematically ($G \sim 1/r^2$):

$$\partial_t \rho_p + \mathrm{v}_0 \vec{\nabla} \cdot \left(\rho_p \vec{n} \right) = \vec{\nabla} \cdot D(\alpha) \vec{\nabla} \rho_p$$

$$\left(\partial_t + \mathrm{v}_0 \vec{n} \cdot \vec{\nabla} \right) n_i = w \partial_i \rho_p + K(\alpha) \nabla^2 n_i$$
$$+ \lambda \int_{\vec{r}\,'} \nabla_i G_{jk}(\vec{r} - \vec{r}\,') \nabla'_l \left[\alpha\, n_k n_l + \beta \left(\partial'_k n_l + \partial'_l n_k \right) \right]$$

$\mathrm{v}_0 \sim f$ self-propulsion intrinsic to polar systems; $\beta \sim \mathrm{v}_0$

$\alpha \sim f$ from active hydrodynamic forces: $\alpha < 0$ for pullers, $\alpha > 0$ for pushers

Microscopic expressions for various parameters (D, K, w) that are renormalized by activity

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Nonlocal hydrodynamics

Long-range hydrodynamics interactions ($F \sim 1/r^2$) yield nonlocal hydrodynamic equations.

$$\underbrace{J_\alpha(\vec{r})}_{\text{current}} = \int d\vec{r}\,' \underbrace{K(\vec{r} - \vec{r}\,')}_{\text{nonlocal interaction}} \underbrace{\Phi_\alpha(\vec{r}\,')\, \Phi_\beta(\vec{r})}_{\text{hydrodynamic fields}}$$

When the eqs. are linearized, the nonlocality can be truncated in a small q expansion

$$\delta J_\alpha(\vec{r}) \simeq \Phi_{\beta 0} \int d\vec{r}\,' K(\vec{r} - \vec{r}\,')\ \delta\Phi_\alpha(\vec{r}\,')$$
$$\rightarrow \Phi_{\beta 0} \tilde{K}(-\vec{q})\ \delta\tilde{\Phi}_\alpha(\vec{q}) \simeq \Phi_{\beta 0} \left[\tilde{K}_0 + iq\tilde{K}_1 + \ldots \right] \delta\tilde{\Phi}_\alpha(\vec{q})$$

small & large distance cutoffs

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Some Results

- Derivation of (nonlocal) hydrodynamics for pushers & pullers with microscopic expressions for parameters

- Steady-state solution of hydrodynamic eqs yields bulk states: **no bulk ordered state** from **pairwise hydrodynamic interactions**

→Isotropic state: ρ=const, P=Q=0

→**Steric effects** yield **nematic** order at high concentration

→**No polar state:** need **external** symmetry breaking, e.g., chemotaxis?

- Linearization around bulk states reveals instability of isotropic and ordered states → **pattern formation**.

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Instability of Isotropic State: different mechanisms for pushers & pullers

Pullers (α<0)

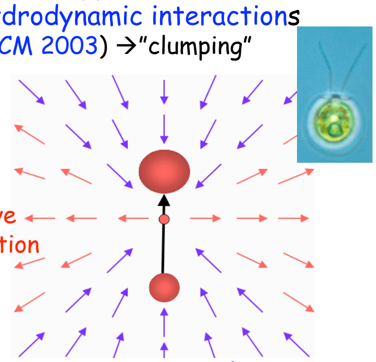
1) **growth of density fluctuations** from a suppression of longitudinal diffusion due to active hydrodynamic interactions (cf. Kruse & Julicher 2000; Liverpool & MCM 2003) →"clumping"

$$\partial_t \delta\rho + v_0 \vec{\nabla}\cdot\vec{P} = (D - |\alpha|\rho_0)\nabla^2\delta\rho$$

Controlled by Peclet number:

$$\frac{|\alpha|}{D} \sim \frac{(f/\zeta)L}{D} \sim \frac{vL}{D} = Pe$$

2) above a critical v_0: propagating **"sound-like" density waves**



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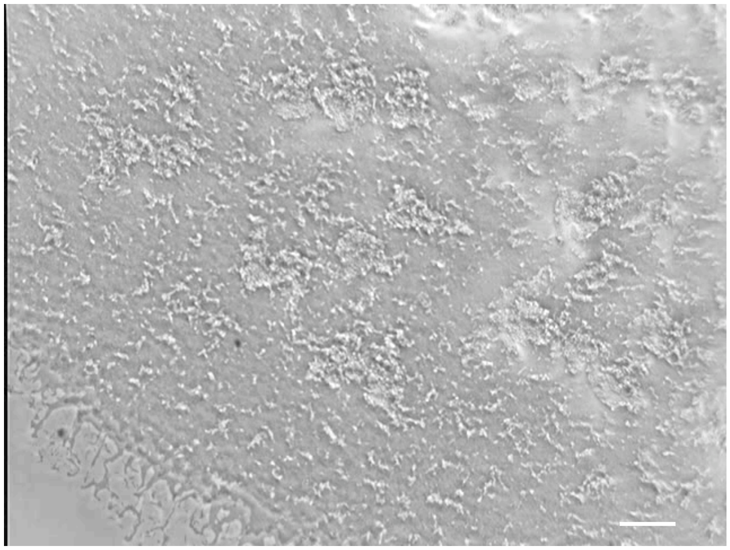

Late stages of Myxo on starvation agar 1 mm
Welch's lab, Syracuse University

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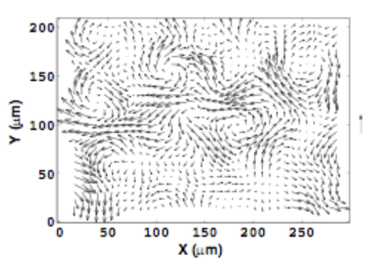
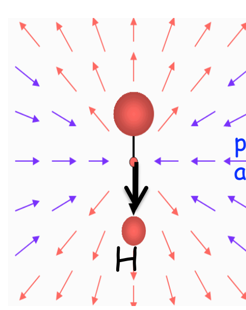
Instability of Isotropic state

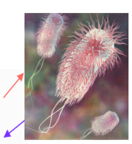
Pushers (α>0)
orientational fluctuations are unstable on all scales when $\alpha_R > D_R$ (cf. Saintillan & Shelley, 2008).

$$\partial_t Q_{\parallel\perp} = -(D_R - \alpha_R) Q_{\parallel\perp} + \ldots$$



Dombrowski et al, PRL 2004:
"turbulence" in a drop of Bacillus Subtilis





parallel alignment

perpendicular alignment

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Fluctuations in the Ordered state

- Ordered state **always** unstable on all scales due to coupling of orientation and flow: “generic instability” (Simha & Ramaswamy, PRL 2002)
  - Contractile / Puller : Splay fluctuations
  - Tensile / Pusher : Bend fluctuations

- Generic instability consequence of $1/r^2$ interactions. Can be suppressed by:
  - Viscoelastic medium (screening)
  - Frictional substrate

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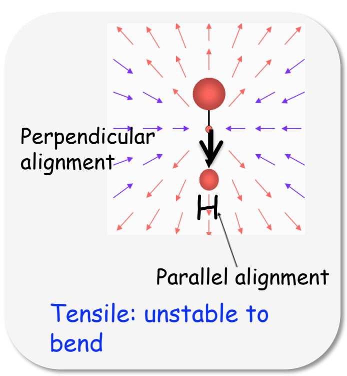
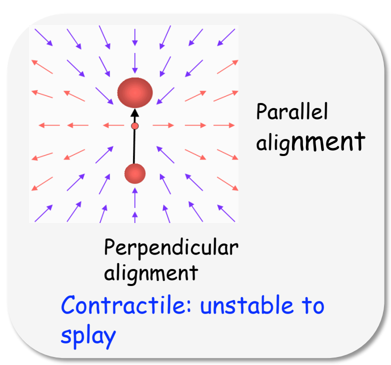
Ordered states

Ordered states of movers & shakers are unstable on all scales due to the coupling of orientation and flow

→ “generic” instability (Ramaswamy & Simha, 2002)





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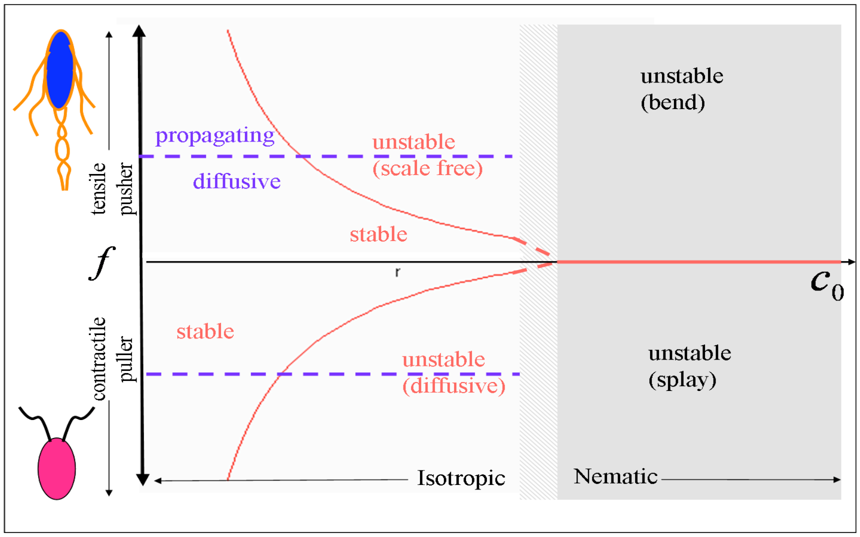

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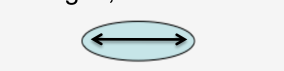
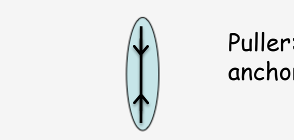
Conclusions

- Derivation of continuum theory from simple physical models yields unified description of many noneq. phenomena
- No physical mechanism for bulk polar order yet
- Insight into physical origin of emergent behavior in active systems and classification of such behavior

A future direction: incorporate the effect of boundaries (method of images, cf. Berke et al, 2008)



pusher: parallel anchoring



Puller: normal anchoring

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