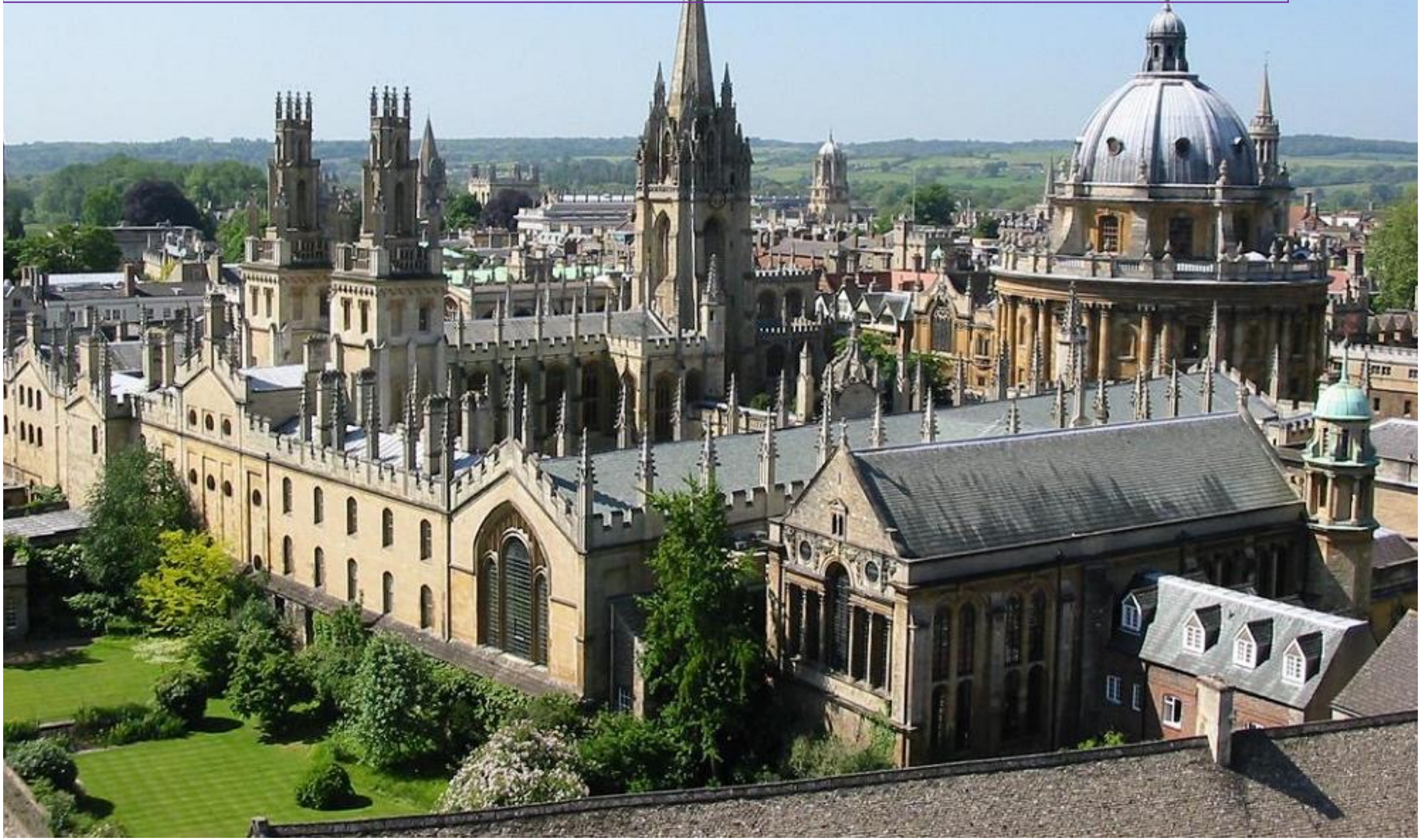
Active Matter Models of Mechanobiology

Julia Yeomans
University of Oxford



1. Introduction

2. Active turbulence: the basics

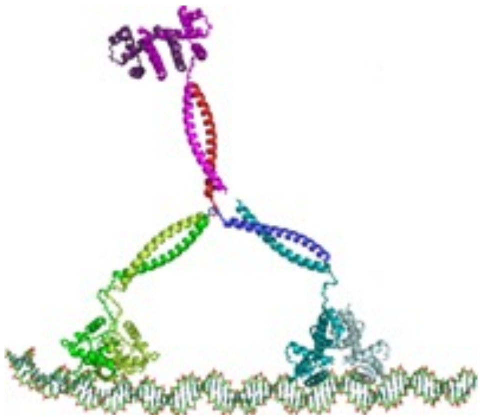
- Background 1: Swimming at low Re
- Background 2: nematic liquid crystals
- Active stress and active instabilities
- Active topological defects
- P. Mirabilis spreading
- 3D

3. Active turbulence: details (other instabilities, confinement)

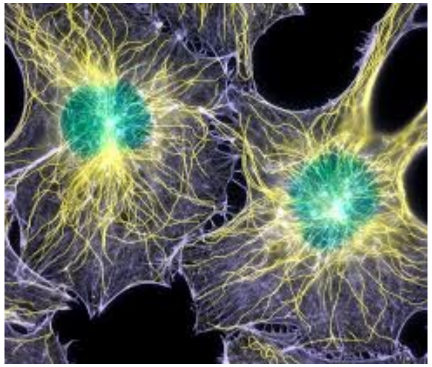
4. Mechanobiology

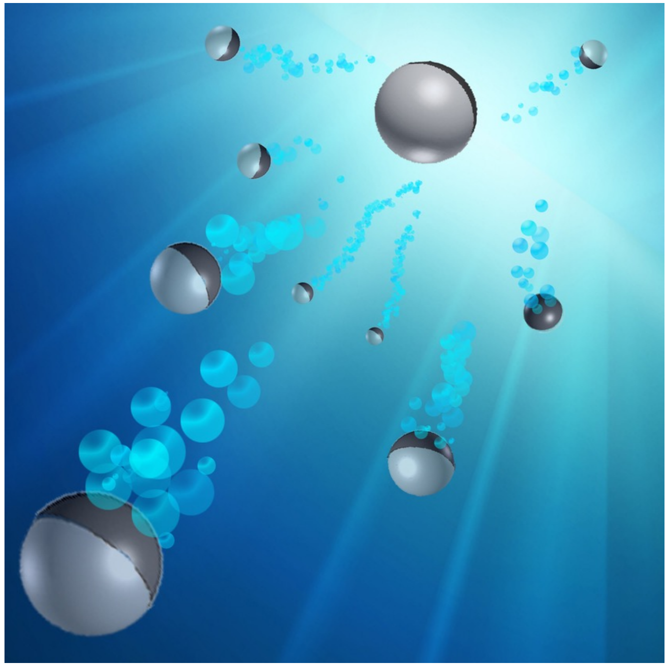
Active matter:
takes energy from the surroundings on a single particle level
remains out of thermodynamic equilibrium

molecular motors



cells



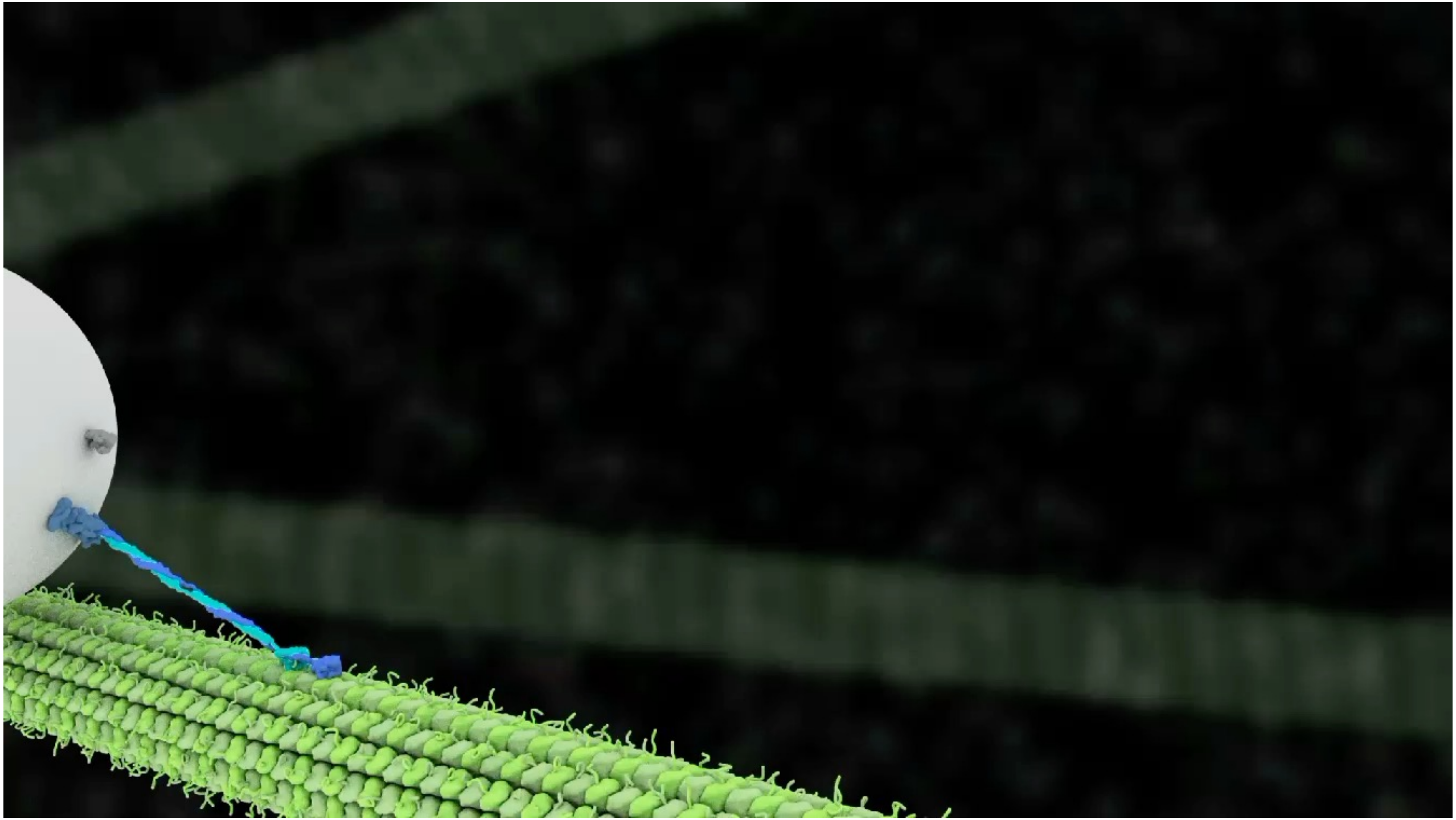


active colloids

microswimmers

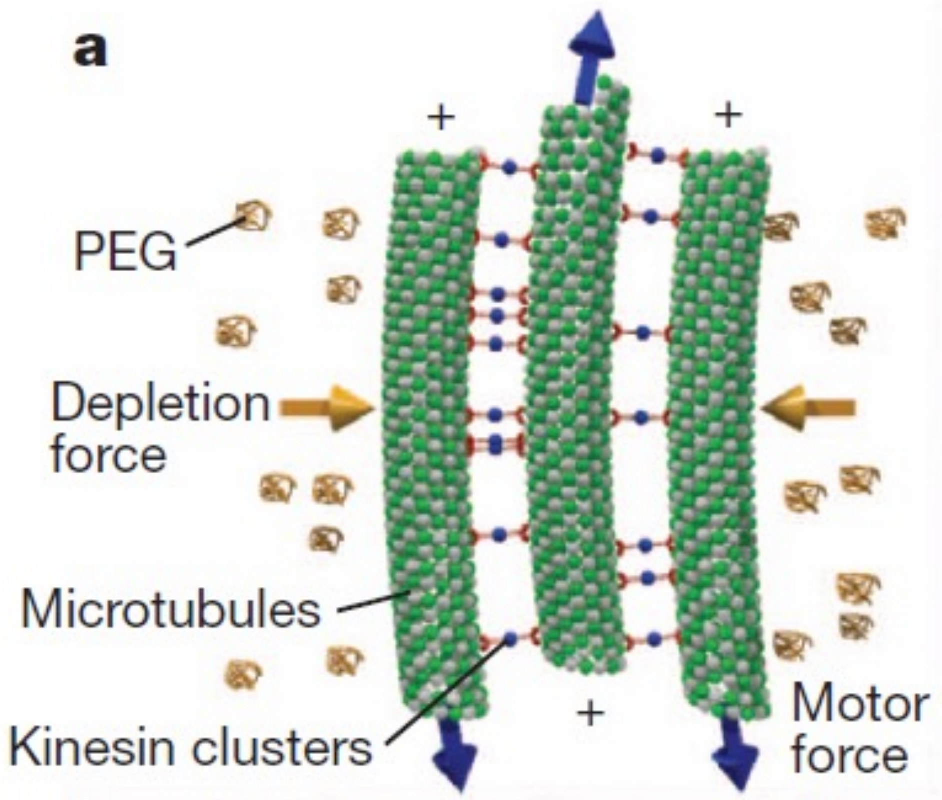
animals

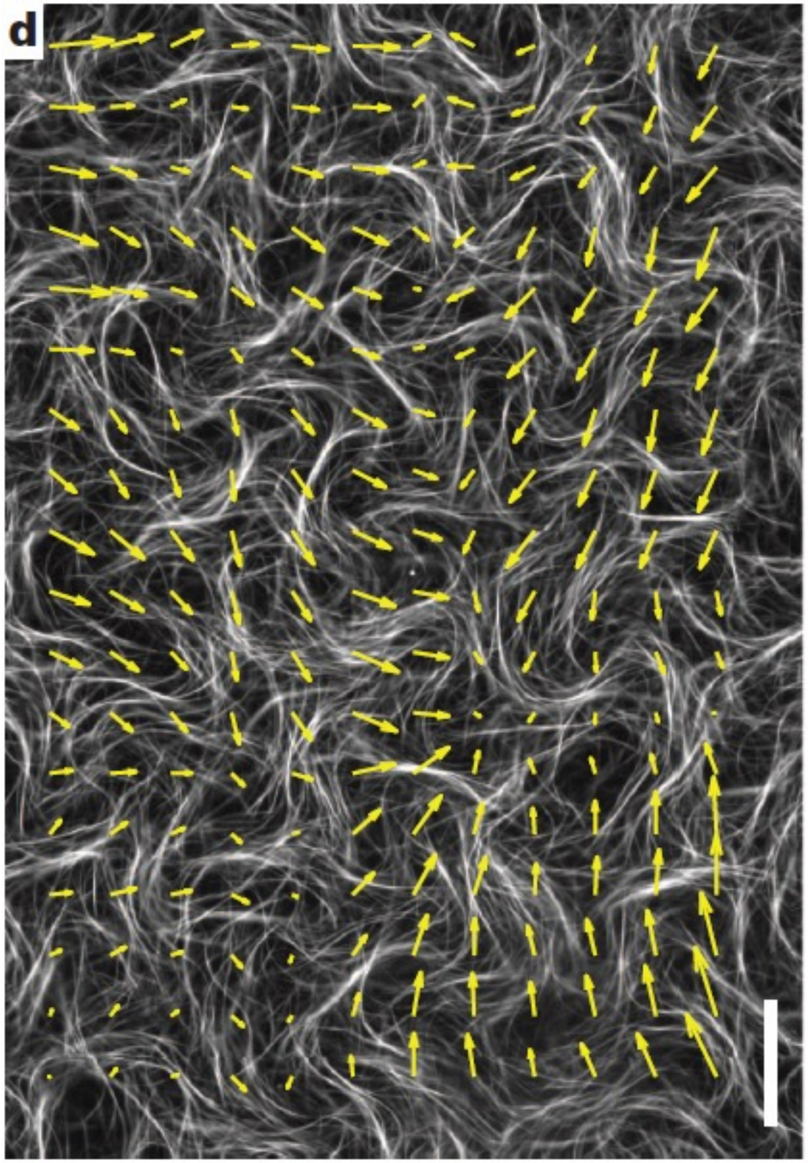
Molecular motors (kinesin)



Erik Schäffer Lab
Animation by Janet Iwasa

Microtubule-motor protein mixtures



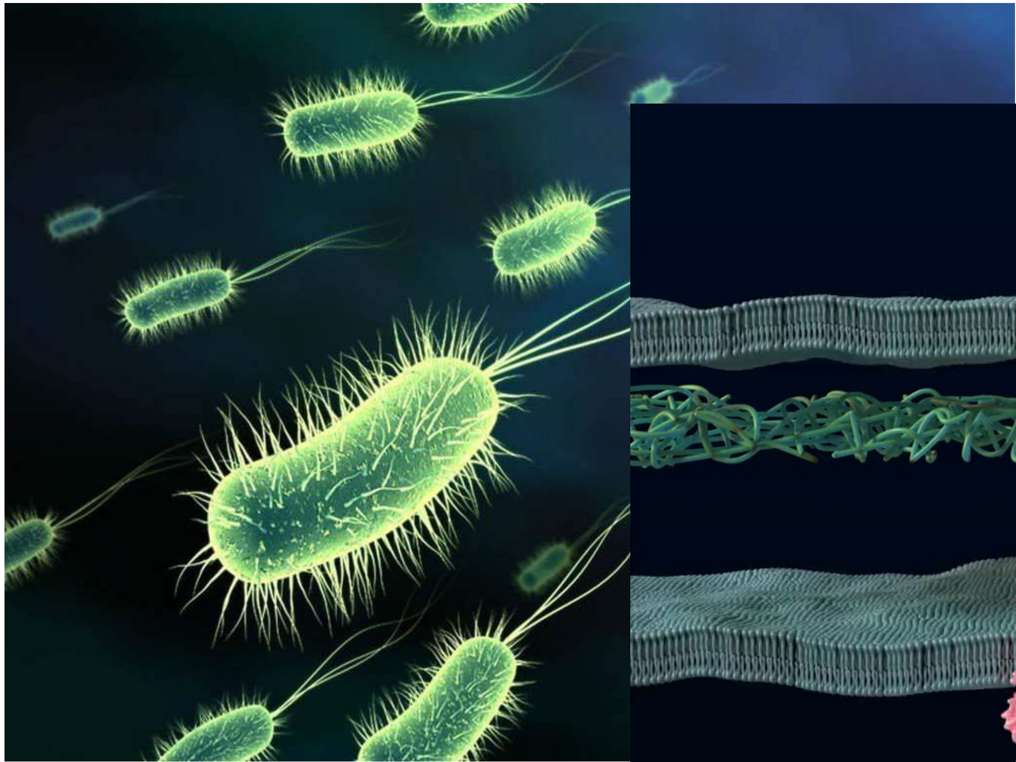


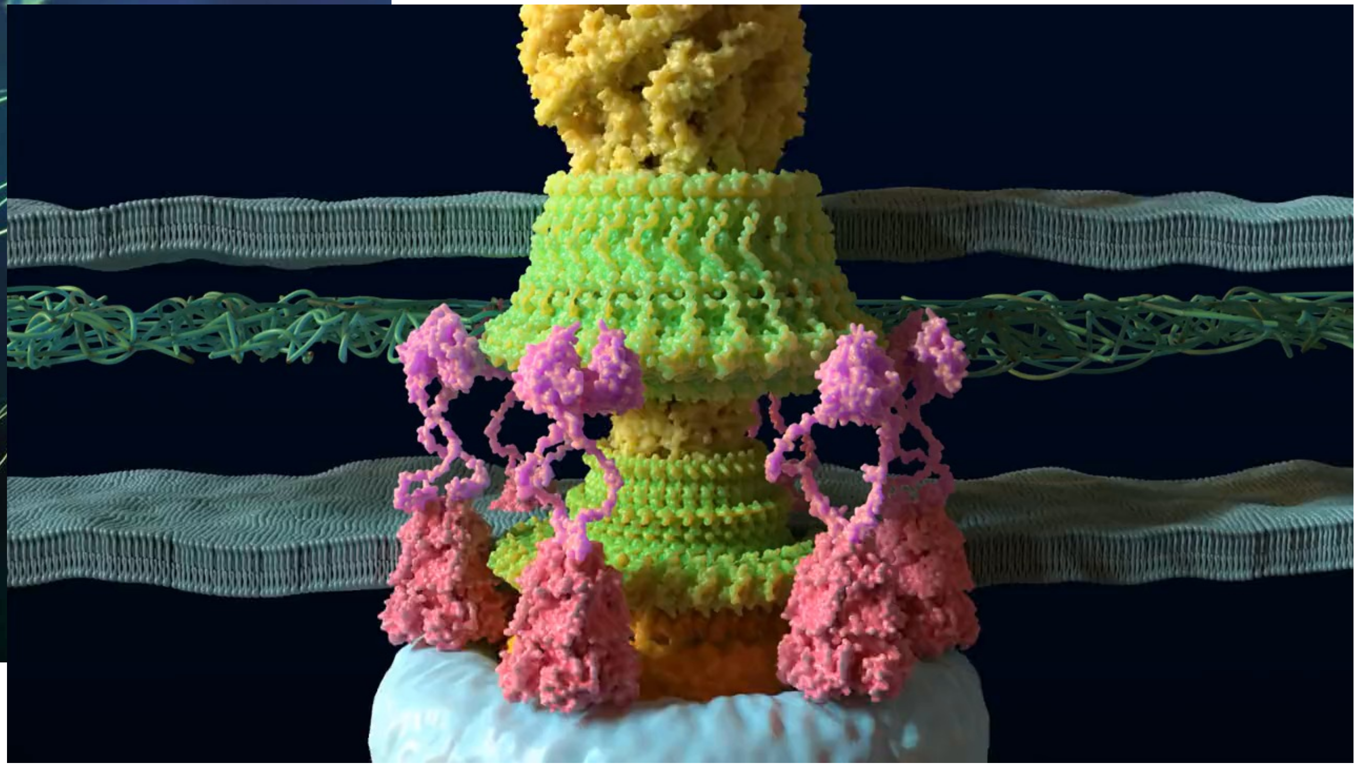
Sanchez, Chen, DeCamp, Heymann, Dogic, Nature 2012

Microtubule-motor protein mixtures mixtures

Francesc Sagues
Pau Guillamat
Jordi Ignes-Mullol

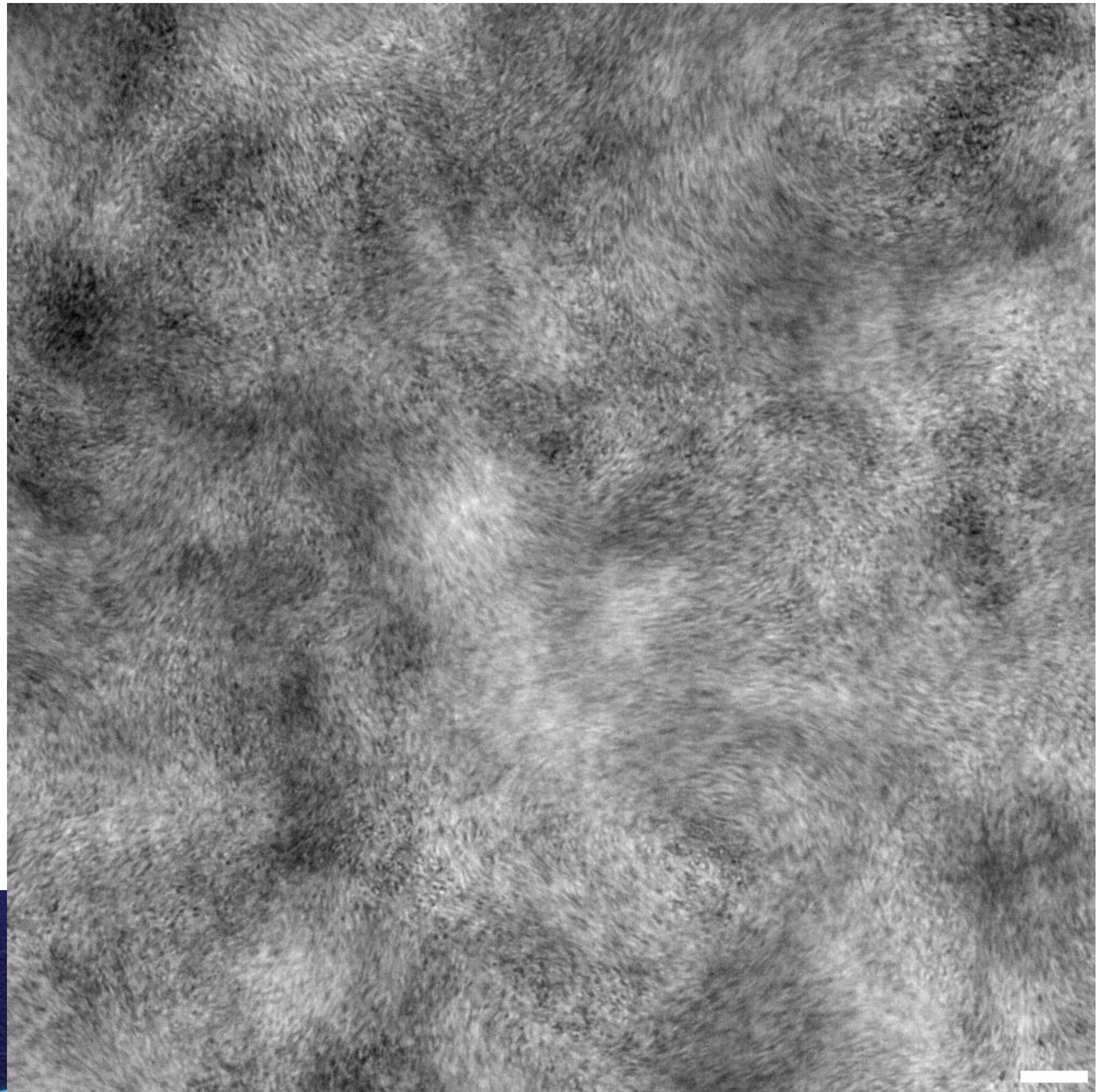
Bacteria

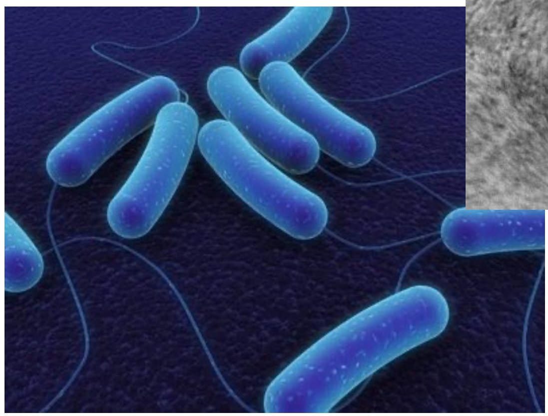




Animation by Matthew Clark, University of Oxford
Richard Berry group

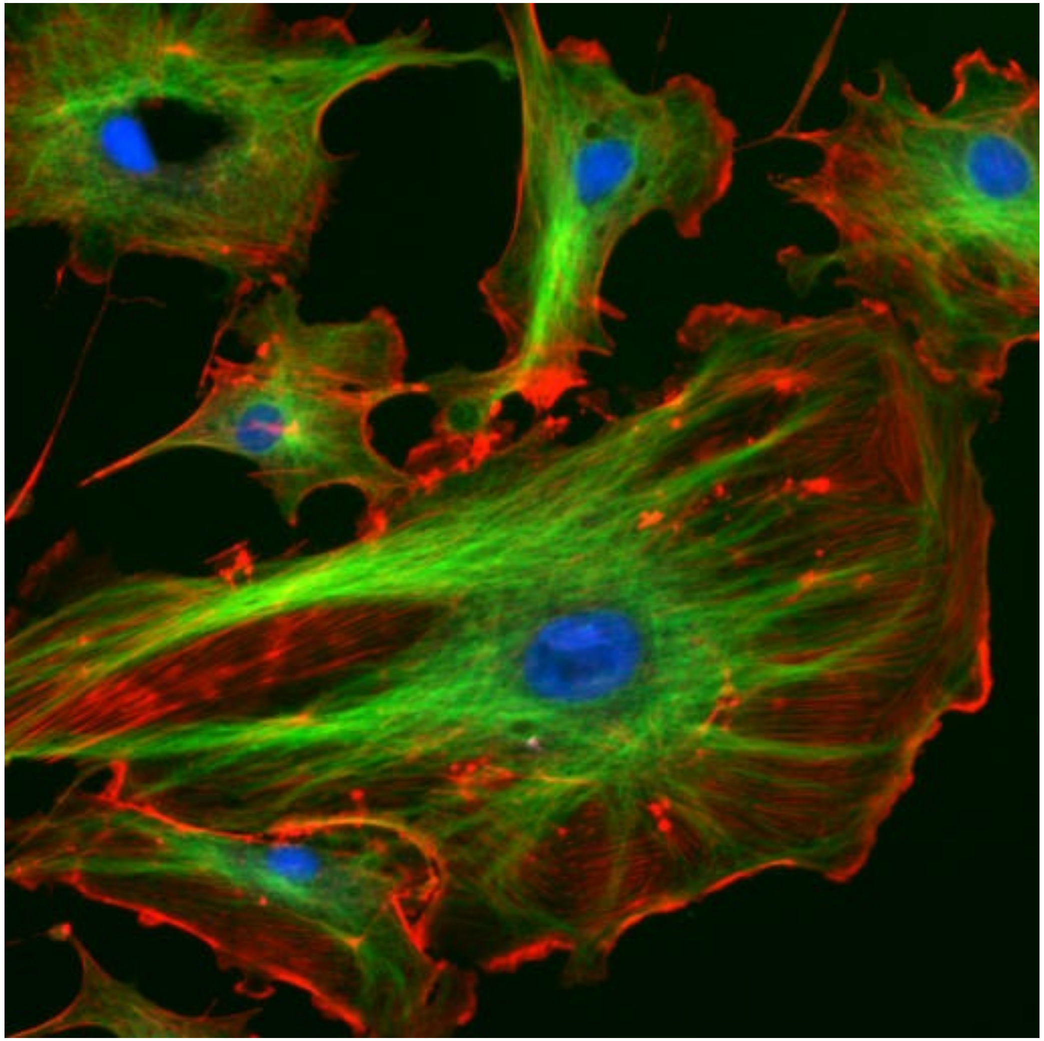
Active turbulence: bacteria





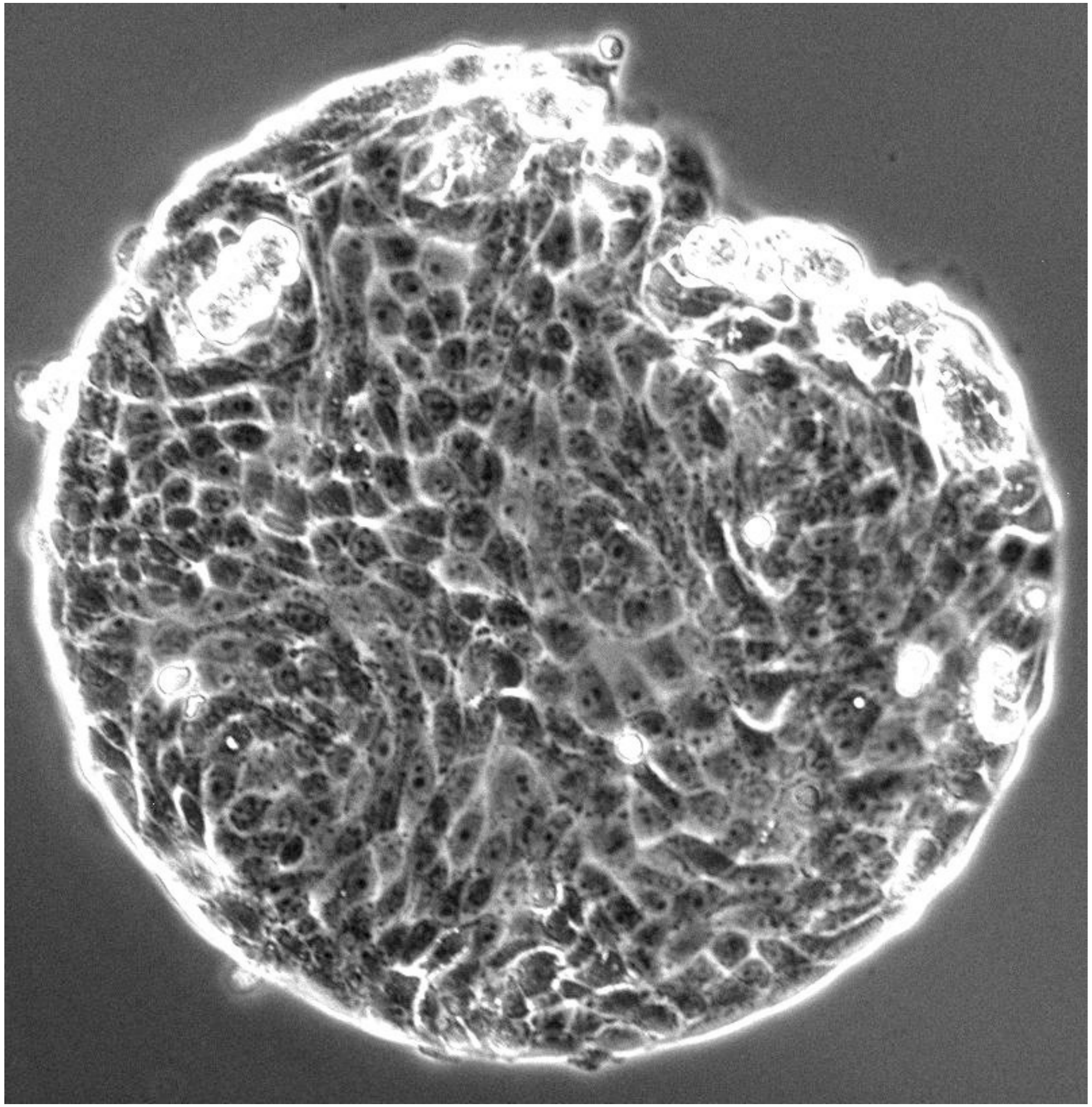
Dense suspension of microswimmers
Yi Peng, Zhengyang Liu & Xiang Chen
Science Advances 7, 2021

Eukarytic cells



Ladoux and Nicholas Rep Prog Phys 2012

Eukaryotic cells: active turbulence

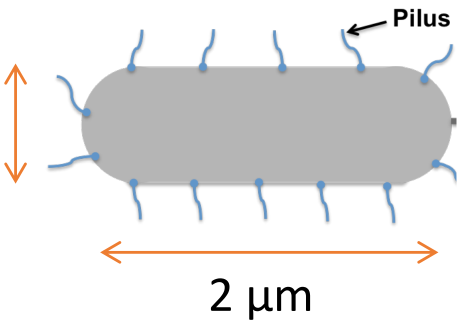


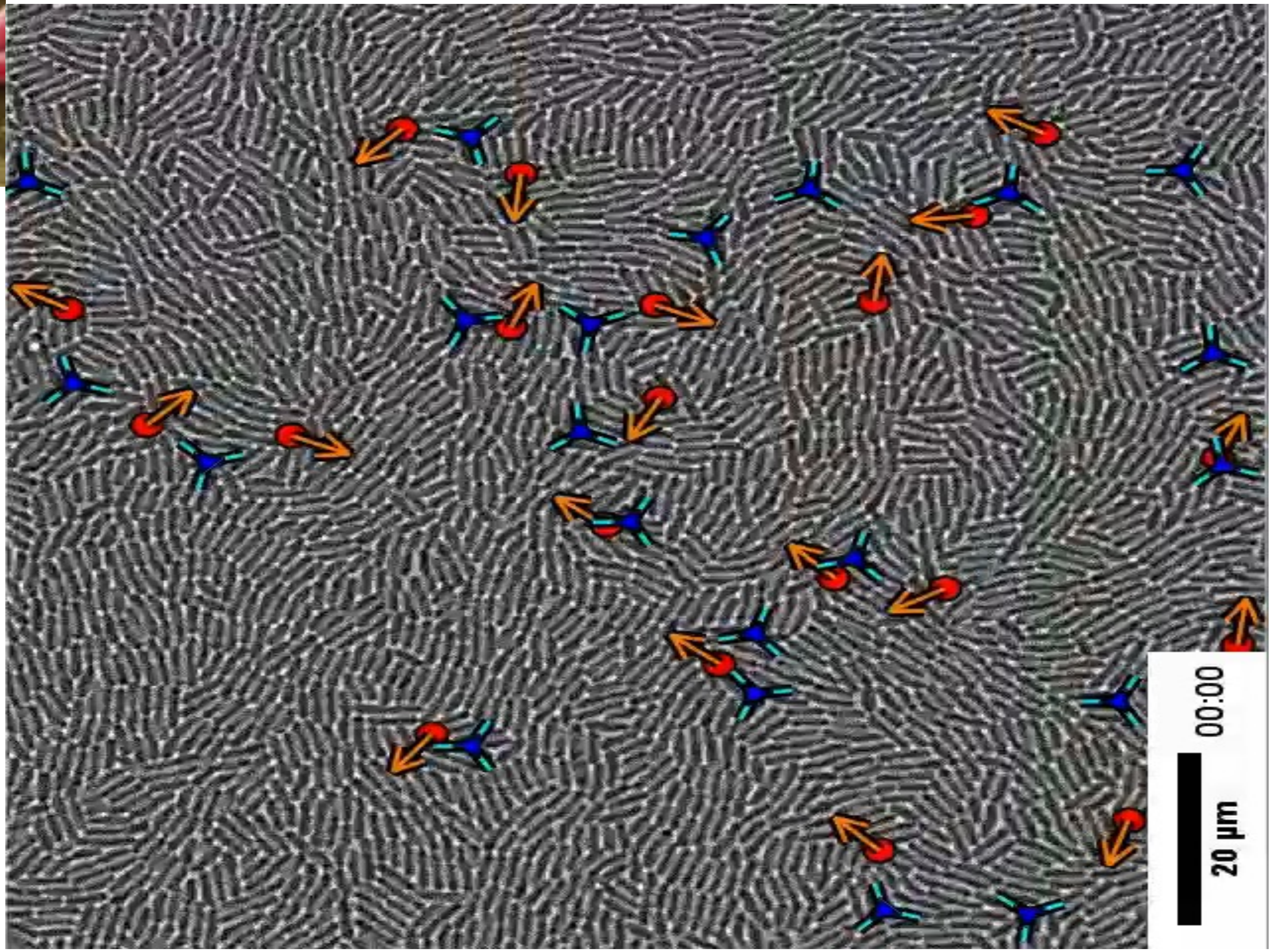
Bacteria: active turbulence

Pseudomonas aeuriginosa

twitching motility using Type IV Pili

reversals





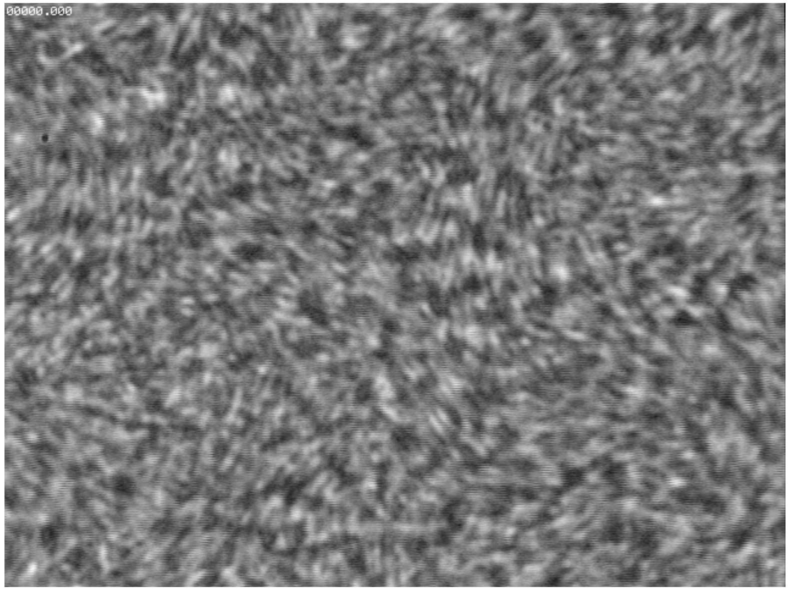
Active matter

Meant to be out of thermodynamic equilibrium

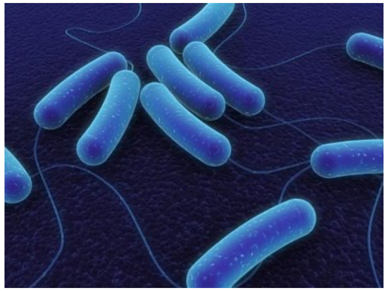
Why is it interesting?

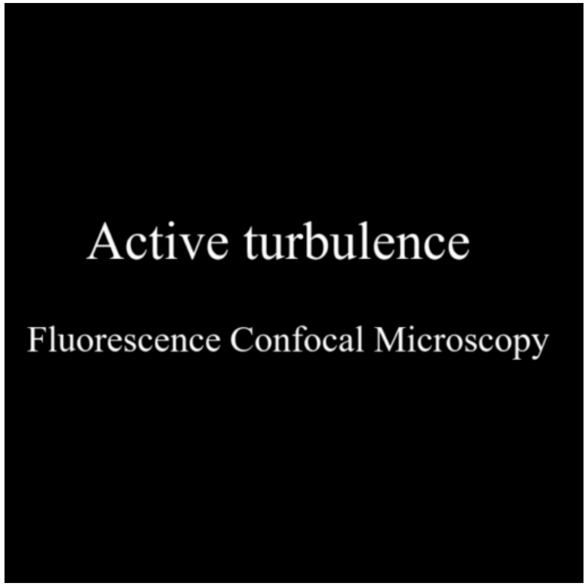
- to understand biological systems: biomechanics and self-assembly
- To create new types of micro-engines
  Internally-driven microchannel flow
- As examples of non-equilibrium statistical physics

Active turbulence



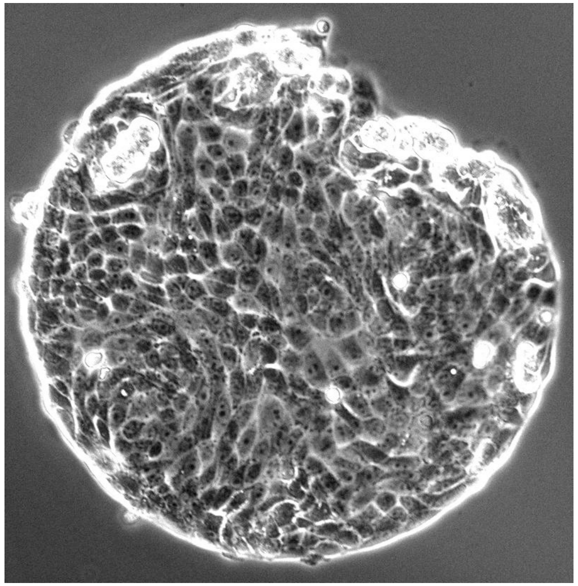
Dense suspension of microswimmers





Microtubules driven by motor proteins

Confluent cell layer



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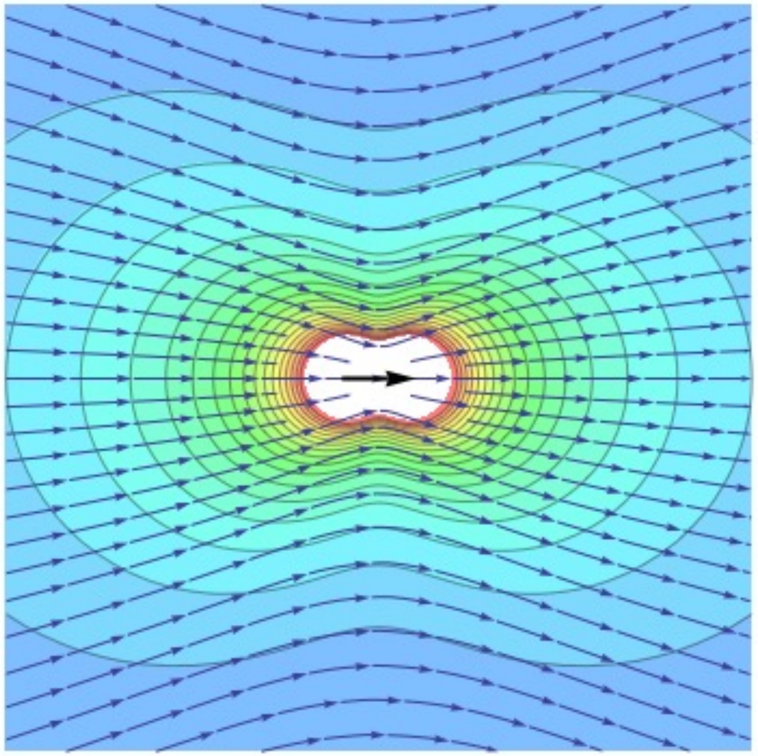
4. Mechanobiology

Stokes equations

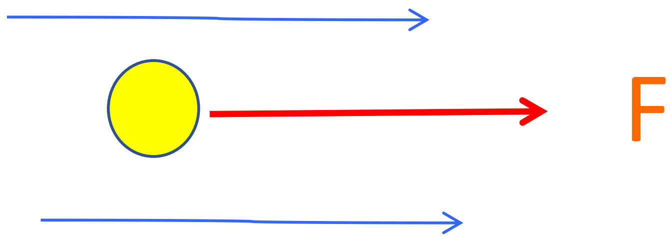
$$\nabla p = \mu \nabla^2 \mathbf{v} + \mathbf{f}$$



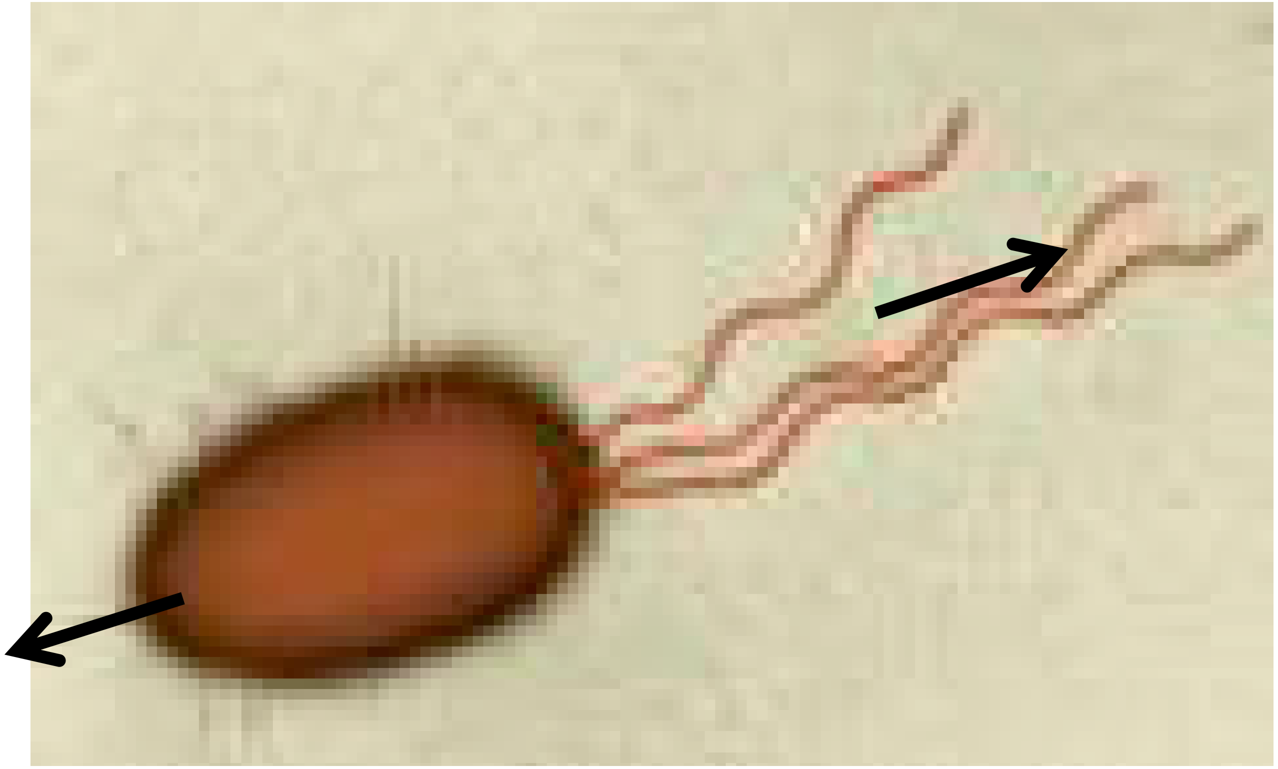
Stokeslet

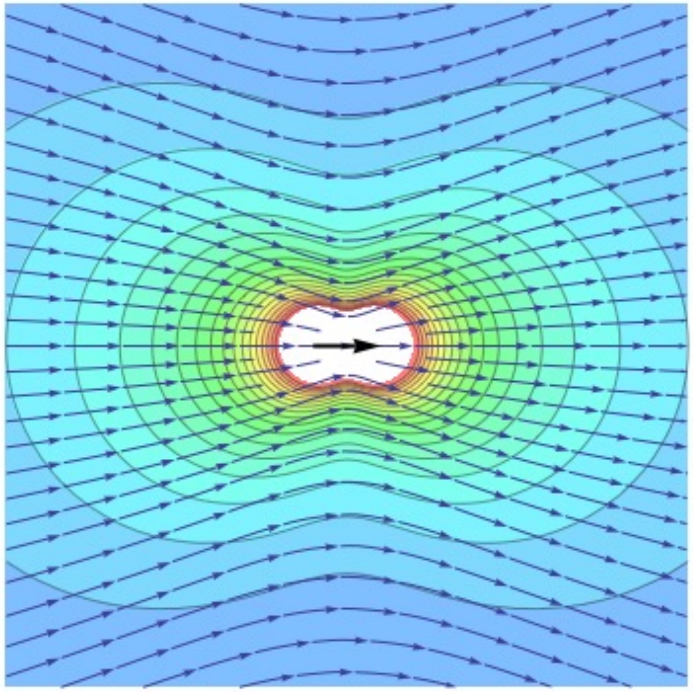
$$\mathbf{v} = \frac{\mathbf{f}}{8\pi\mu} \cdot \left(\frac{\mathbf{I}}{r} + \frac{\mathbf{rr}}{r^3} \right)$$

$$v_i(\mathbf{r}) = \frac{f_j}{8\pi\mu} \left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3} \right)$$

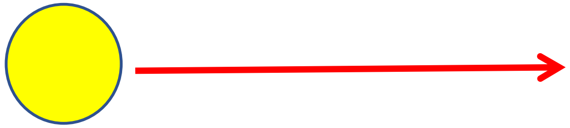


Swimmers have no net external forces or torques acting on them.
So, to leading order, the far flow field ~ $1/r^2$



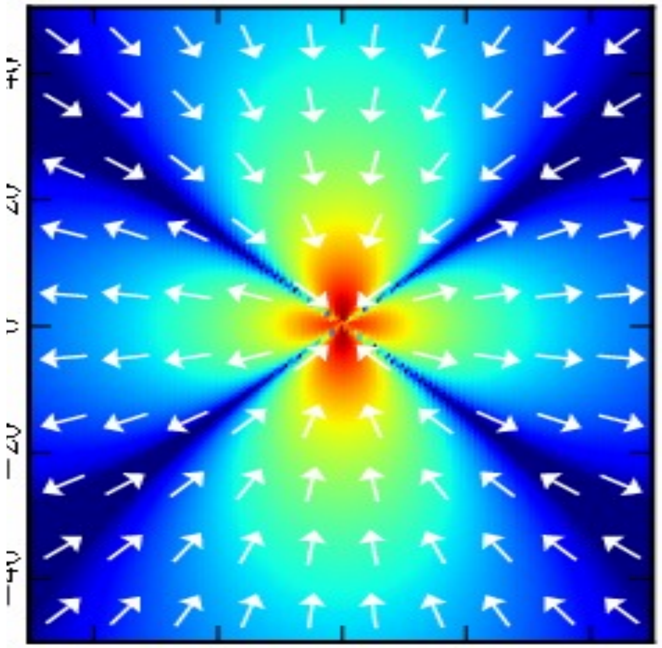


colloid flow field

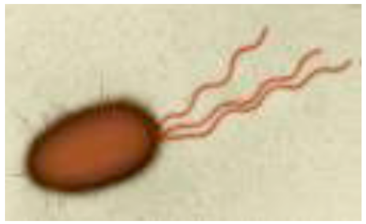


F

$$\mathbf{v} = \frac{\mathbf{f}}{8\pi\mu} \cdot \left(\frac{\mathbf{I}}{r} + \frac{\mathbf{rr}}{r^3} \right)$$



F

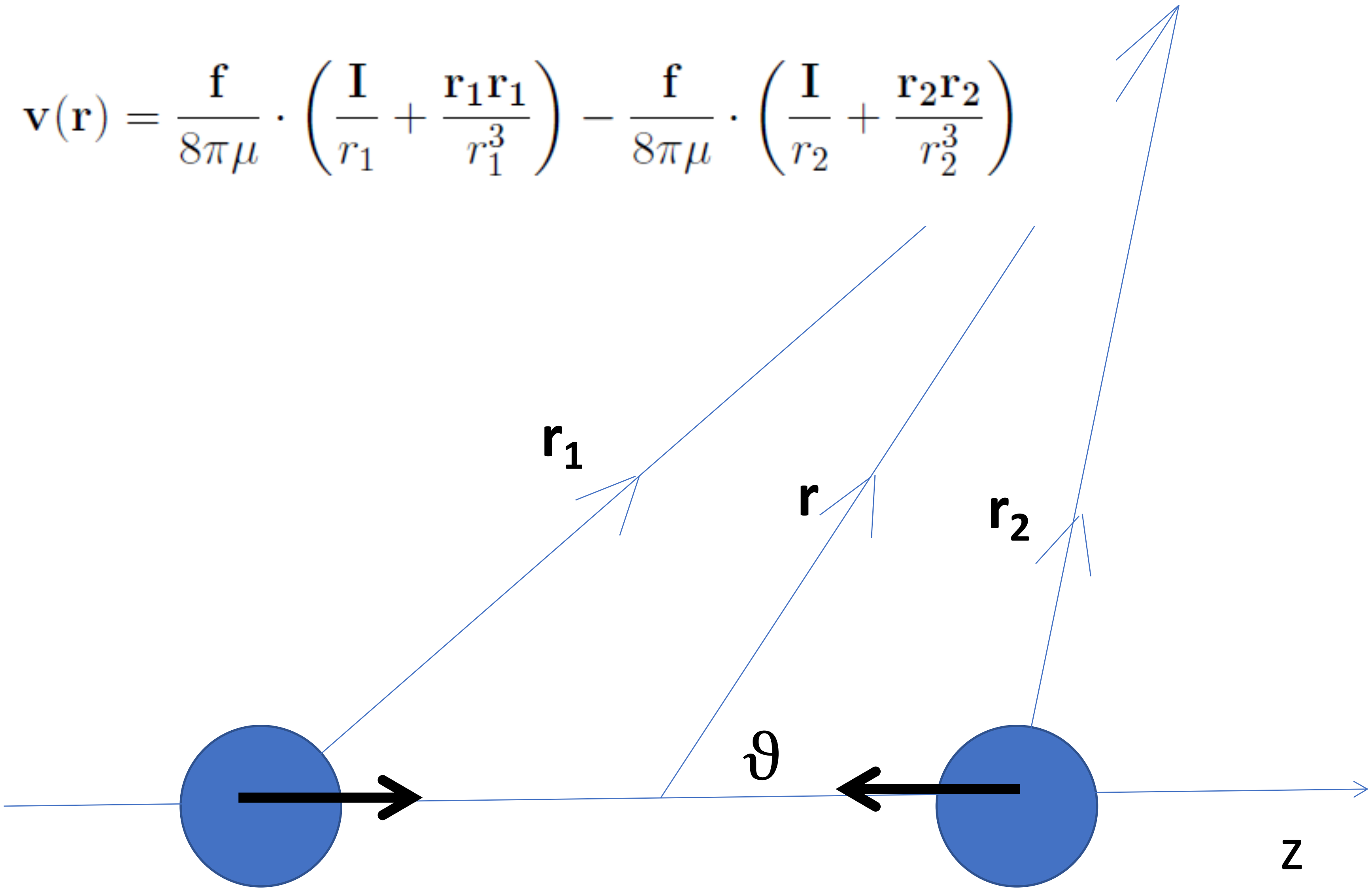


F

swimmer flow field

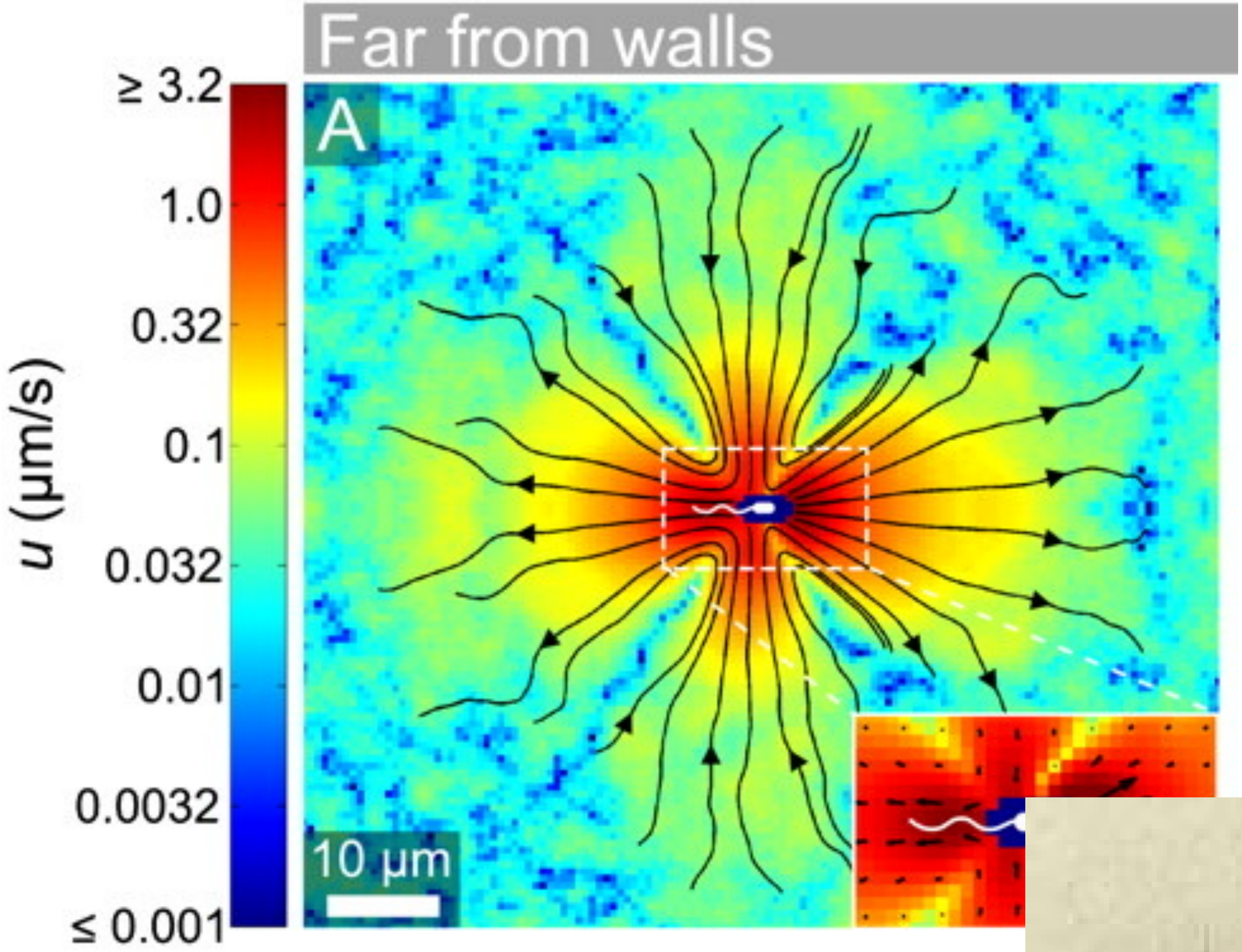
nematic symmetry

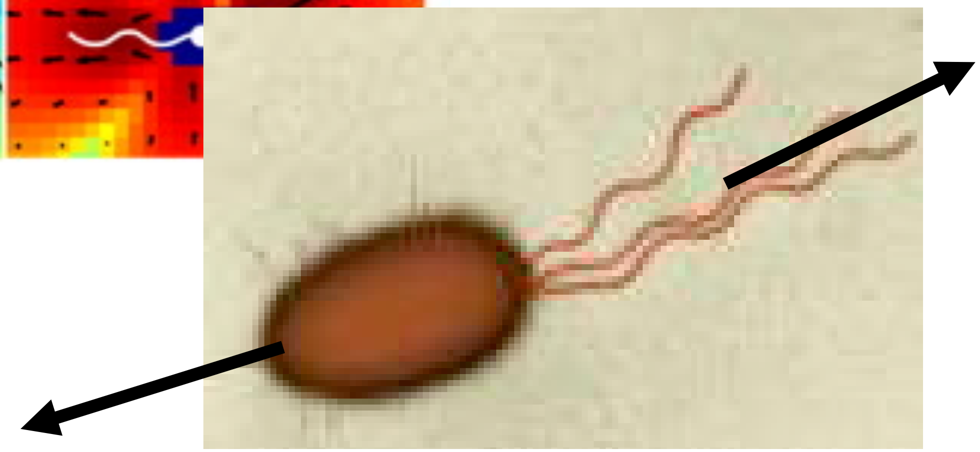
$$\mathbf{v}(\mathbf{r}) = \frac{\mathbf{f}}{8\pi\mu}\cdot\left(\frac{\mathbf{I}}{r_1}+\frac{\mathbf{r}_1\mathbf{r}_1}{r_1^3}\right) - \frac{\mathbf{f}}{8\pi\mu}\cdot\left(\frac{\mathbf{I}}{r_2}+\frac{\mathbf{r}_2\mathbf{r}_2}{r_2^3}\right)$$



$$v_r = \frac{f}{4\pi\mu}\,\frac{L}{r^2}\,\left(3\cos^2\theta - 1\right)$$

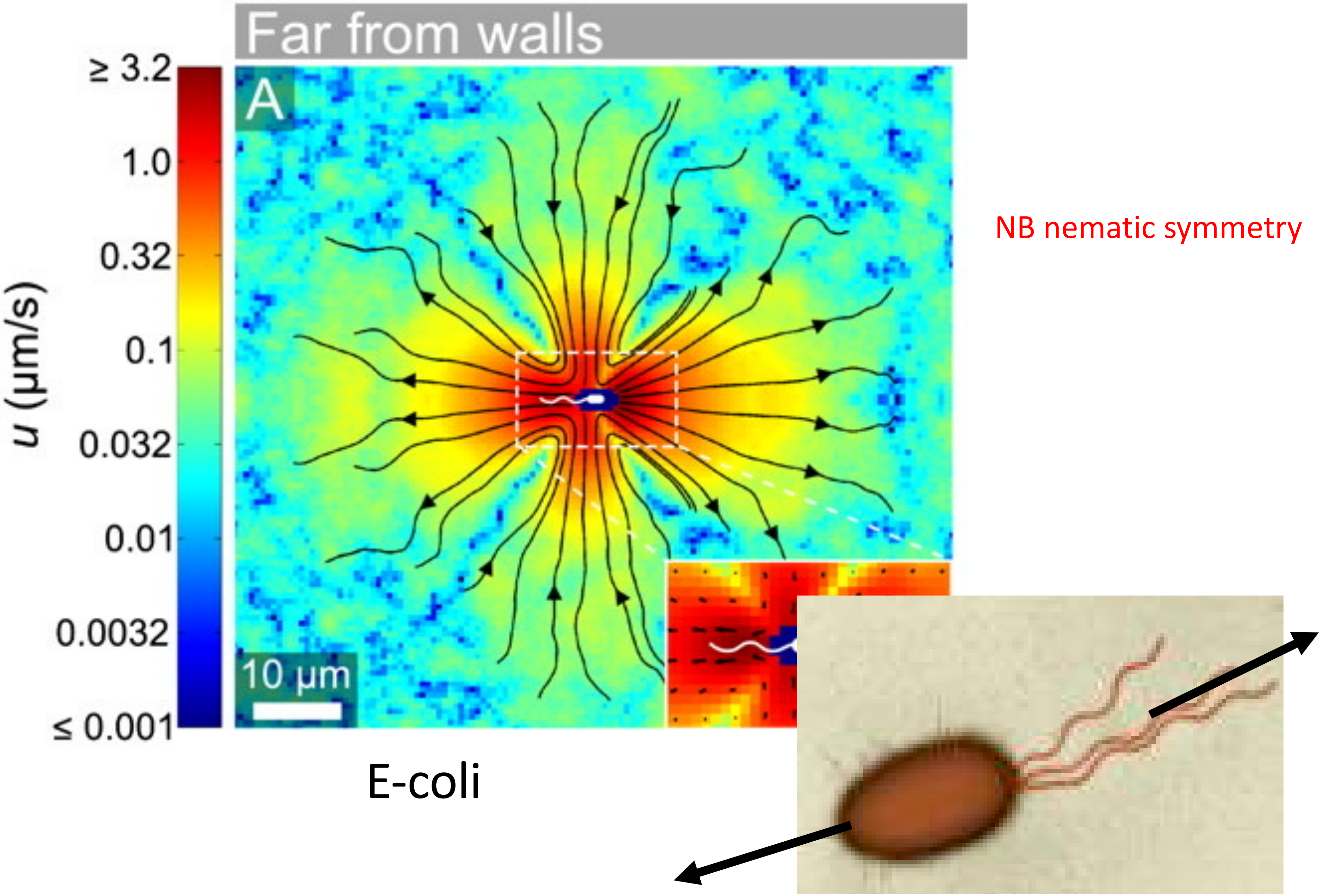
Swimmers have dipolar far flow fields because they have no net force acting on them





E-coli

Goldstein group, Cambridge



NB nematic symmetry

E-coli

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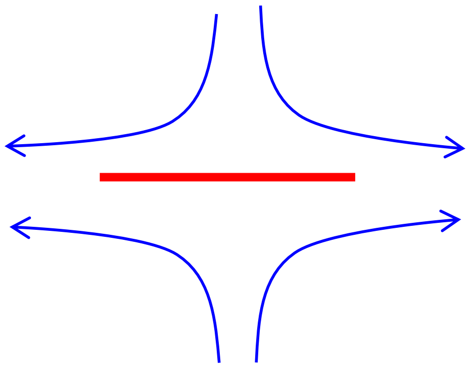
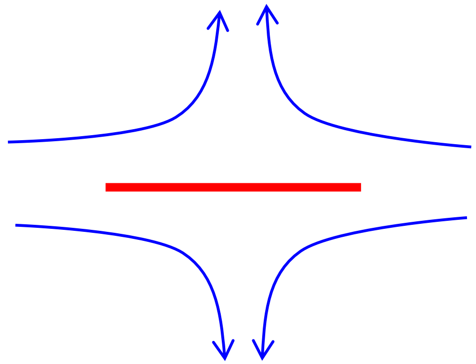


Extensile
pusher



Contractile
puller

Nematic ordering

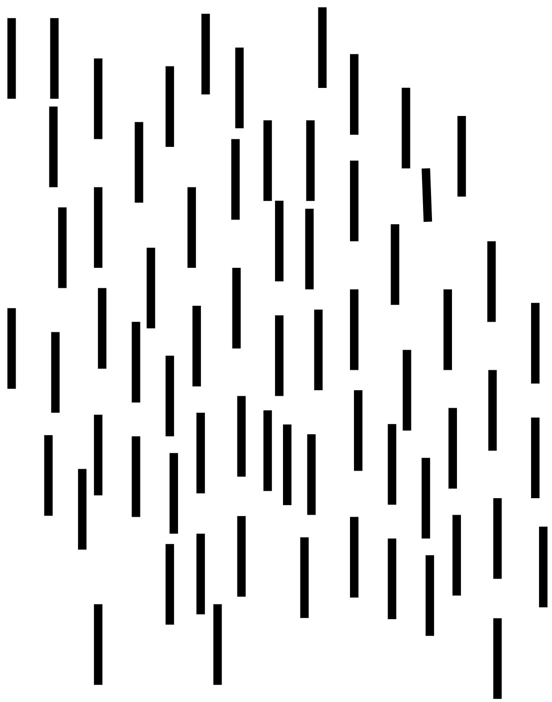
ordered nematic

$$Q_{ij} = \frac{3}{2}\langle n_i n_j - \frac{\delta_{ij}}{3}\rangle$$

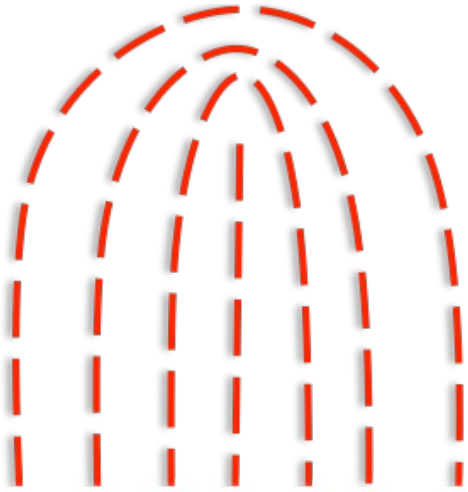
Small and unimportant defects

localised distortion
easy to restore order

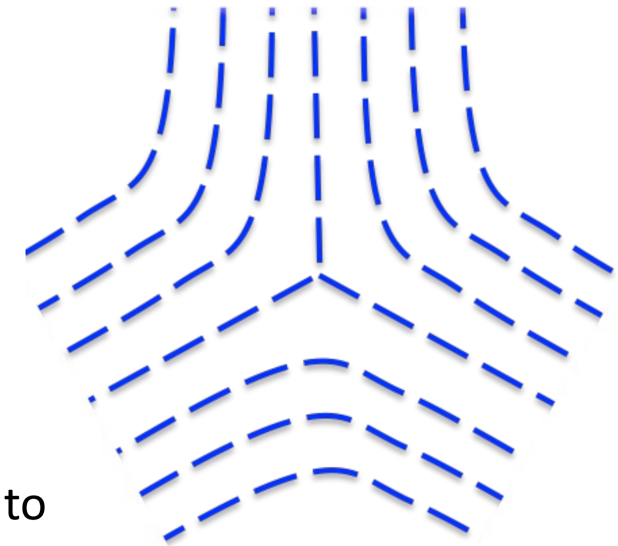
Topological defects



$$m = +\frac{1}{2}$$



$$m = -\frac{1}{2}$$



defects annihilate in pairs to give perfect nematic order

Continuum equations of liquid crystal hydrodynamics

$$(\partial_t + u_k\partial_k)Q_{ij} - S_{ij} = \Gamma H_{ij}$$

$$S_{ij} = (\lambda E_{ik} + \Omega_{ik})(Q_{kj} + \delta_{kj}/3) +$$

$$(Q_{ik} + \delta_{ik}/3)(\lambda E_{kj} - \Omega_{kj}) - 2\lambda(Q_{ij} + \delta_{ij}/3)(Q_{kl}\partial_k u_l)$$

$$E_{ij} = (\partial_i u_j + \partial_j u_i)/2$$

$$\Omega_{ij} = (\partial_j u_i - \partial_i u_j)/2$$

$$H_{ij} = -\delta\mathcal{F}/\delta Q_{ij} + (\delta_{ij}/3)\mathrm{Tr}(\delta\mathcal{F}/\delta Q_{kl})$$

$$\mathcal{F} = K(\partial_k Q_{ij})^2/2 + AQ_{ij}Q_{ji}/2 + BQ_{ij}Q_{jk}Q_{ki}/3 + C(Q_{ij}Q_{ji})^2/4$$

Continuum equations of liquid crystal hydrodynamics

$$\rho(\partial_t + u_k\partial_k)u_i = \partial_j\Pi_{ij}$$

$$\Pi_{ij}^{viscous} = 2\mu E_{ij}$$

$$\Pi_{ij}^{passive} = -P\delta_{ij} + 2\lambda(Q_{ij} + \delta_{ij}/3)(Q_{kl}H_{lk}) - \lambda H_{ik}(Q_{kj} + \delta_{kj}/3)$$
$$-\lambda(Q_{ik} + \delta_{ik}/3)H_{kj} - \partial_i Q_{kl}\frac{\delta\mathcal{F}}{\delta\partial_j Q_{lk}} + Q_{ik}H_{kj} - H_{ik}Q_{kj}$$

Tumbling parameter

Continuum equations of liquid crystal hydrodynamics

$$(\partial_t + u_k \partial_k) Q_{ij} - S_{ij} = \Gamma H_{ij}$$

couples nematic order and shear flows

relaxation to minimum of Landau-de Gennes free energy

$$\rho(\partial_t + u_k \partial_k) u_i = \partial_j \Pi_{ij}$$

viscous + elastic

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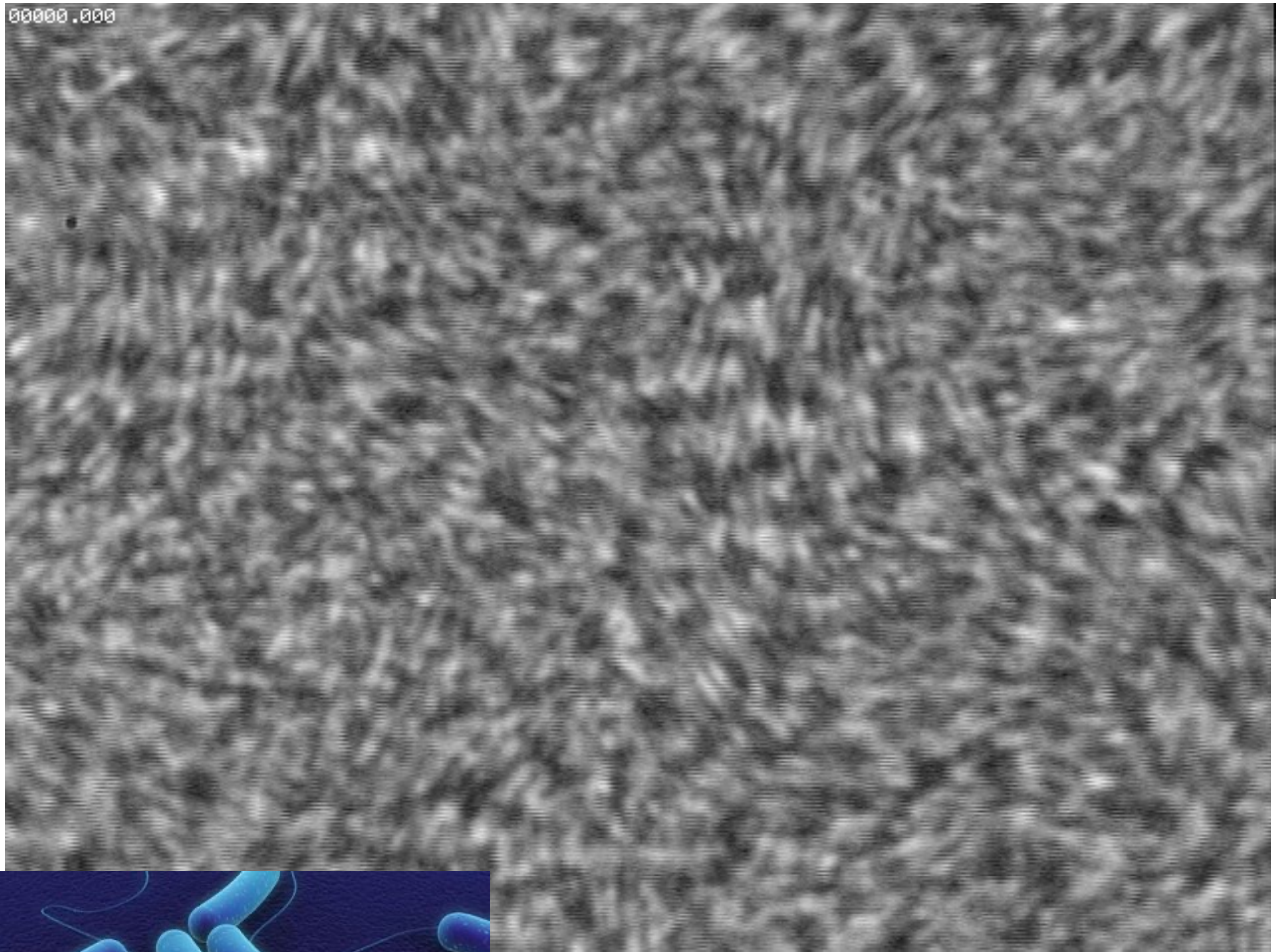
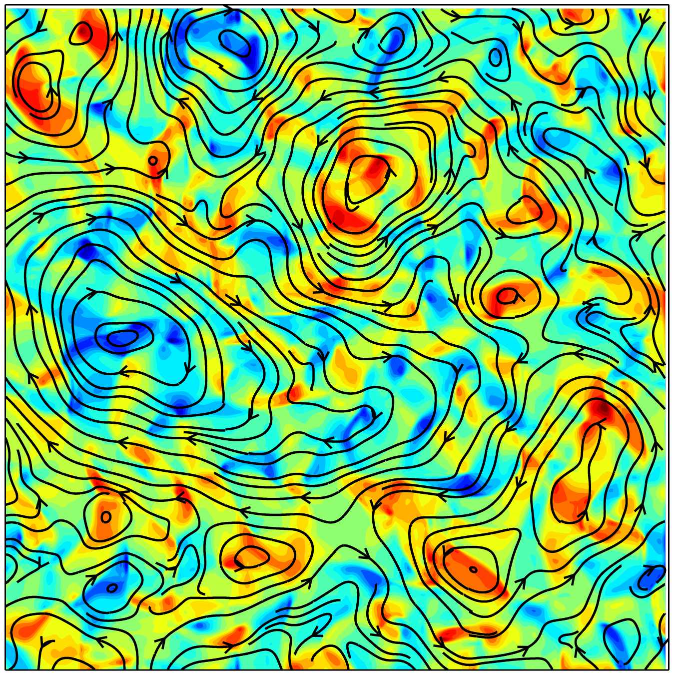
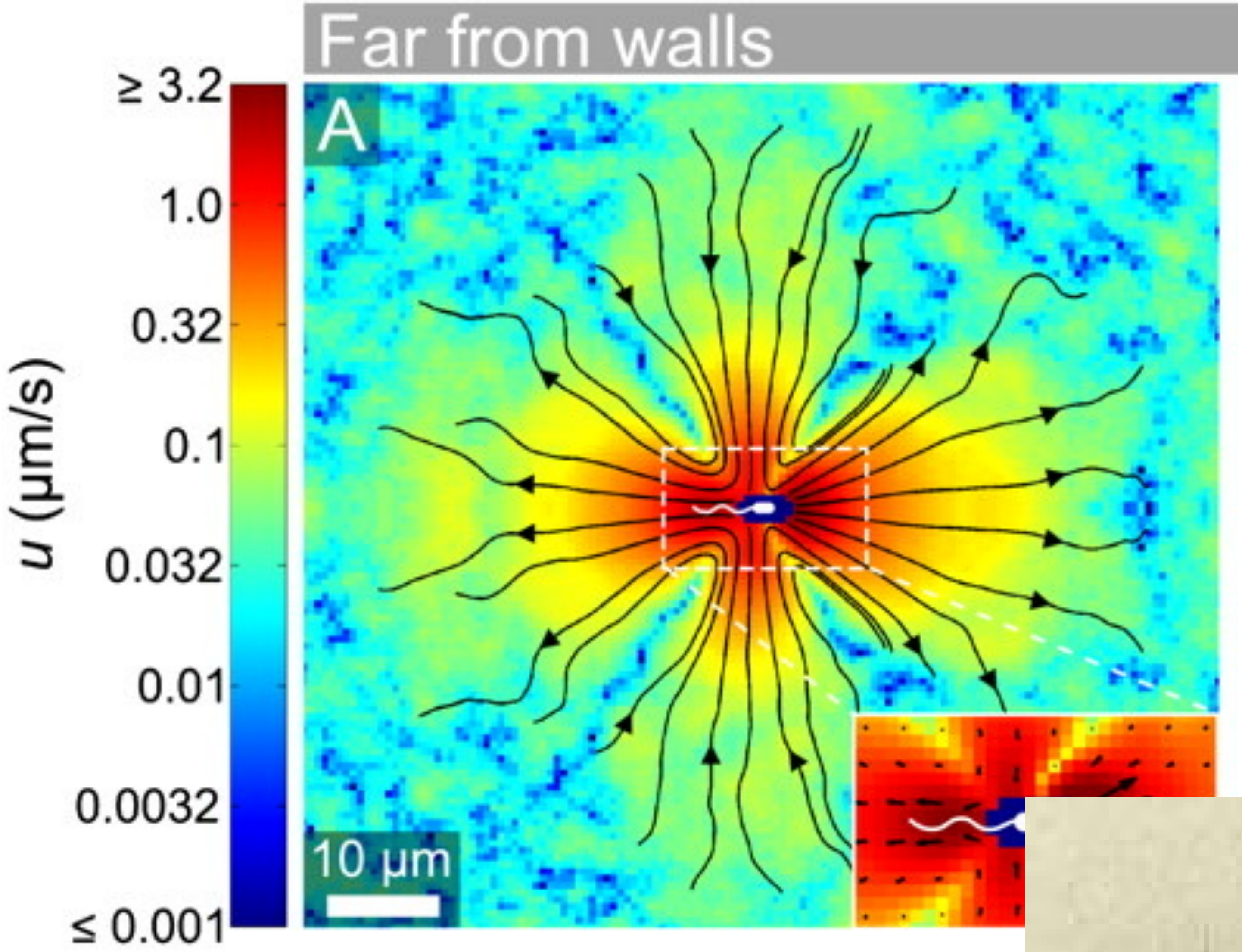
Active turbulence



Dense suspension of microswimmers

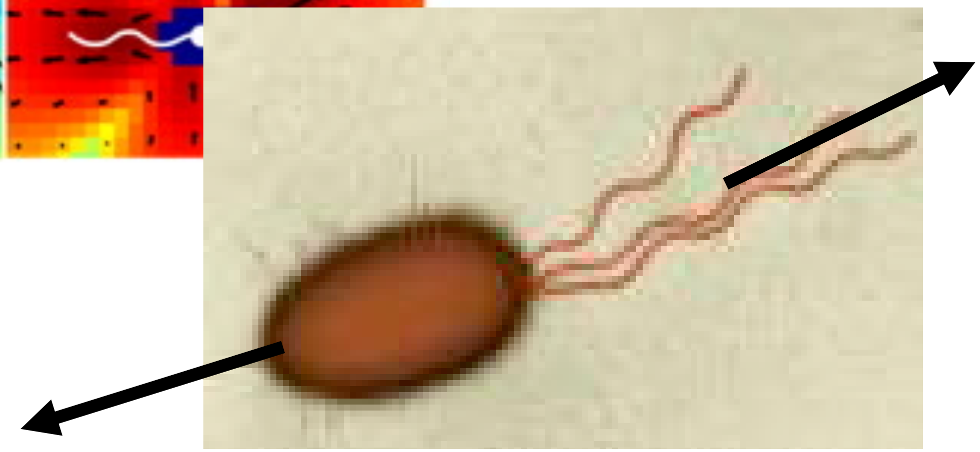
Vorticity field





NB nematic symmetry

E-coli



Goldstein group, Cambridge

Continuum equations of liquid crystal hydrodynamics

$$(\partial_t + u_k\partial_k)Q_{ij} - S_{ij} = \Gamma H_{ij}$$

couples nematic order and shear flows

relaxation to minimum of Landau-de Gennes free energy

$$\rho(\partial_t + u_k\partial_k)u_i = \partial_j \Pi_{ij}$$

viscous + passive

Continuum equations of active liquid crystal hydrodynamics

$$(\partial_t + u_k \partial_k) Q_{ij} - S_{ij} = \Gamma H_{ij}$$

couples nematic order and shear flows

relaxation to minimum of Landau-de Gennes free energy

$$\rho(\partial_t + u_k \partial_k) u_i = \partial_j \Pi_{ij}$$

viscous + passive + active stress

$$\Pi_{ij}^{active} = -\zeta Q_{ij}$$

Active stress

$$\Pi_{ij}^{active} = -\zeta Q_{ij}$$

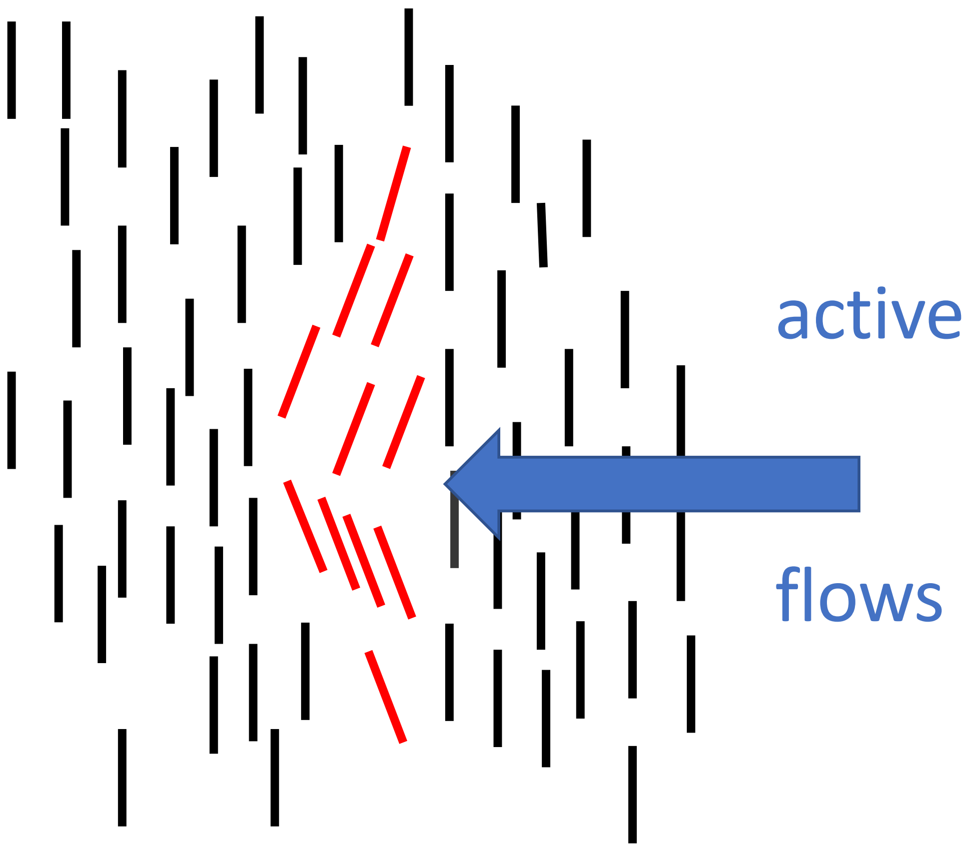
Gradients in the magnitude or direction of the nematic order induce flow.

$\zeta > 0$ extensile

Simha, Ramaswamy, 2001

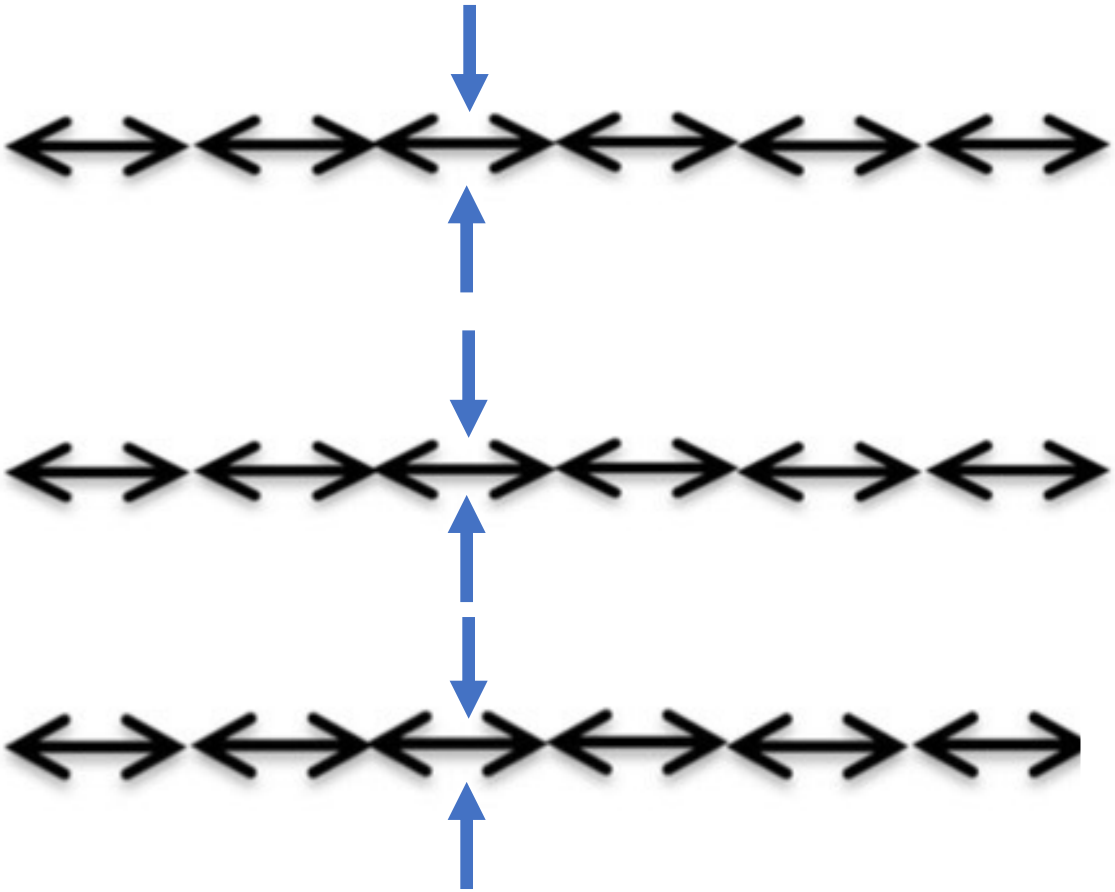
$\zeta < 0$ contractile

nematic ordering is unstable
to active forces

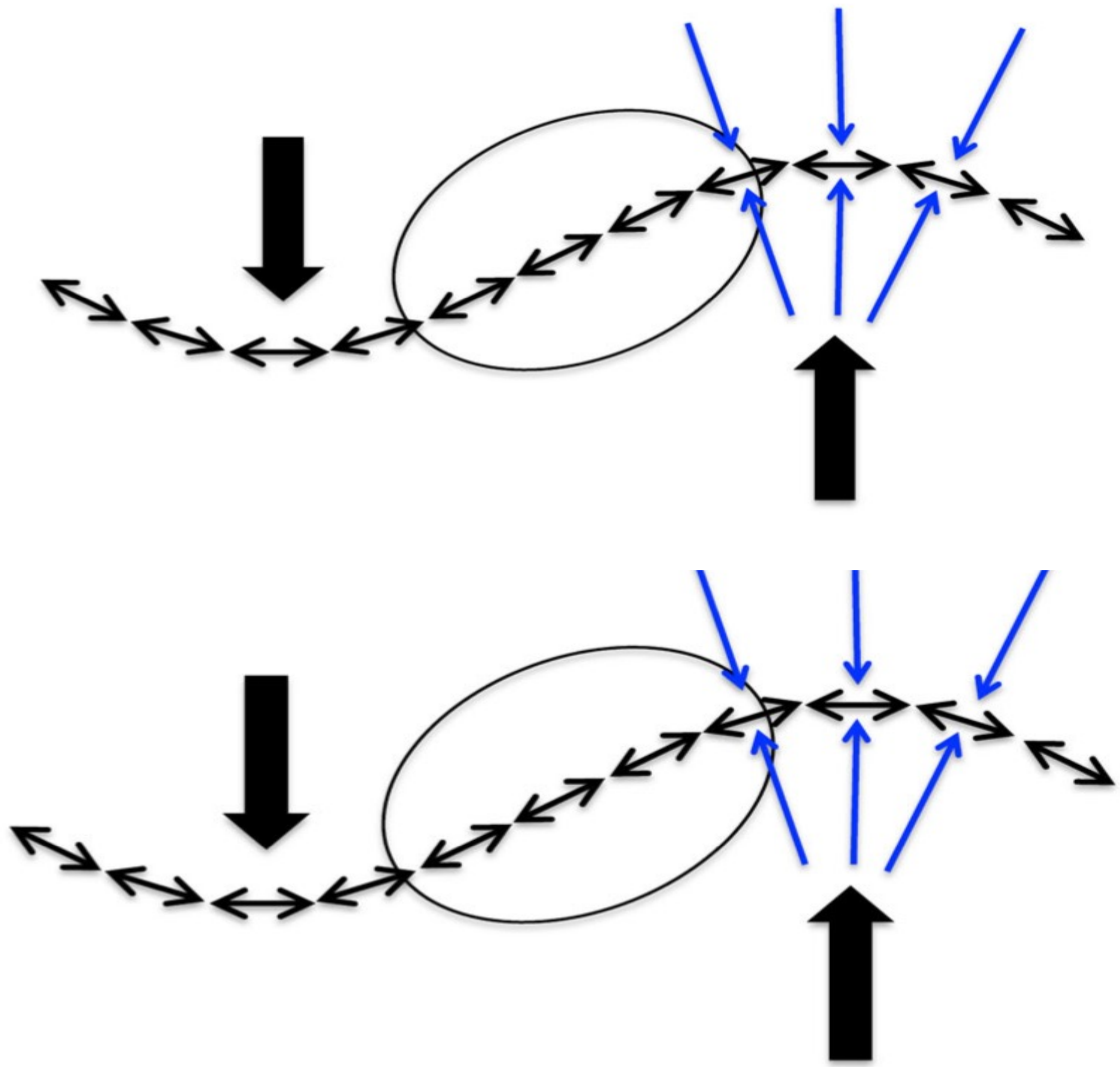


Instability 1

extensile   uniform nematic   no flow



extensile   bend instability => flow



active length scale

activity ζ (units: force/area)

elasticity K (units: force)

length scale $$\sqrt{K/\zeta}$$

Active stress => active turbulence

Active contribution to the stress $$-\zeta \mathbf{Q}$$

Gradients in the magnitude or direction of the order parameter induce flow.

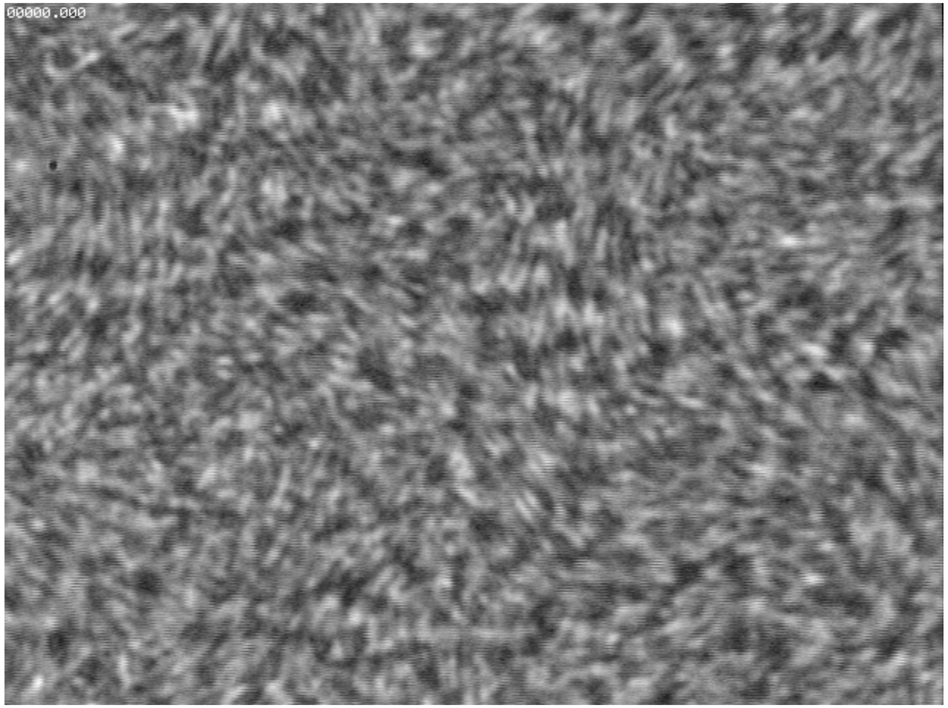
⇒

Linear stability analysis =>
nematic state is unstable to vortical flows

What happens instead is active turbulence

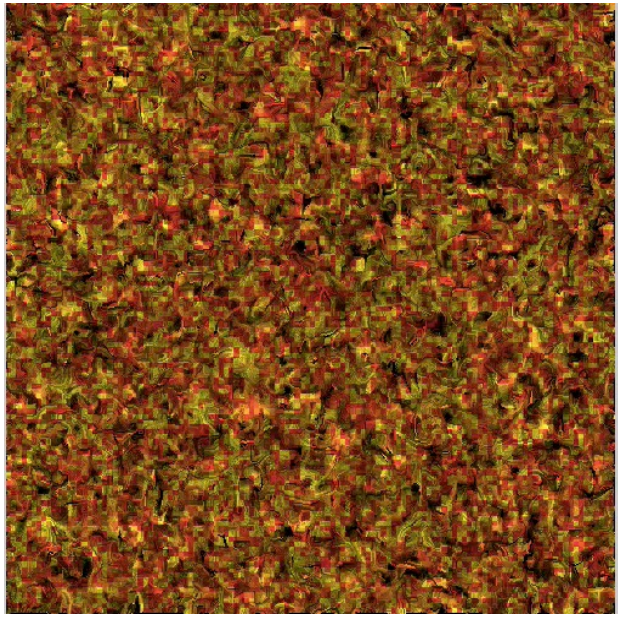
Hatwalne, Ramaswamy, Rao, Simha, PRL 2004

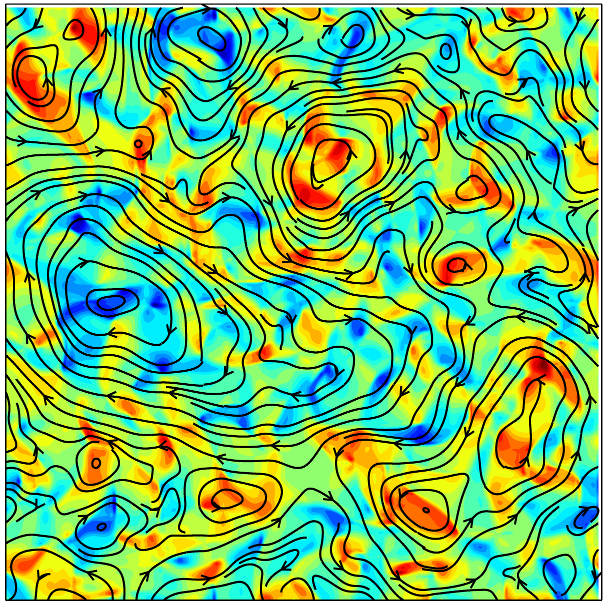
Active turbulence



Dense suspension of microswimmers

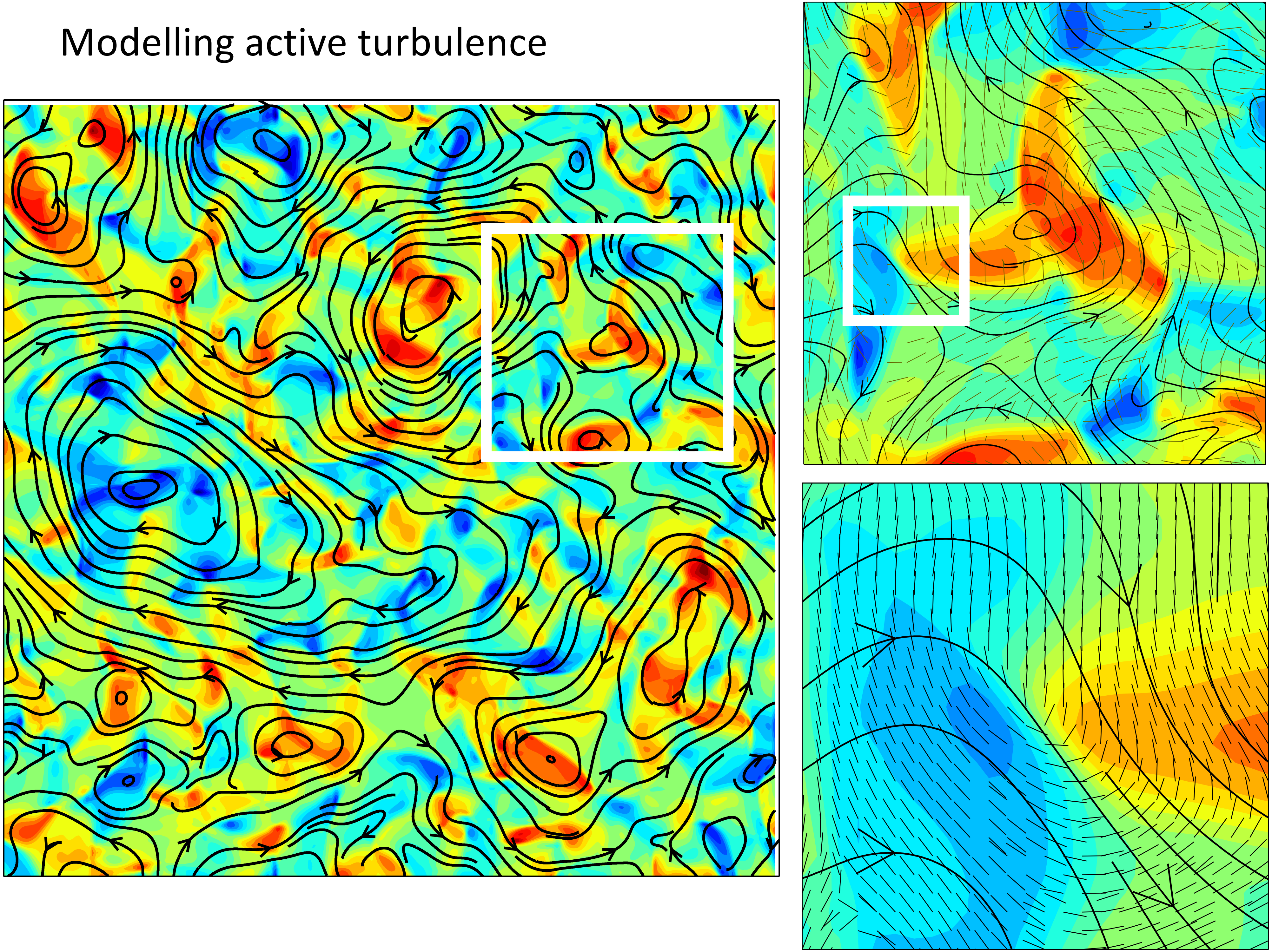
Flow field



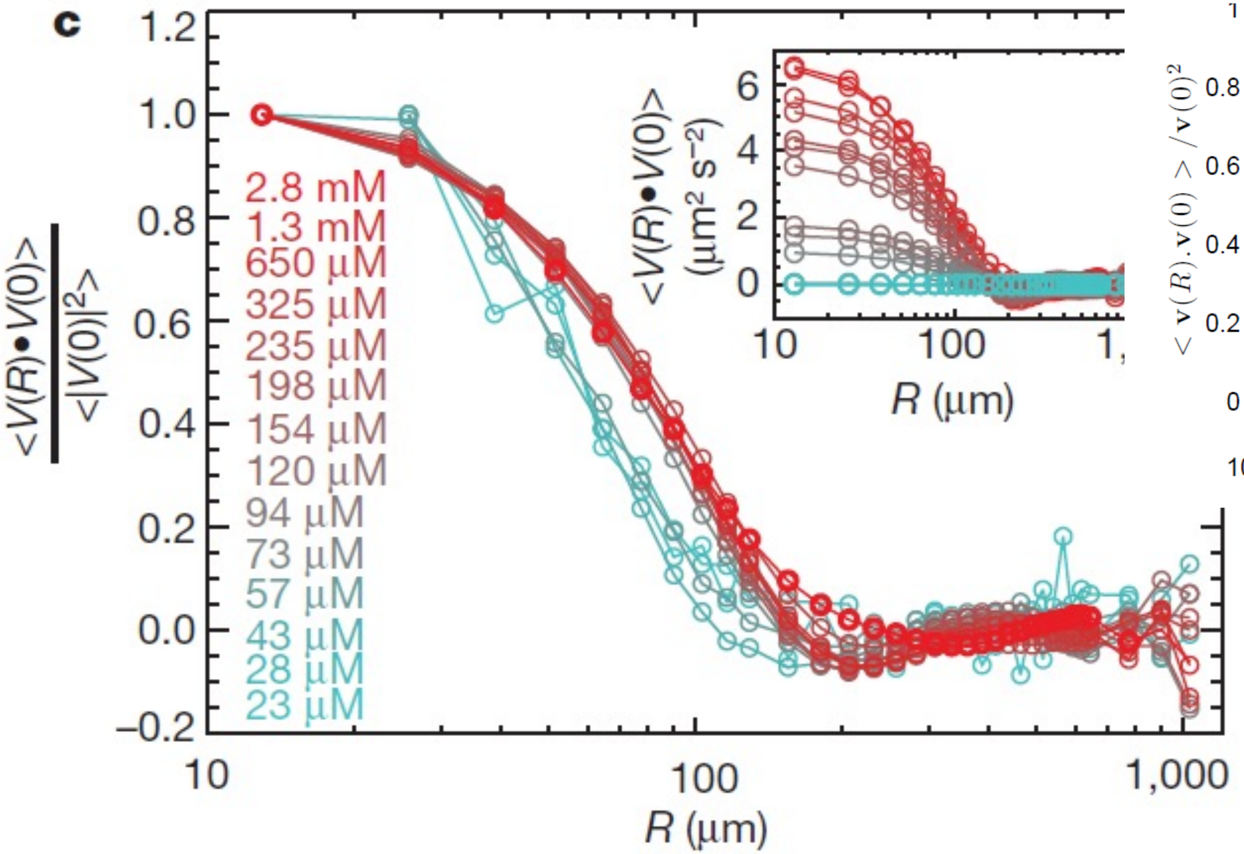


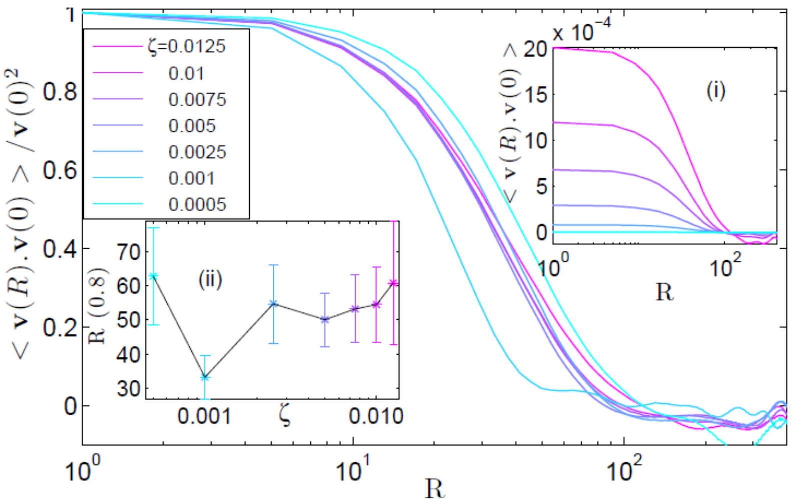
Vorticity field

Modelling active turbulence



Correlations





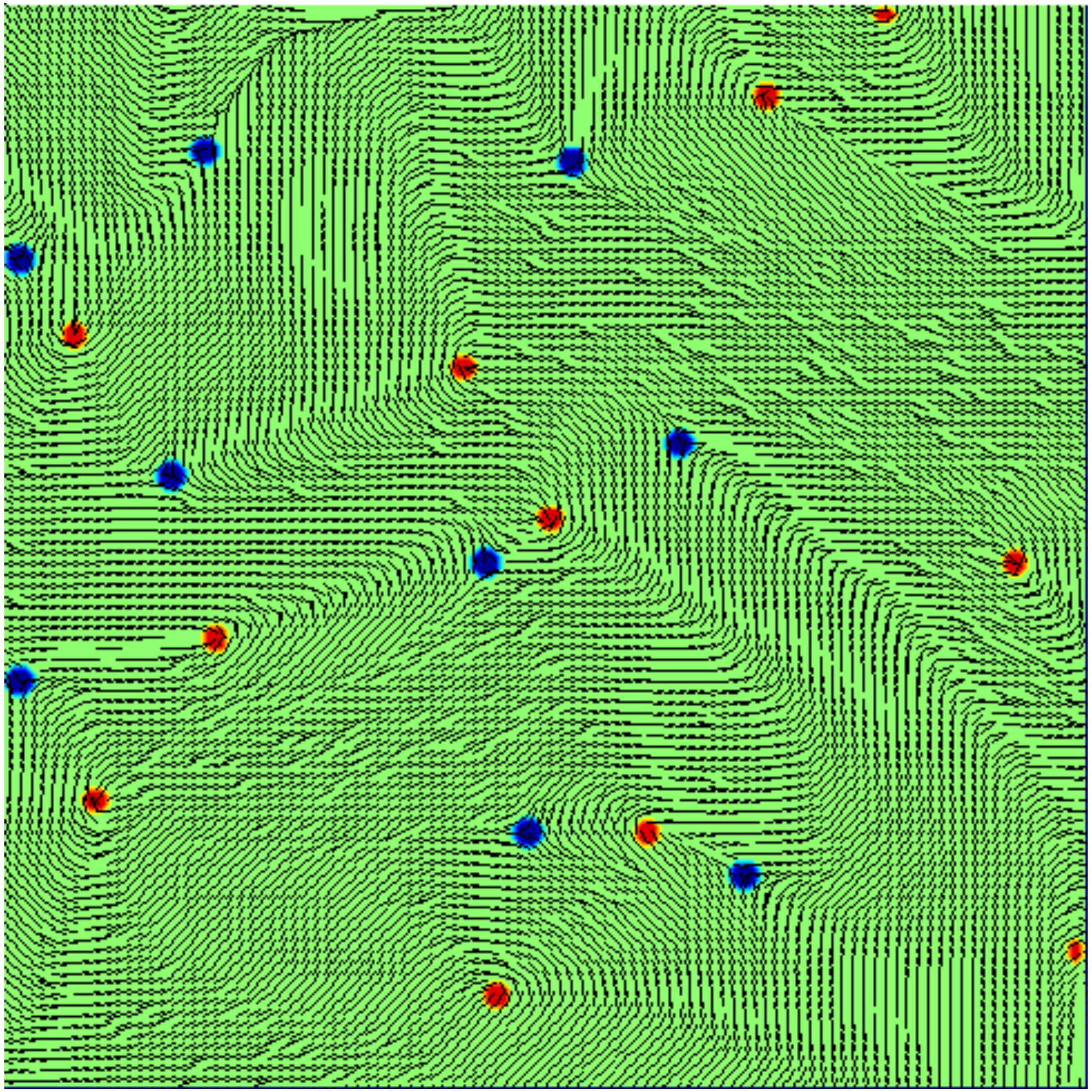
Velocity increases with activity

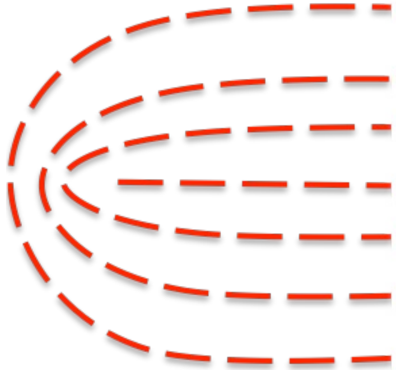
Active length scale:

$$\sqrt{K/\zeta}$$

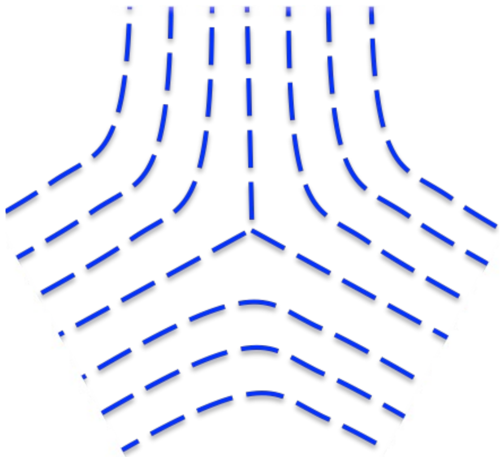
Sanchez, Chen, DeCamp, Heymann, Dogic, Nature 2012

Active turbulence: topological defects are created and destroyed



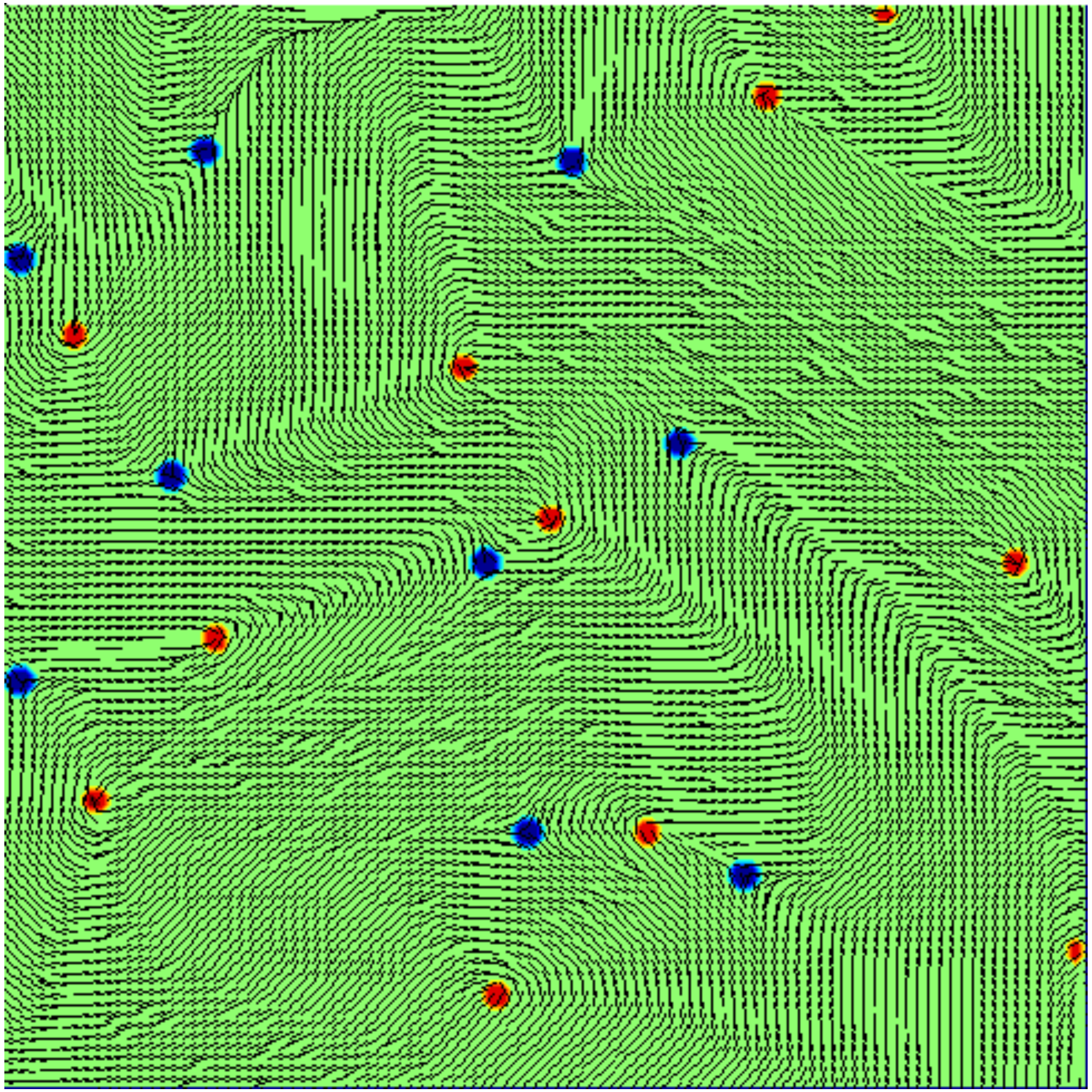


$$m = +\frac{1}{2}$$

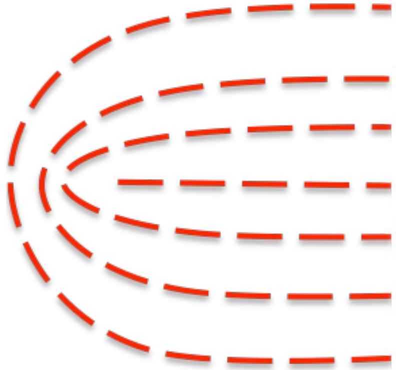


$$m = -\frac{1}{2}$$

Active turbulence: topological defects are created and destroyed



Topological defects are self motile



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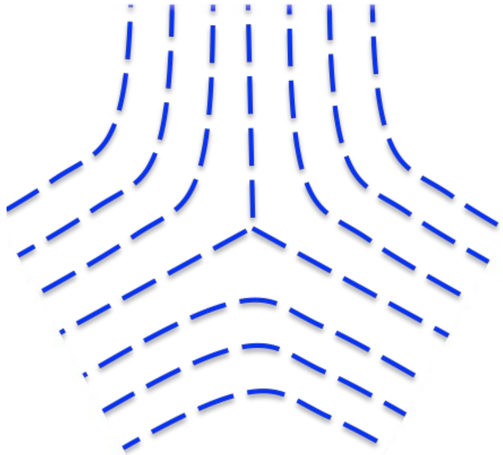
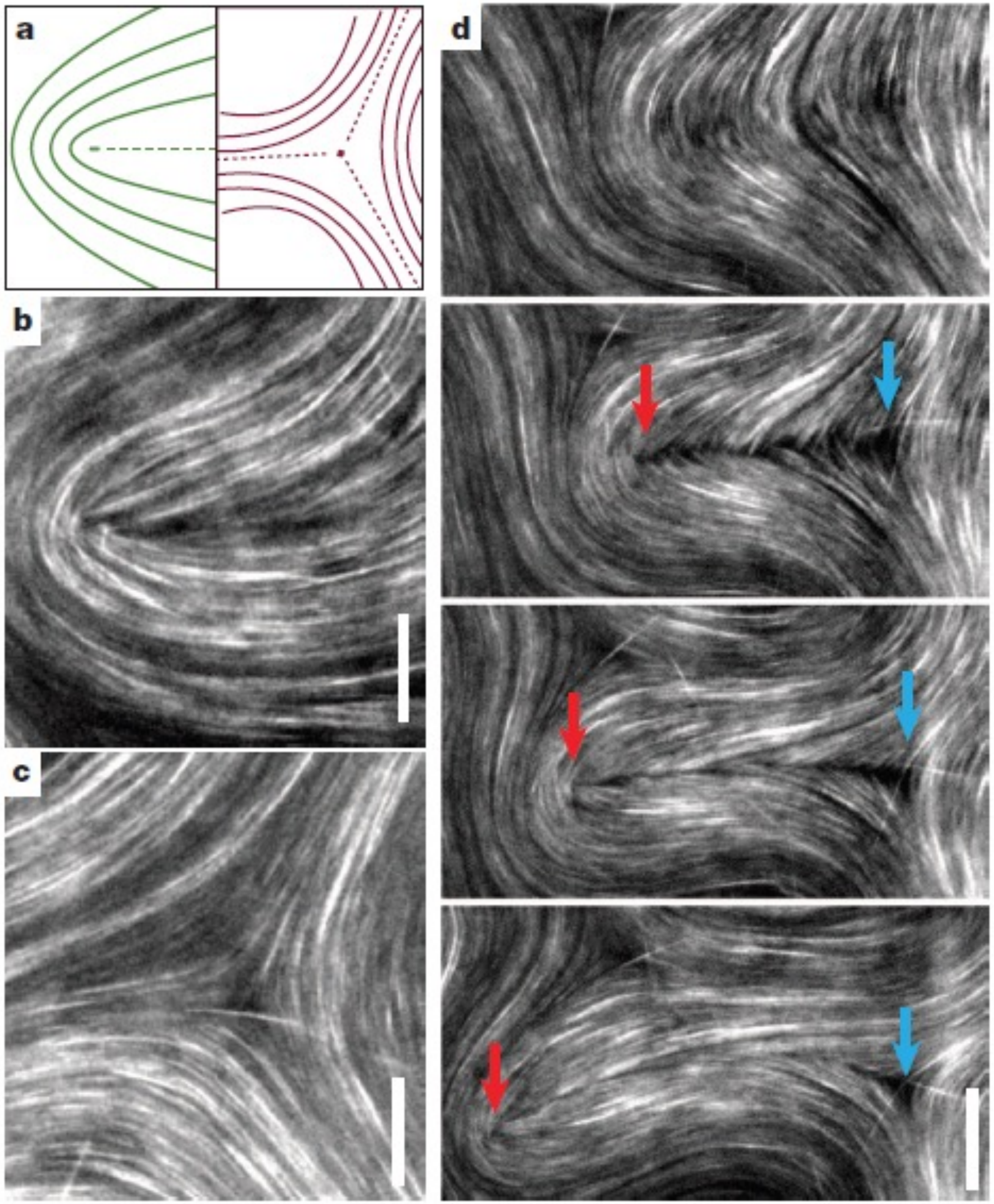
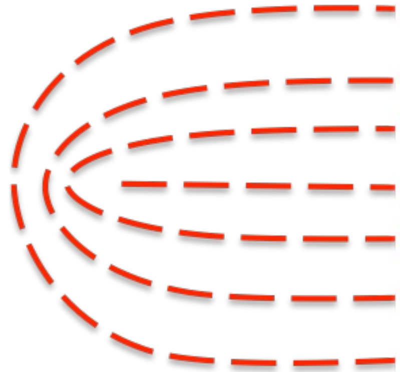
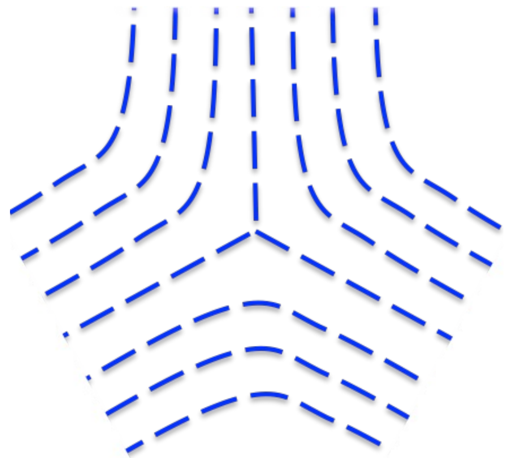


$$m = -\frac{1}{2}$$





$$m = +\frac{1}{2}$$

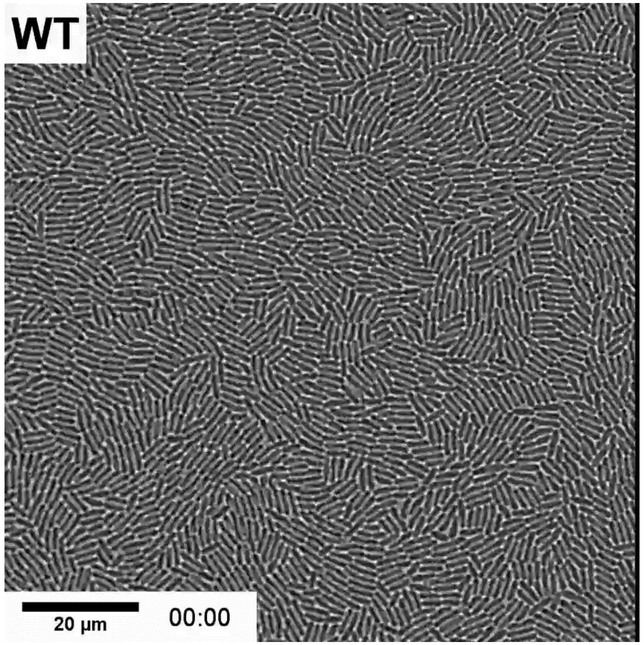


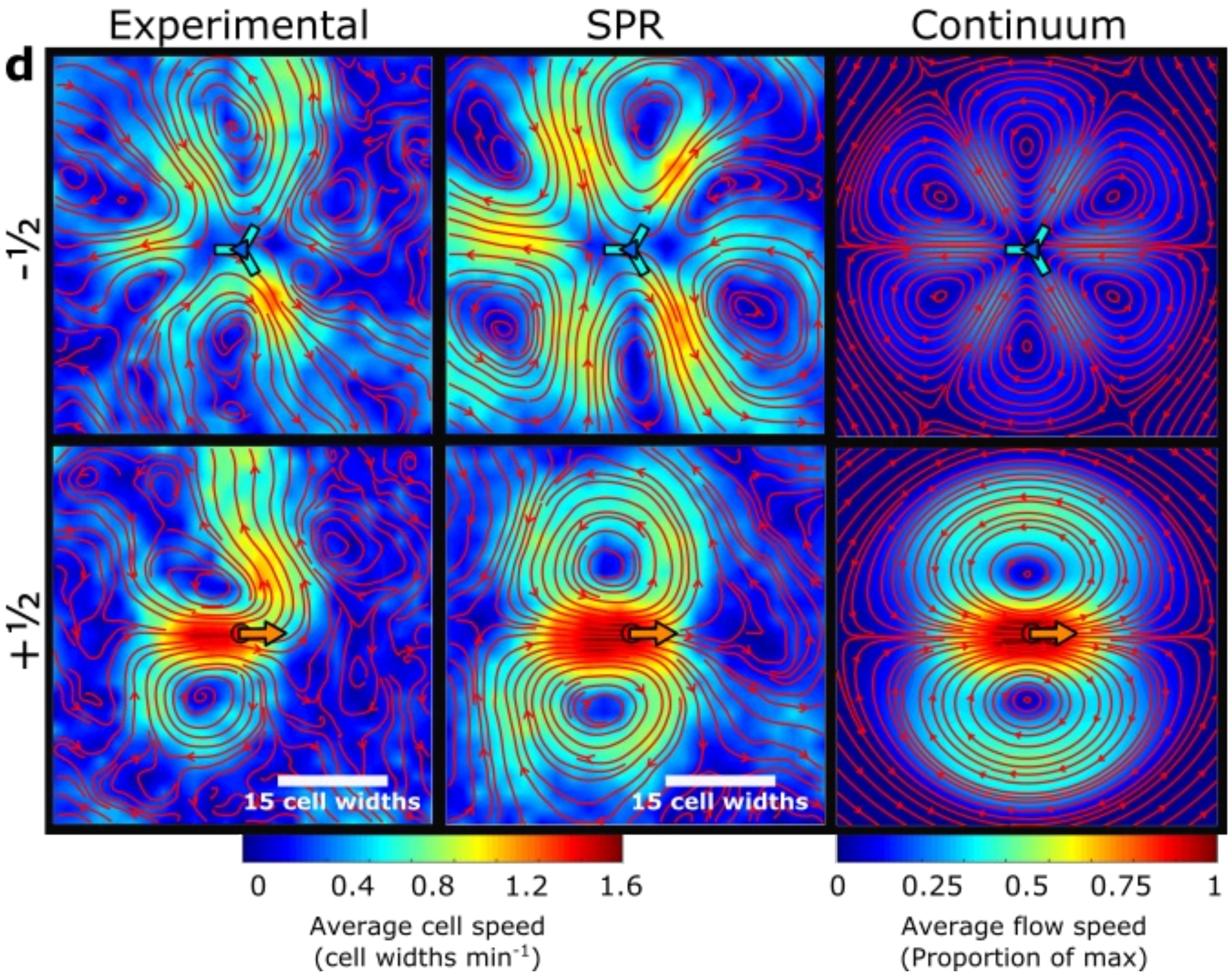
$$m = -\frac{1}{2}$$

Sanchez, Chen, DeCamp, Heymann, Dogic, Nature 2012

L. Giomi, M.J. Bowick, Ma Xu, M.C. Marchetti, PRL 110, 228101

Flow field around defects



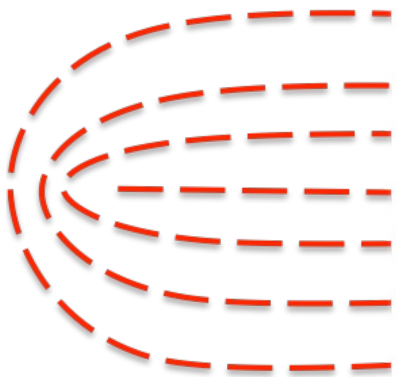


L. Giomi et al *Phil. Trans. A:* 372:0365, 2014

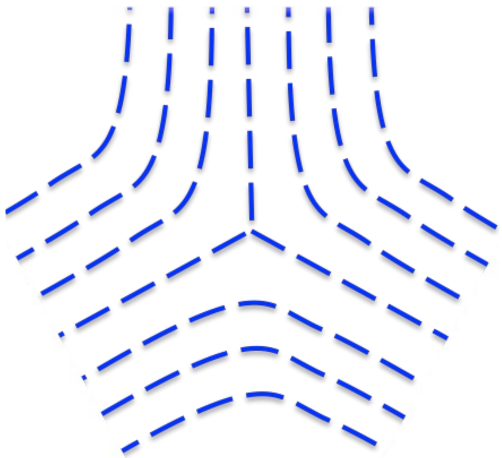
Active nematics:

Gradients in the order parameter => stresses => flows

Active topological defects: the +1/2 defects are self-propelled



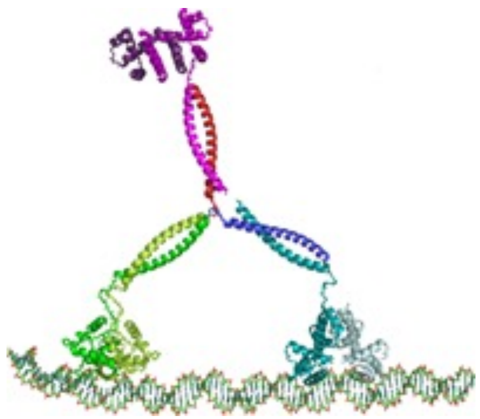
$m = +\frac{1}{2}$



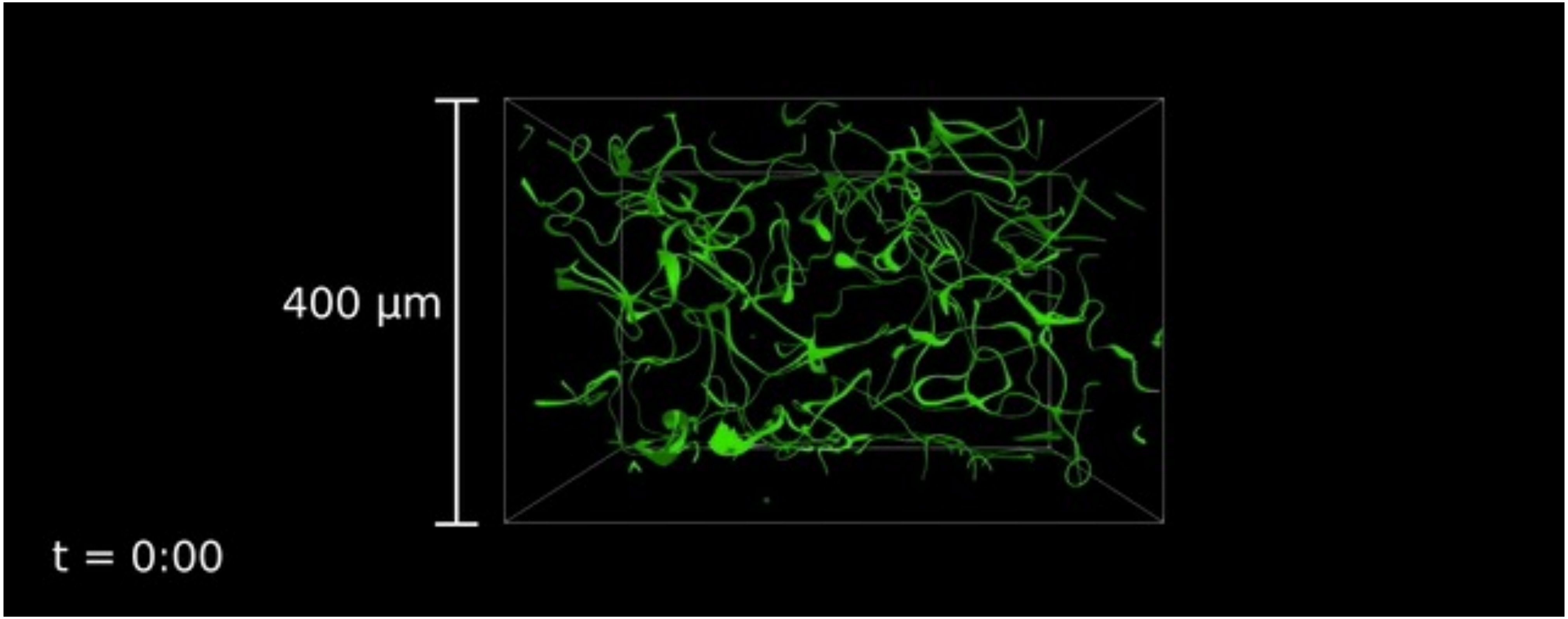
$m = -\frac{1}{2}$

Active nematics review:
A. Doostmohammadi et al. Nature Comms. 9 3246 (2018)

The 2020 motile active matter roadmap
G. Gompper et al 2020 J. Phys.: Condens. Matter 32 193001



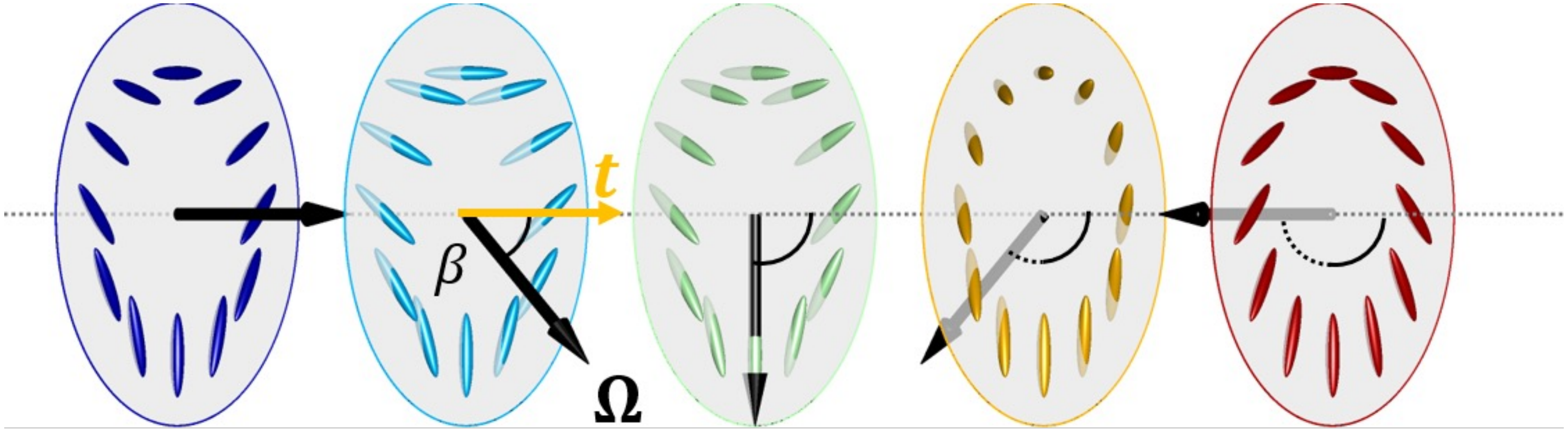
active microtubule bundles in a background of nematic colloids



Duclos et al Science 2020

3D: Disclination Lines

cross section of disclination lines



−1/2 Wedge Twist +1/2 Wedge

Twist angle: 0 $\pi/2$ π