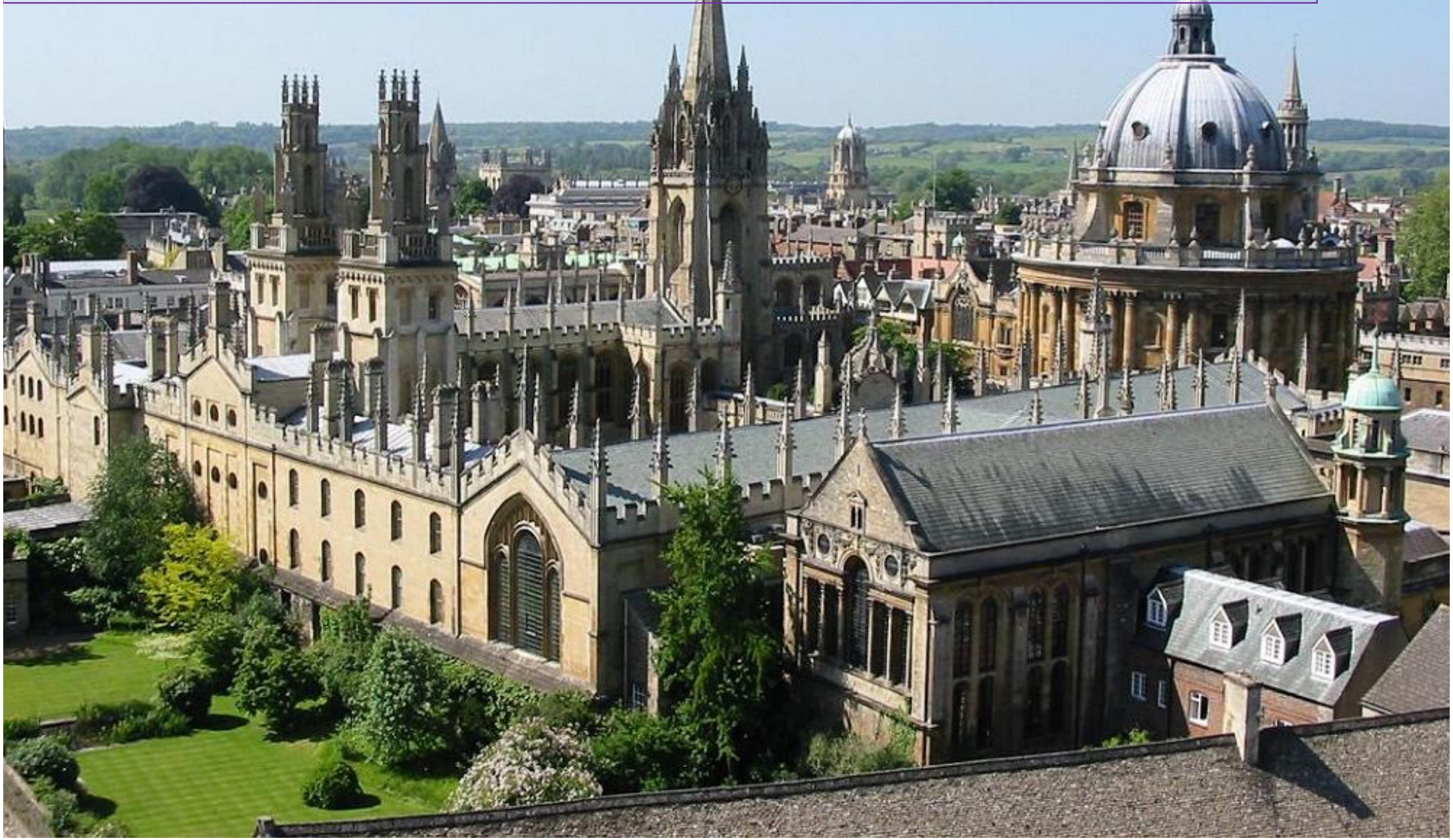
Self-propelled topological defects

Julia Yeomans
University of Oxford



Active nematics

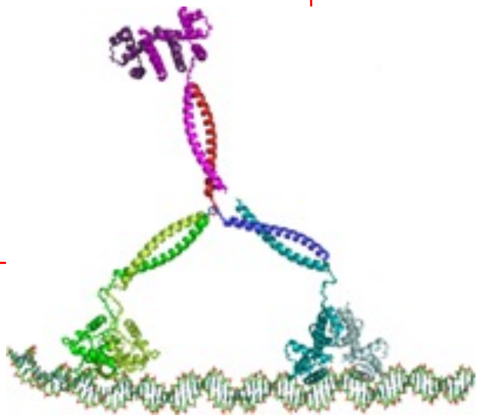
- Active turbulence
- Self propelled topological defects

Topological defects in biological shape changes

- from 2D to 3D
- the morphologies of active droplets

Active topological defects in channels

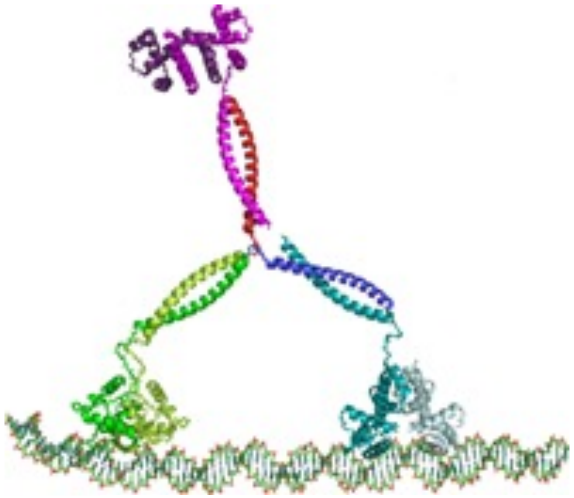
- from laminar flow to active turbulence

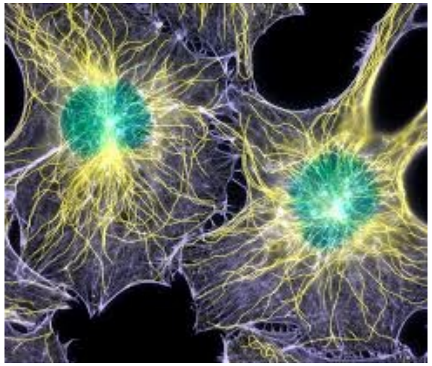


Active matter:

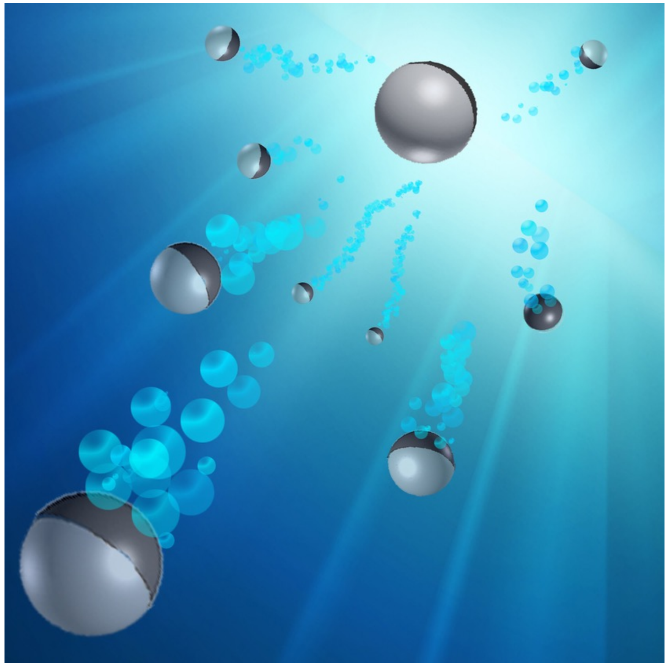
takes energy from the environment on a single particle level and uses it to do work.

molecular motors





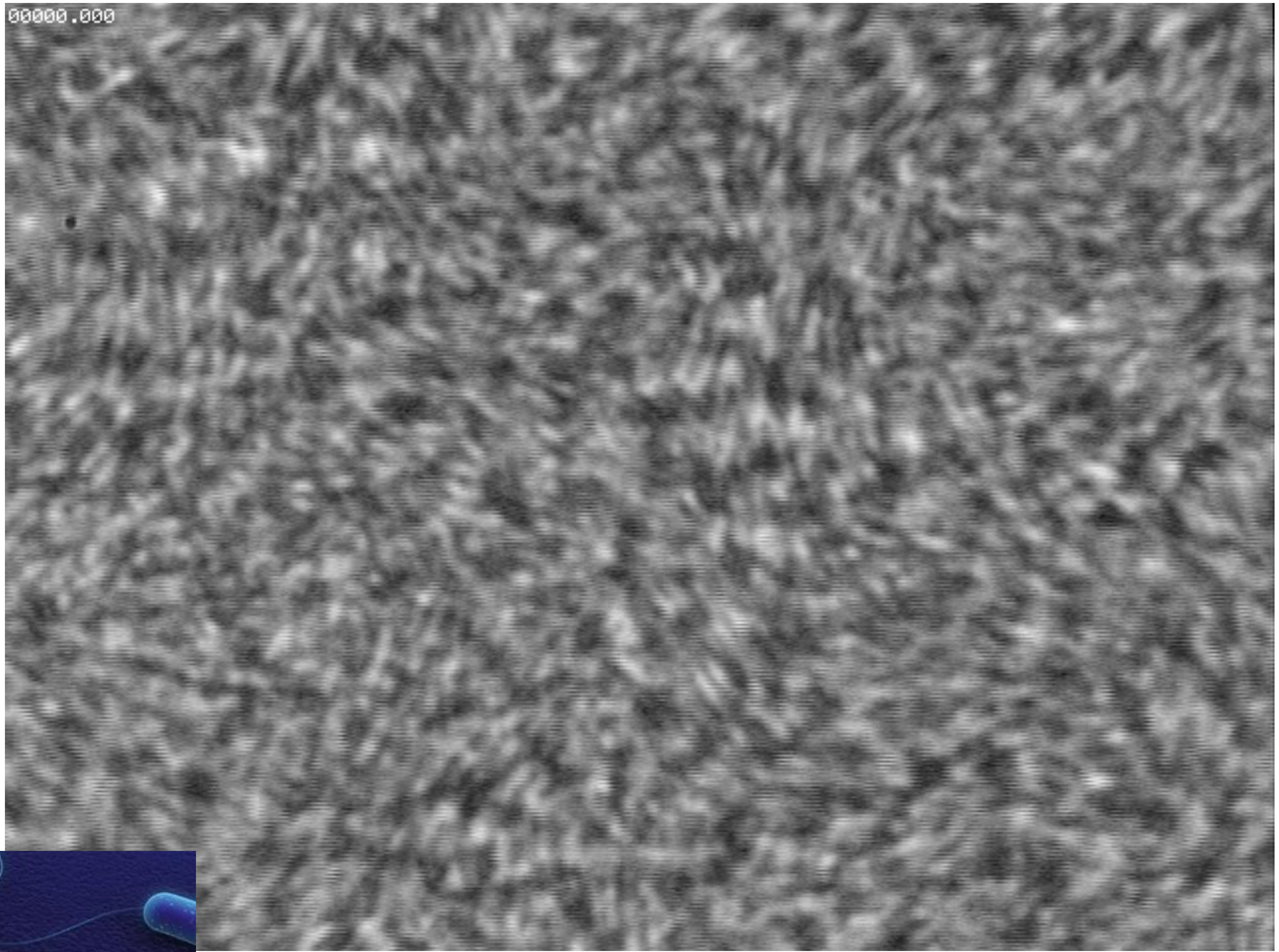
cells



active colloids

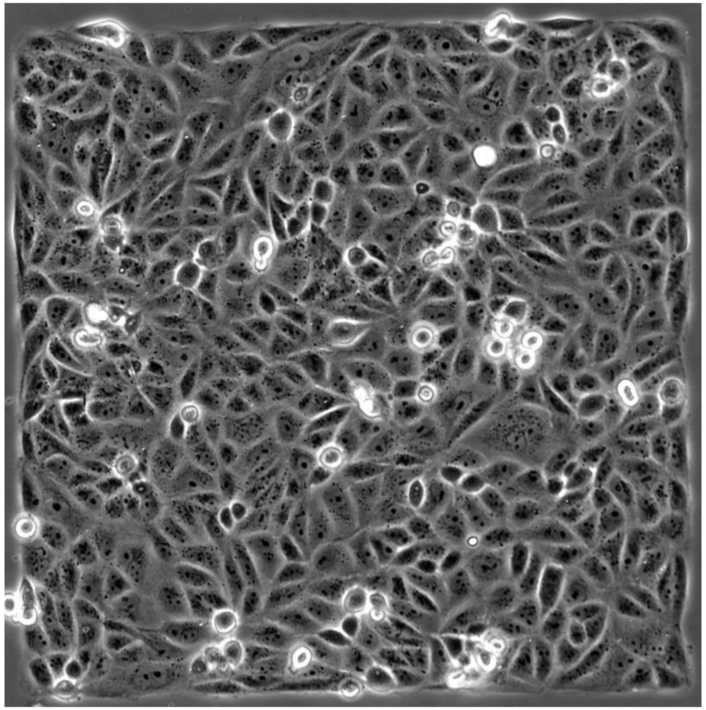
microswimmers

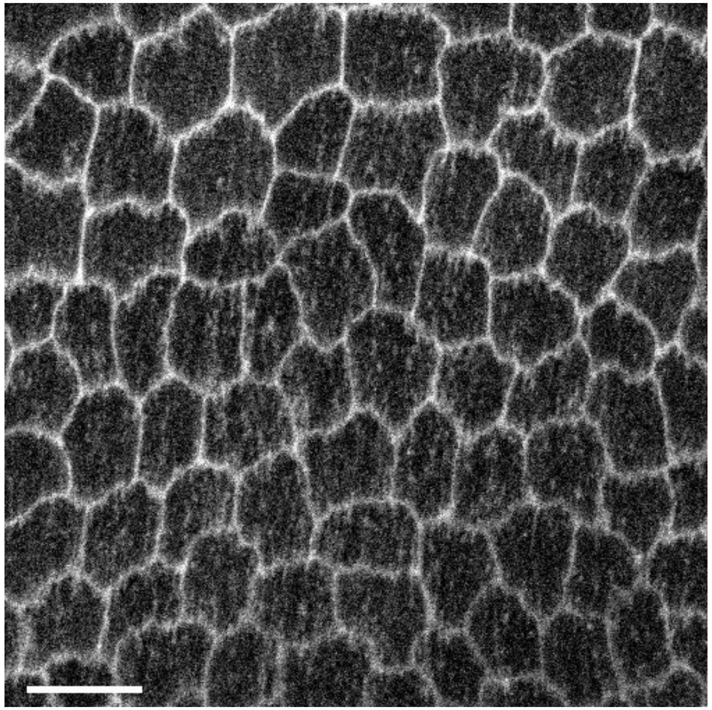
Active turbulence: bacteria



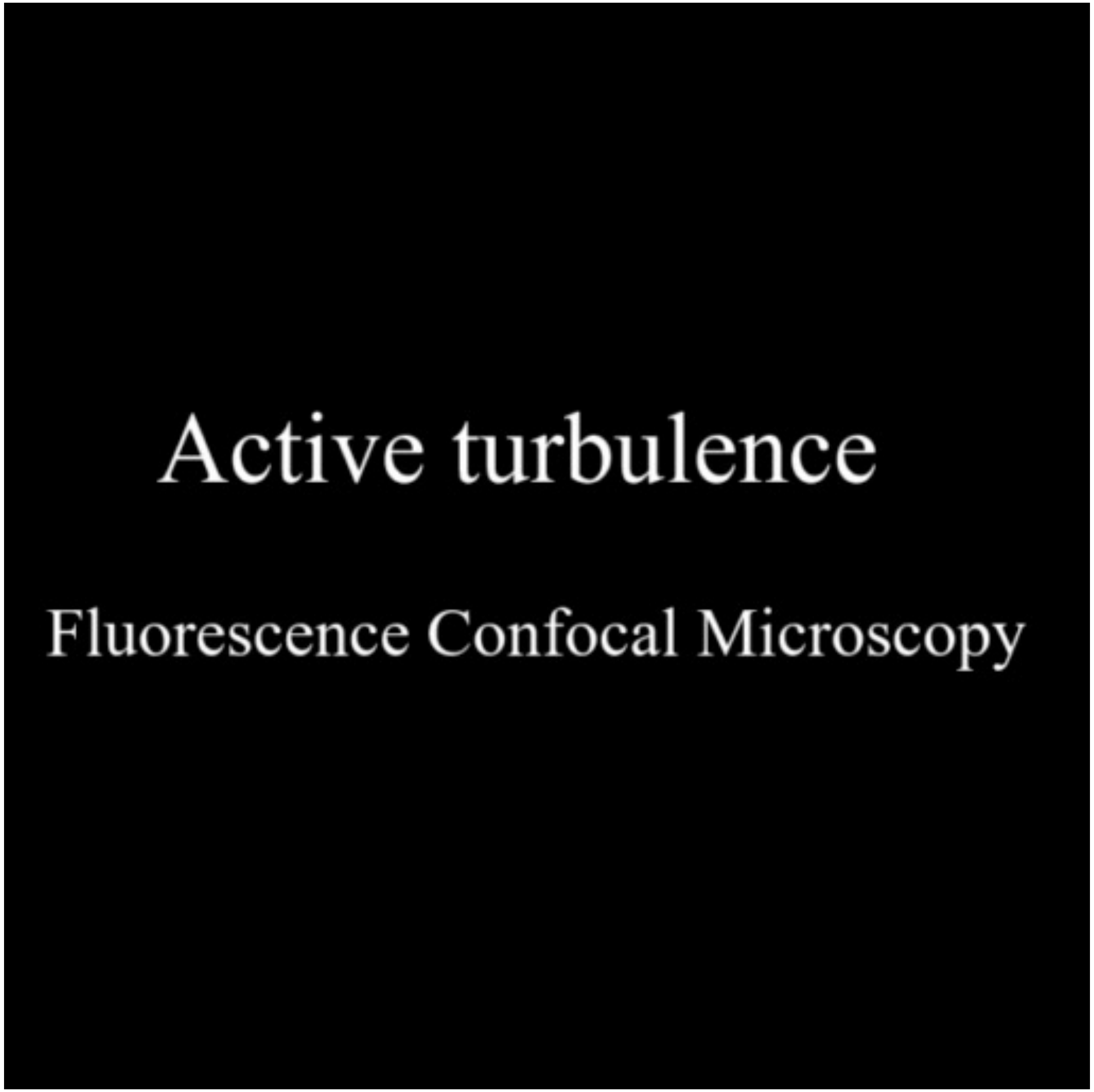
Dense suspension of microswimmers

Active turbulence: epithelial cells

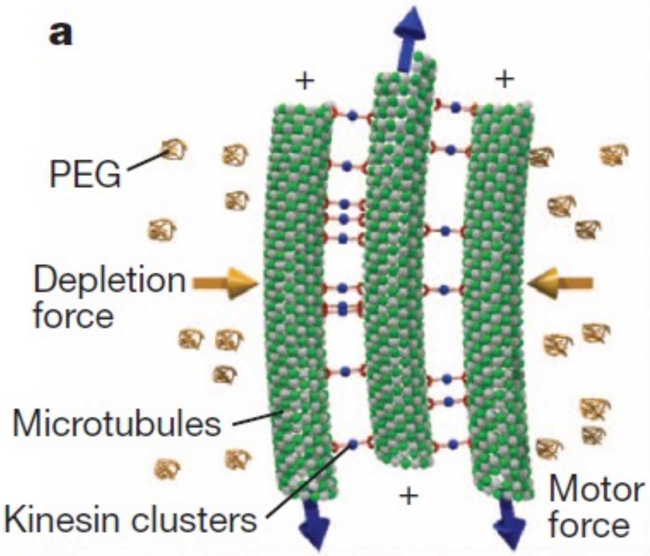




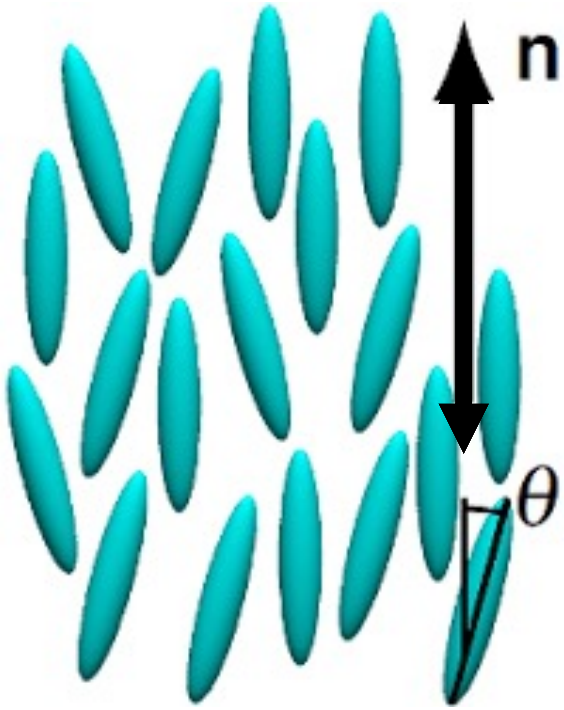
Active turbulence: microtubules & motor proteins



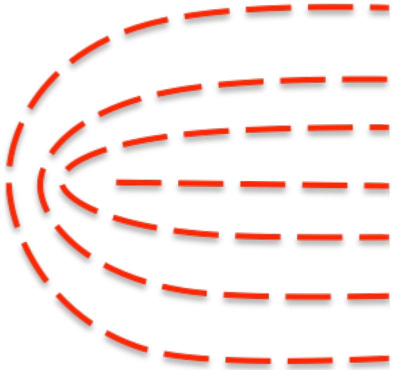
Francesc Sagues
Pau Guillamat
Jordi Ignes-Mullol



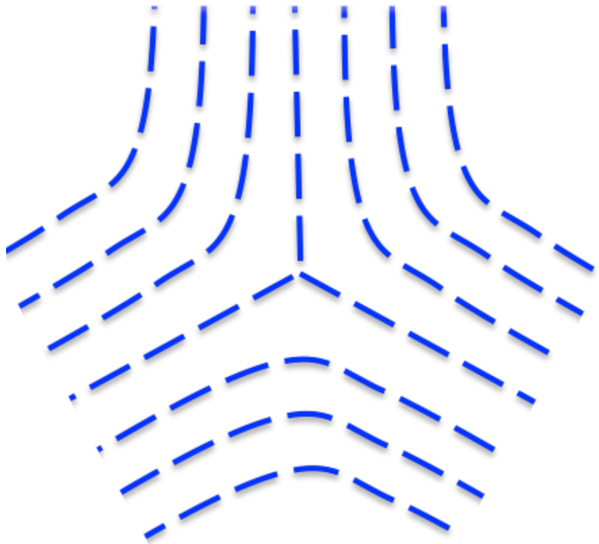
nematic phase



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



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



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

Continuum equations of liquid crystal hydrodynamics

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

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

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

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

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

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

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

Continuum equations of liquid crystal hydrodynamics

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

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

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

Tumbling parameter

Continuum equations of liquid crystal hydrodynamics

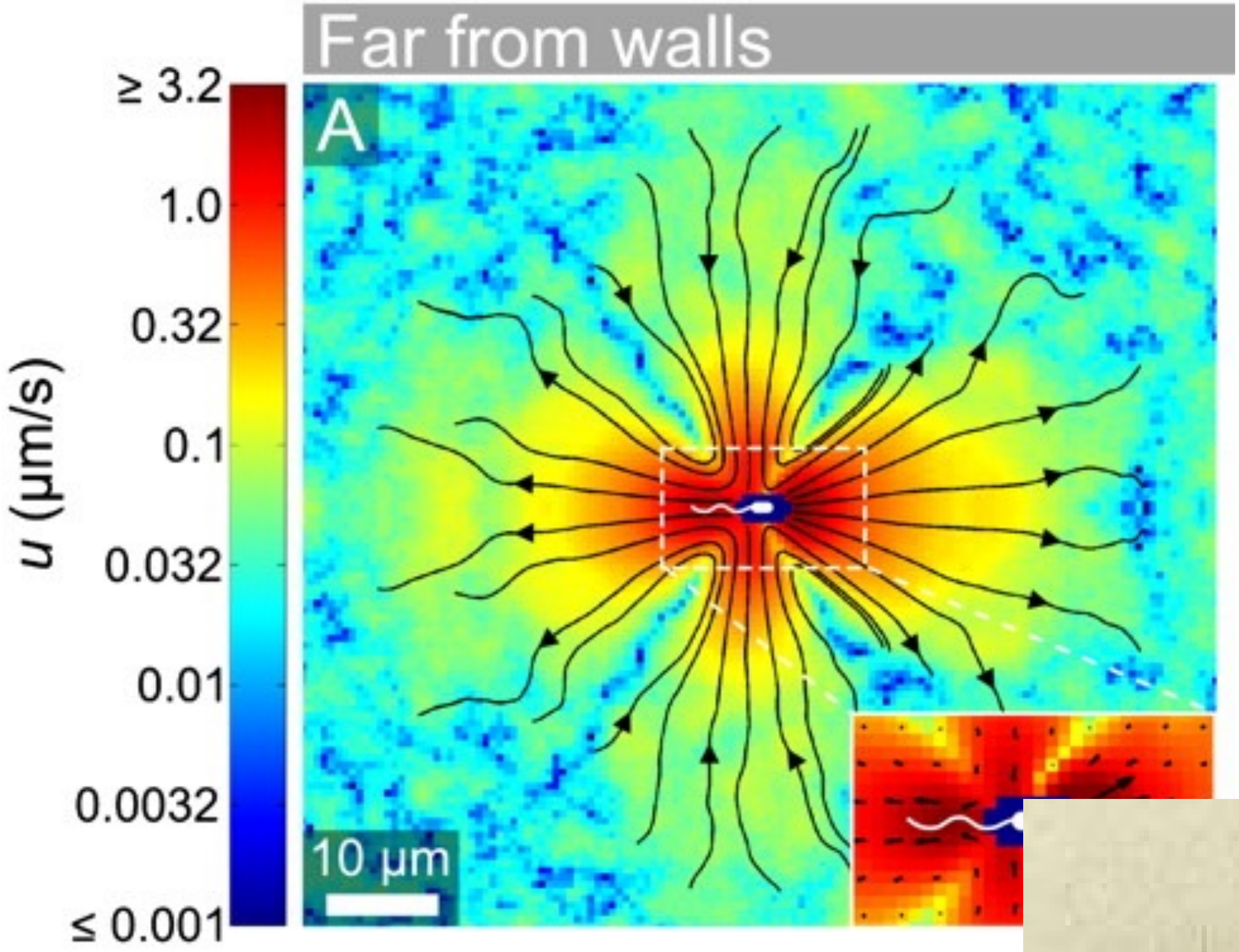
$$(\partial_t + u_k \partial_k) Q_{ij} - S_{ij} = \Gamma H_{ij}$$

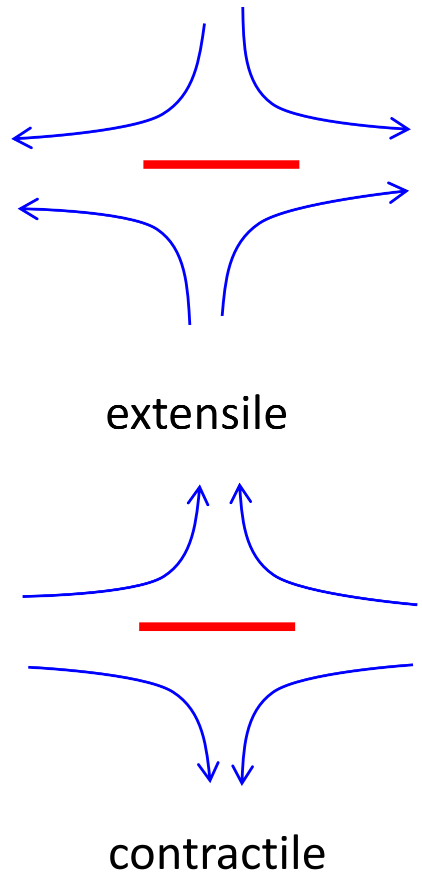
couples nematic order and shear flows

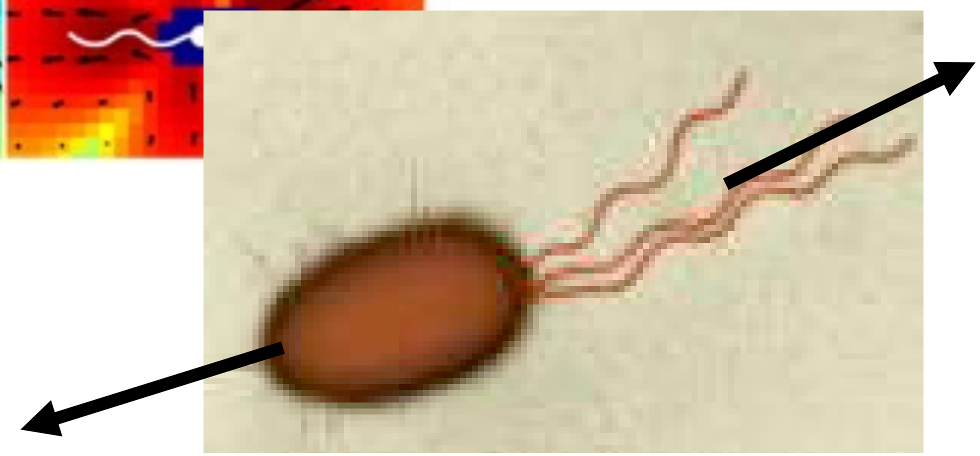
relaxation to minimum of Landau-de Gennes free energy

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

viscous + passive







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 => active turbulence

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

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

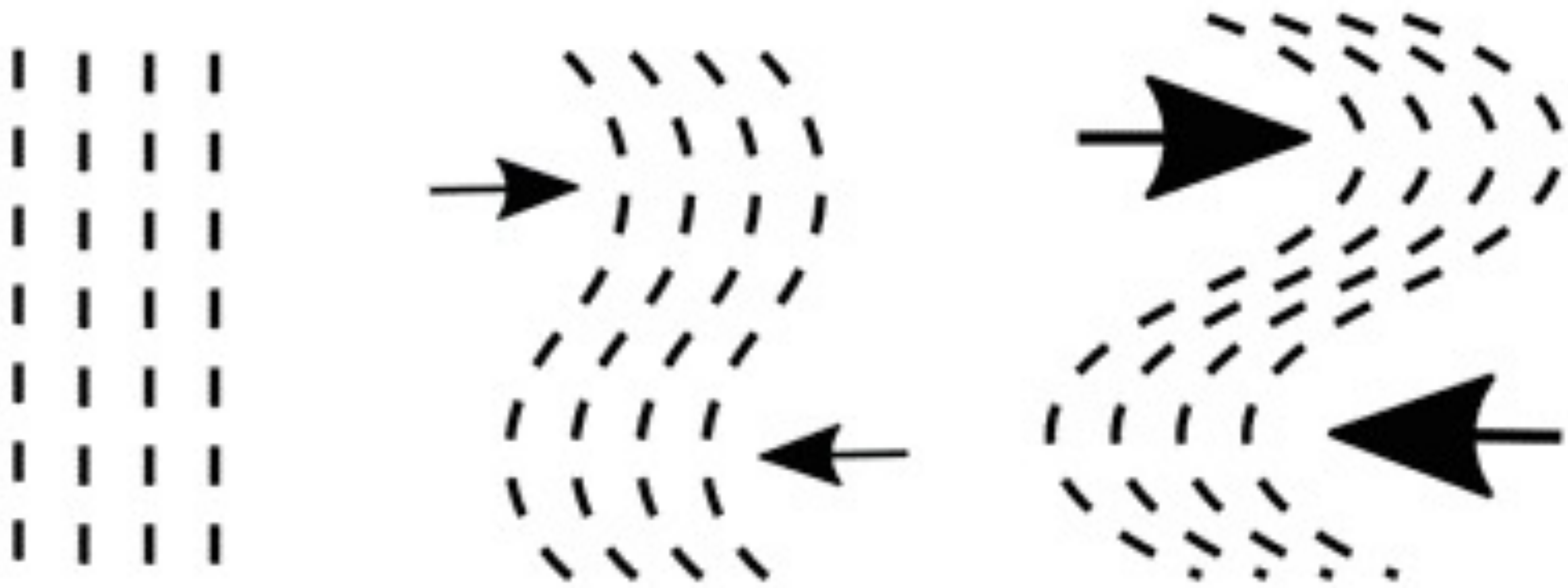
Hatwalne, Ramaswamy, Rao, Simha, PRL 2004

Instability 1: nematic ordering is unstable to bend instabilities

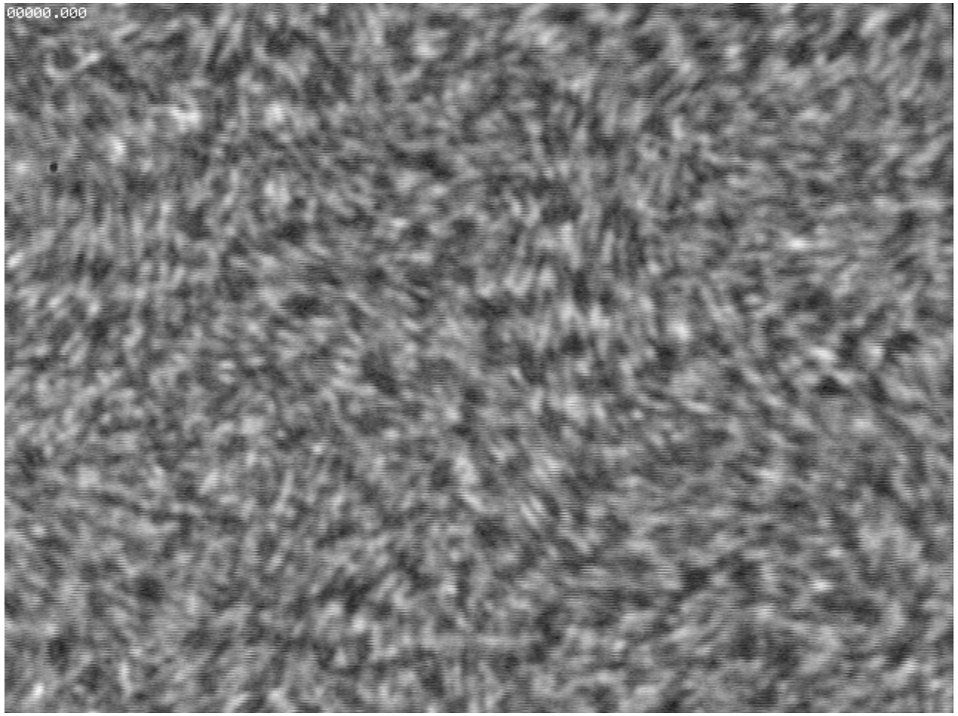
(extensile)

splay instabilities

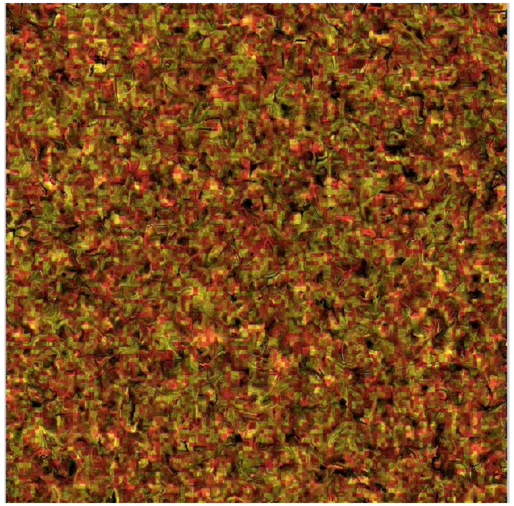
(contractile)

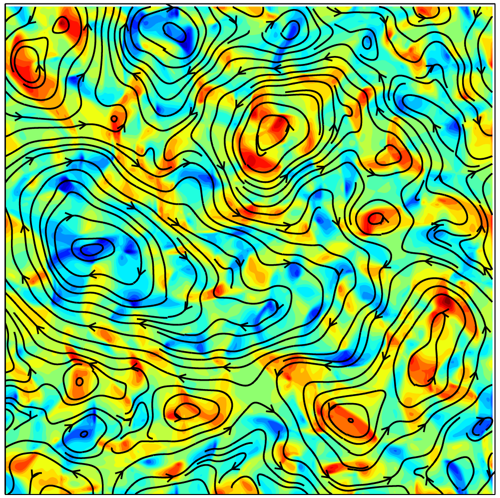


Active turbulence



Microswimmers: E-coli



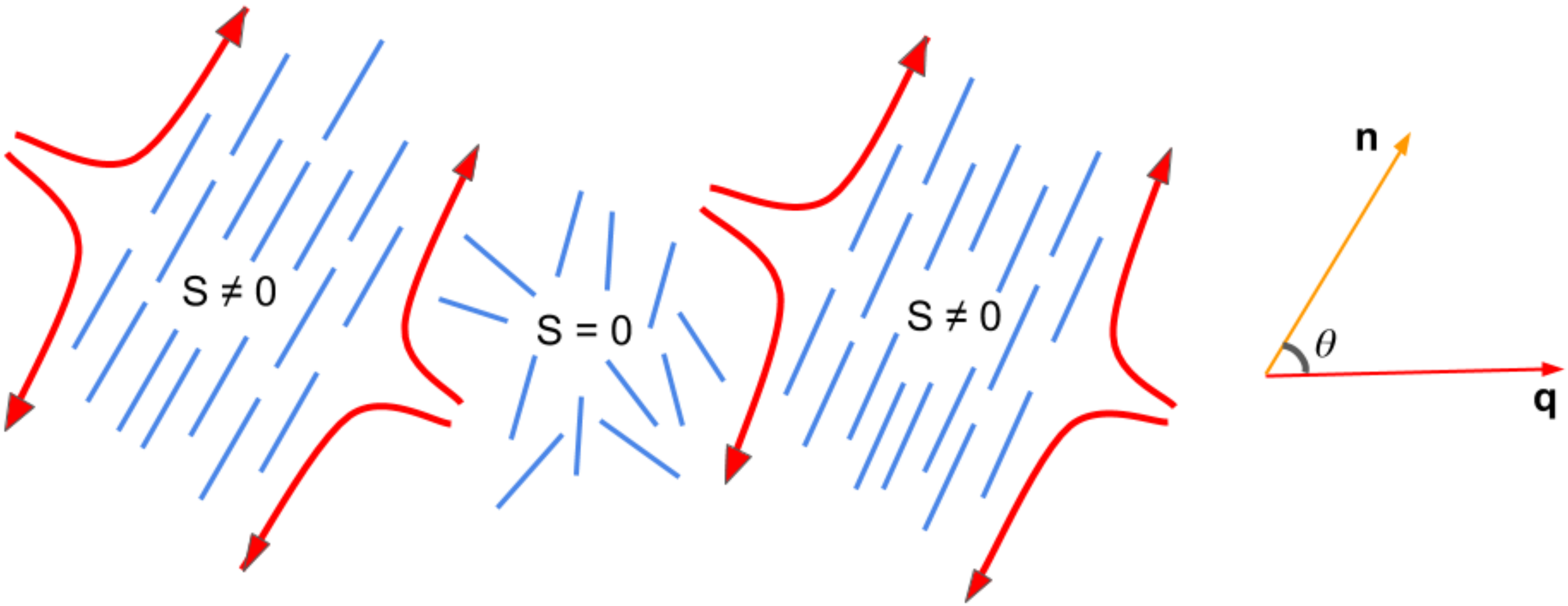


Flow field and vorticity field from solving the continuum equations

BUT

No real reason for thermodynamic ordering in many active systems

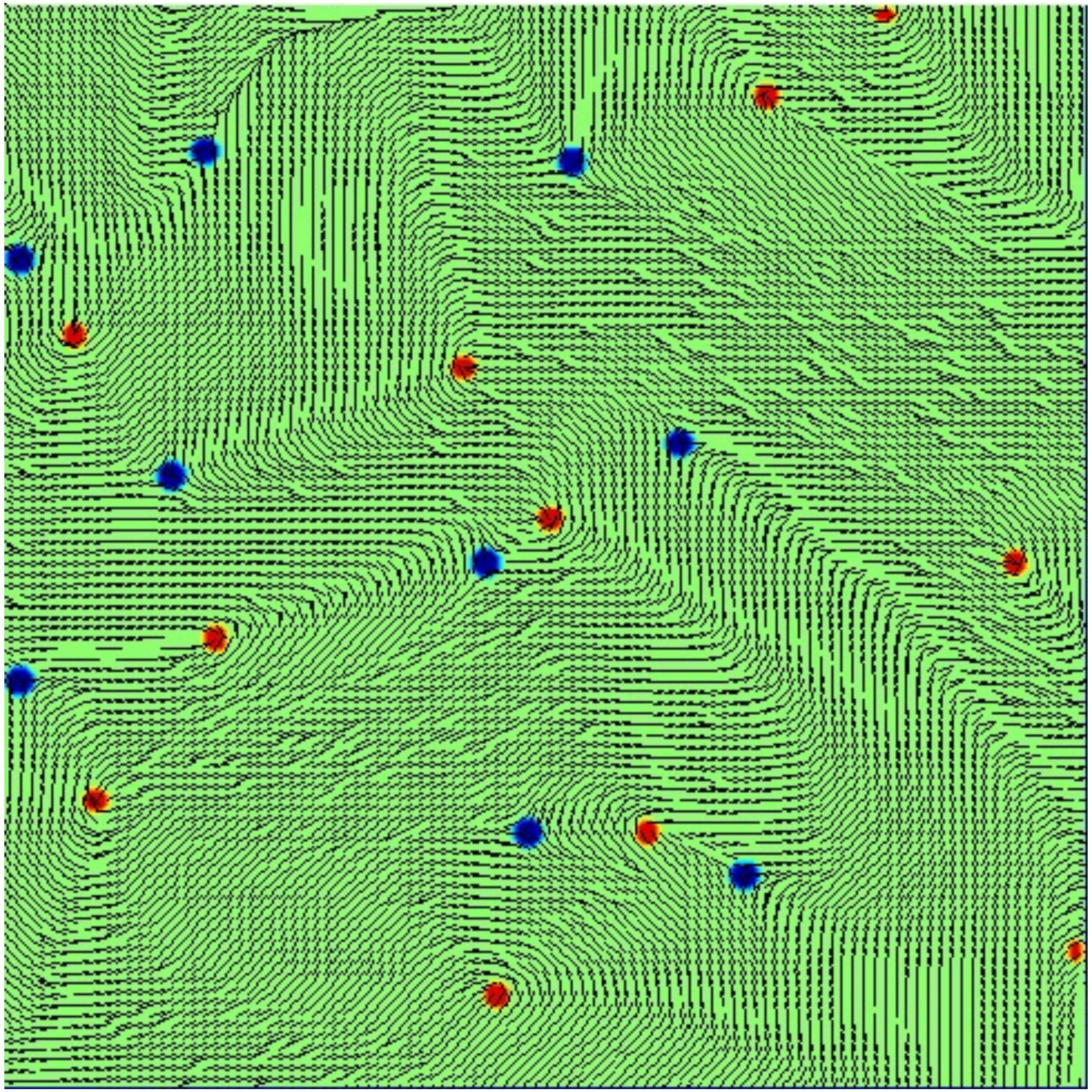
Instability 2: isotropic state is unstable to nematic order

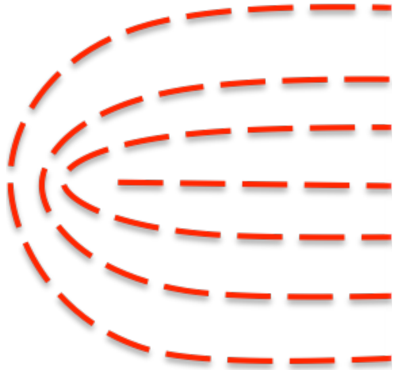


Even if the passive system is isotropic, can still get active turbulence
(for extensile rod-like particles or contractile disc-shaped particles)

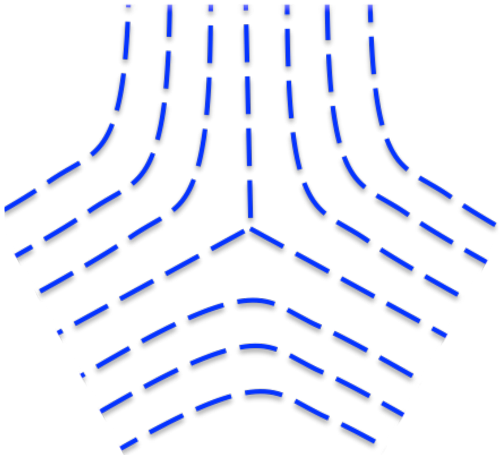
Santhosh et al J Stat Phys 2020

Active turbulence: topological defects are created and destroyed



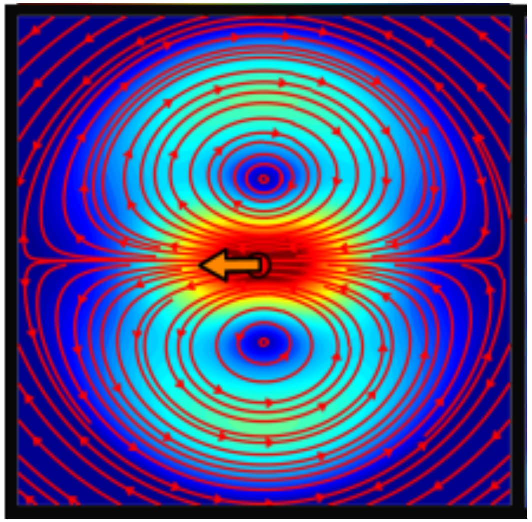


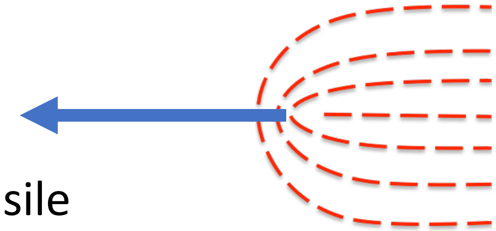
$m = +\frac{1}{2}$



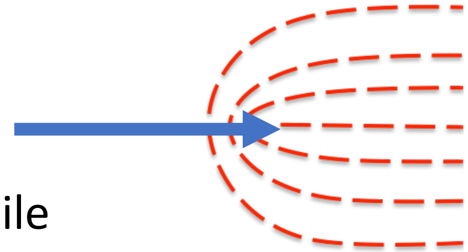
$m = -\frac{1}{2}$

Flow fields around +1/2 defect

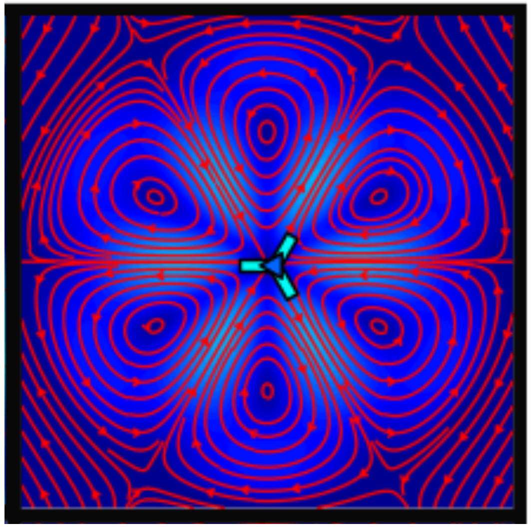


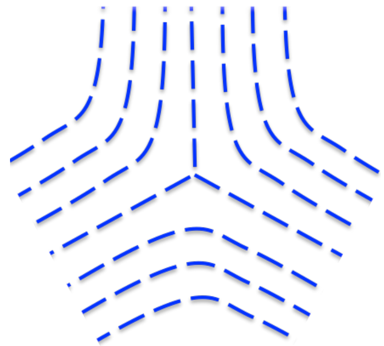


extensile



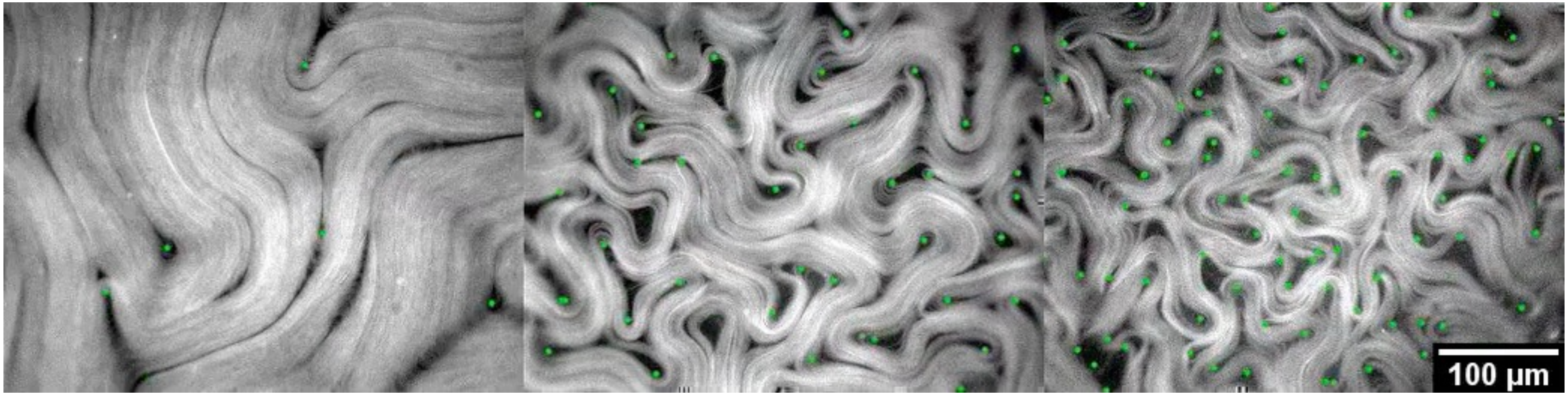
contractile

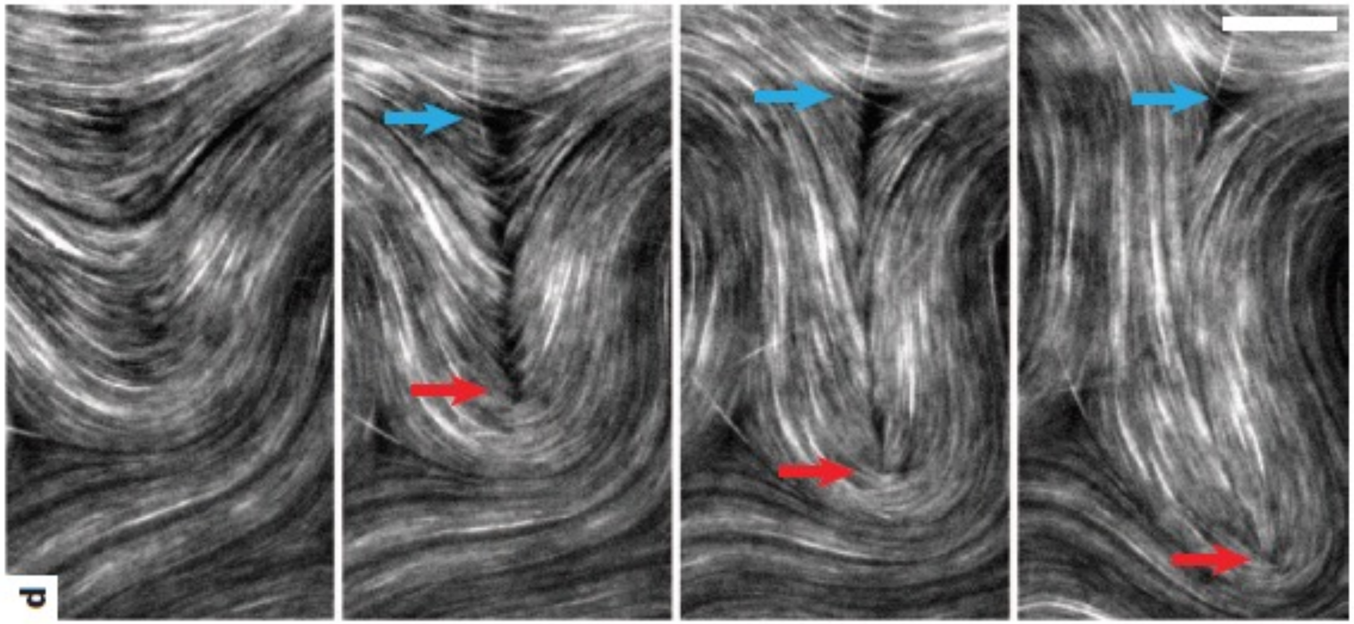


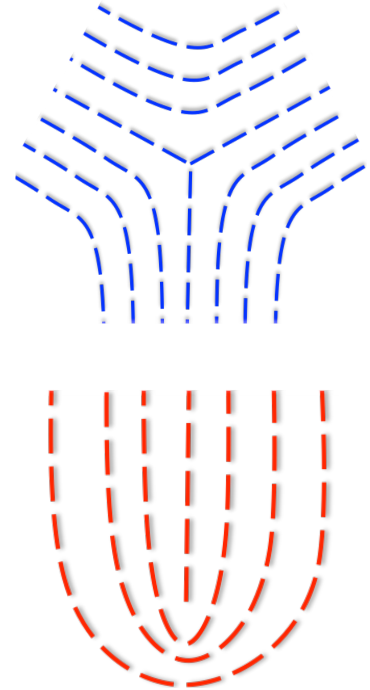


L. Giomi

F. Sagues group





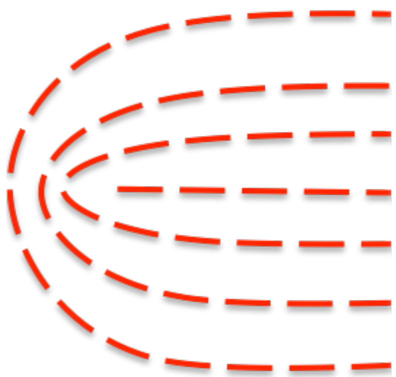


Z. Dogic group

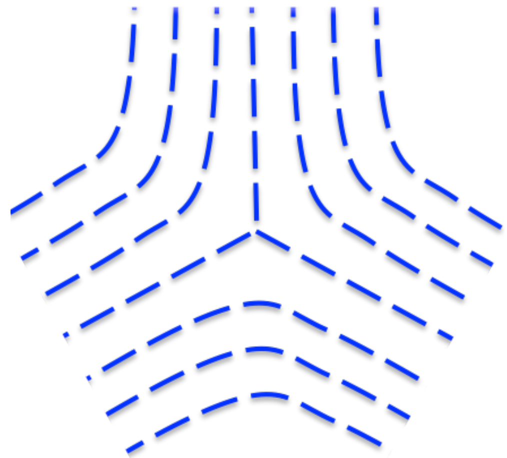
Active nematics:

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

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- the morphologies of active droplets

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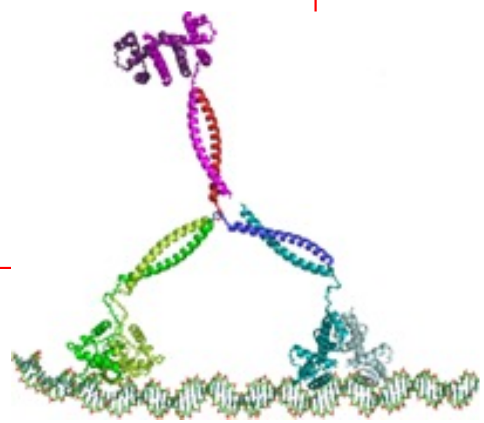
- from laminar flow to active turbulence

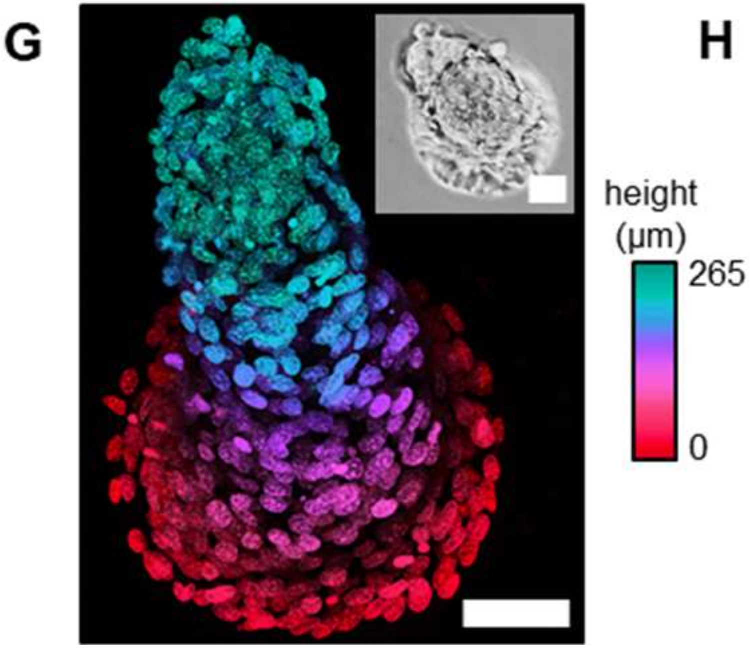


Thank You

Liam Ruske

Mehrana Nejad

From 2D to 3D



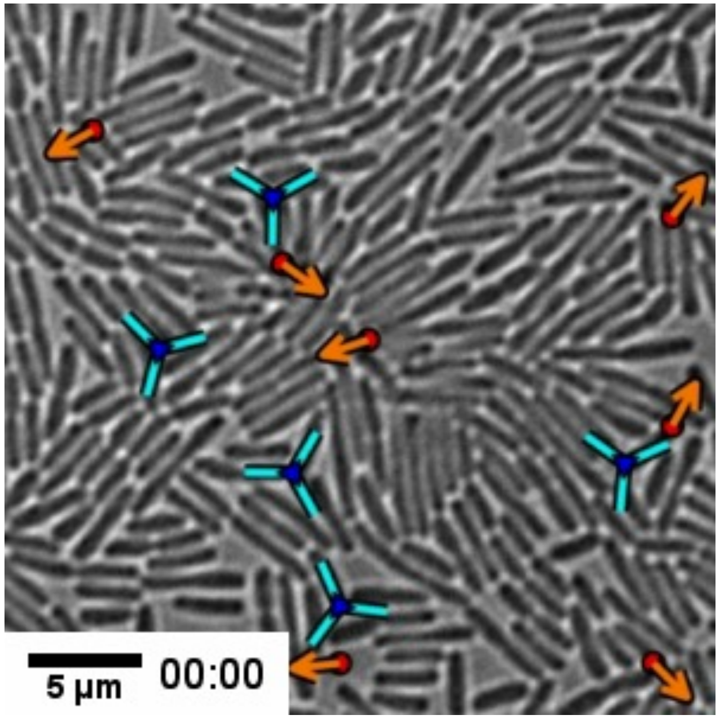
Guillamat, Blanch-Mercader, Kruse, Roux
bioRxiv preprint 129262

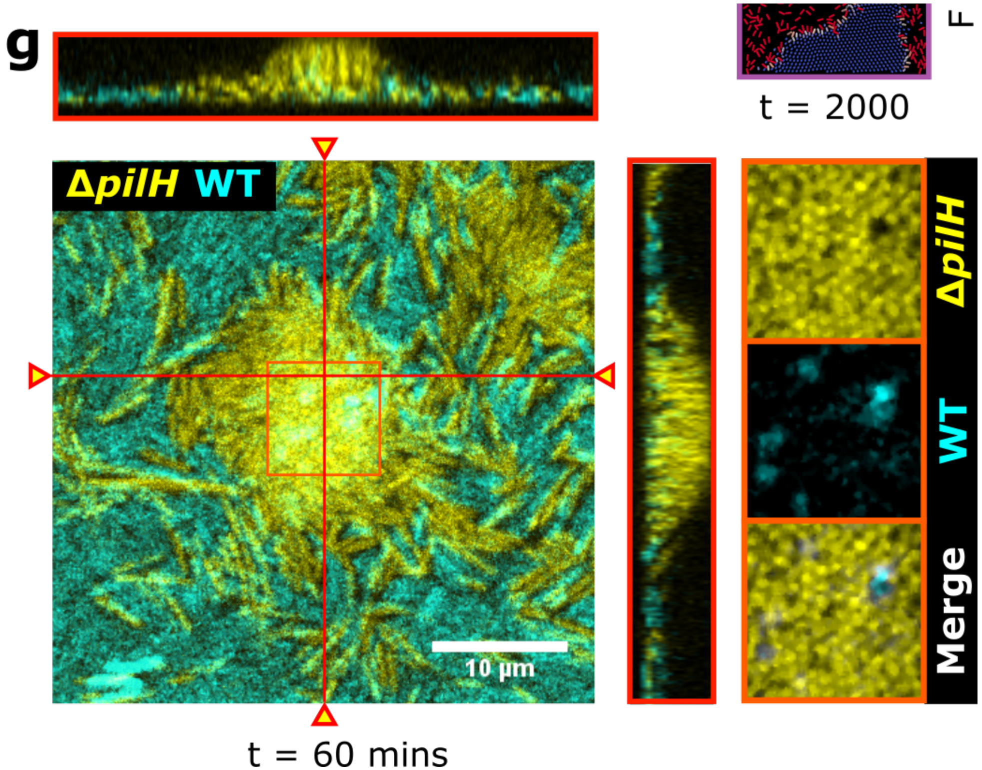
C2C12 myoblasts seeded on small discs

Vertical colonies form at virtual +1 defects in *pseudomonas*

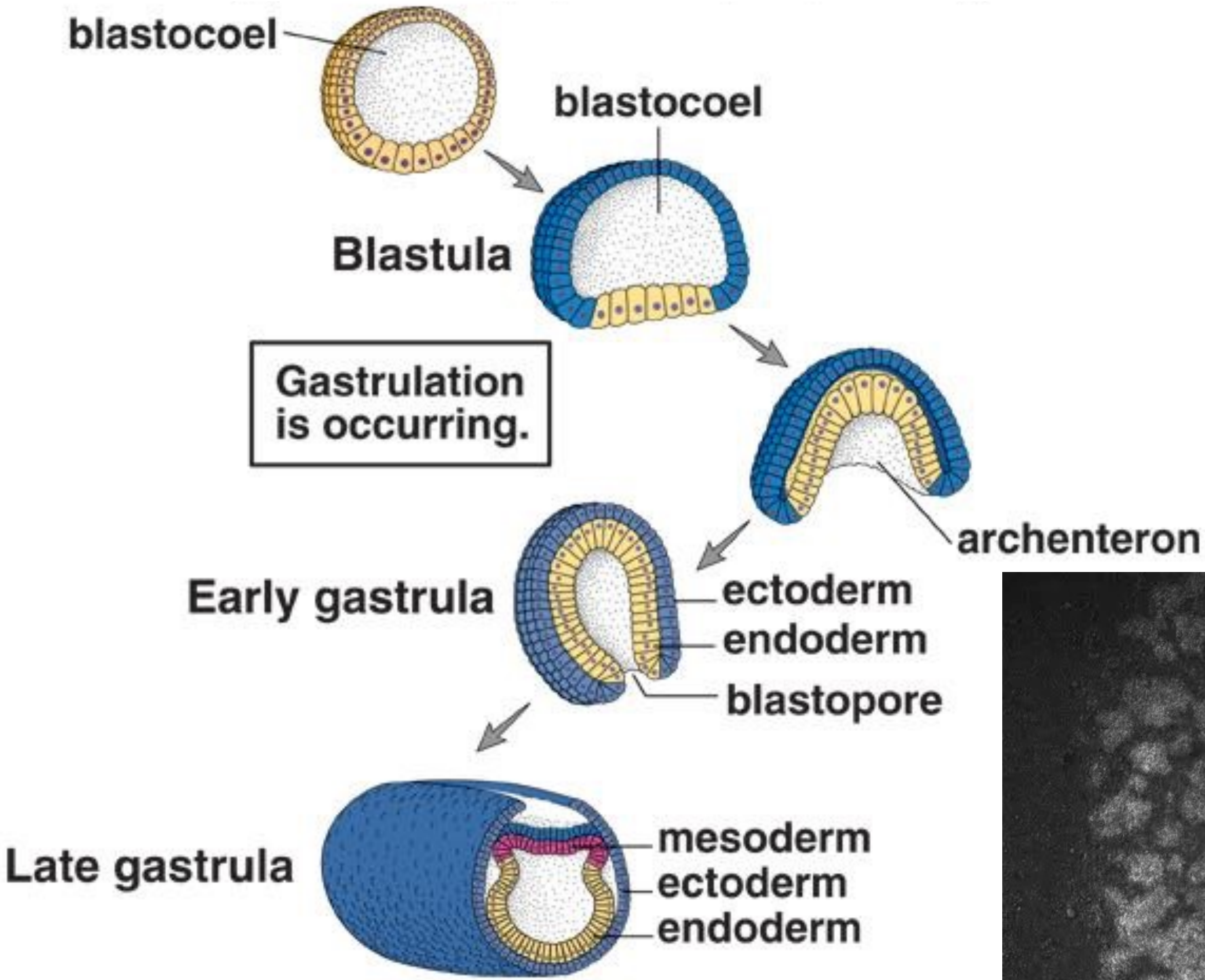
Meacock, Doostmohammadi, Foster, Yeomans, Durham
Nature Physics **17** 205 (2021)

Regions where cells stand on end nucleate at places where two +1/2 defects approach each other

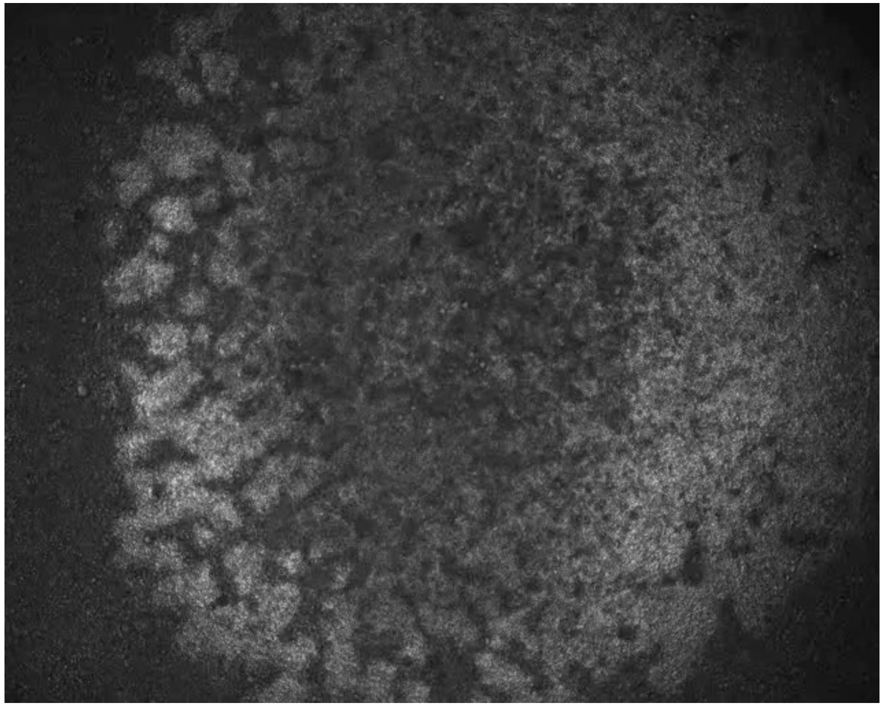




Shape changes in early embryogenesis



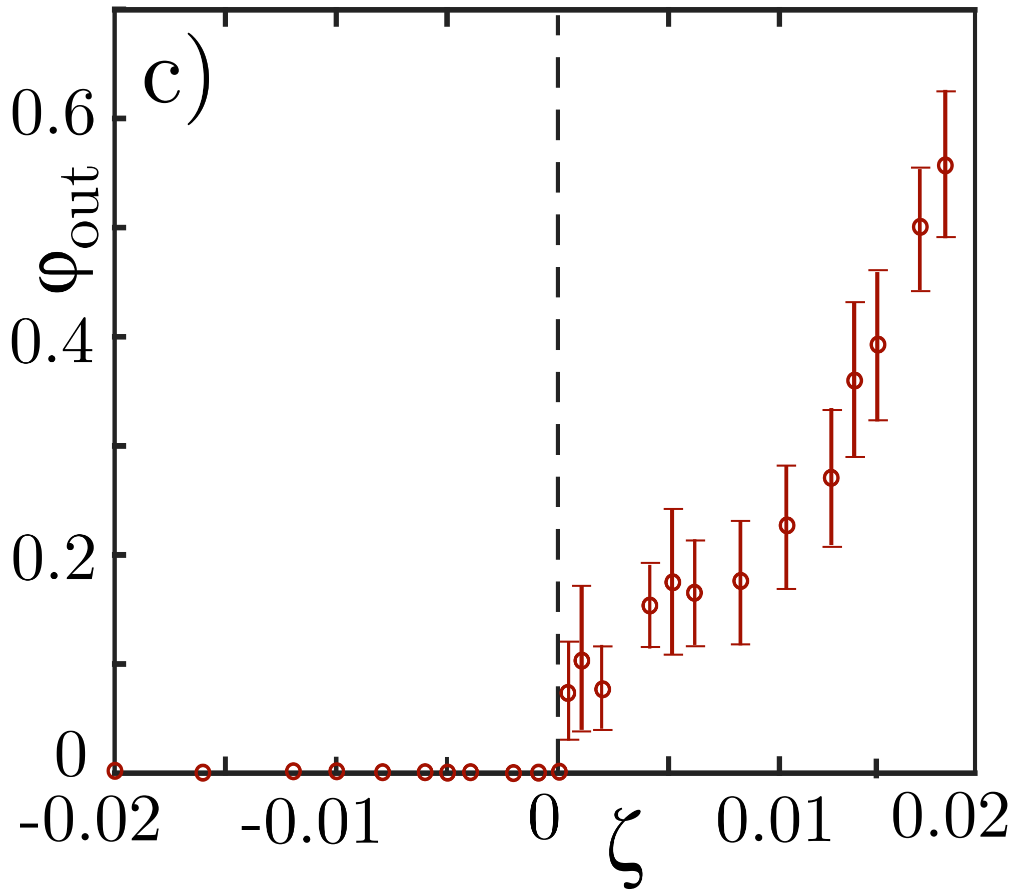
C.J. Weijer, Developmental Biology 2005



From 2D to 3D

2D layer, director and flow field 3D

fraction of nematogens pointing out of the plane



activity

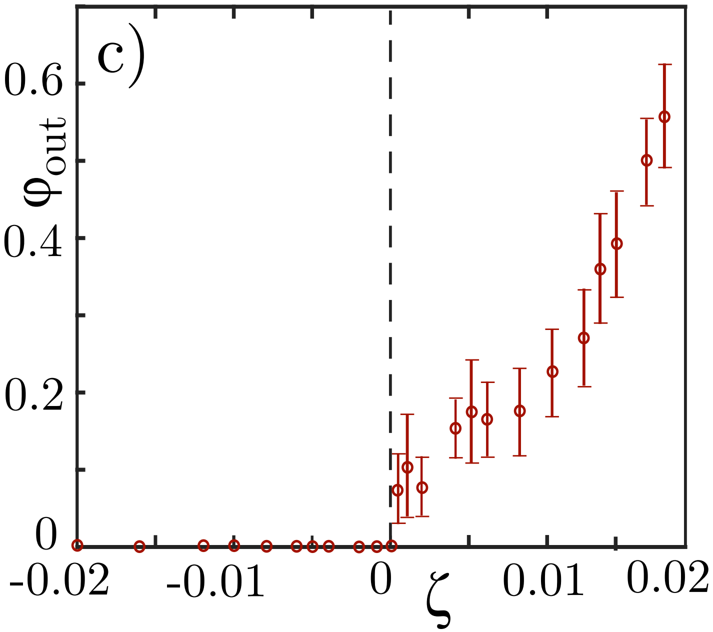
From 2D to 3D

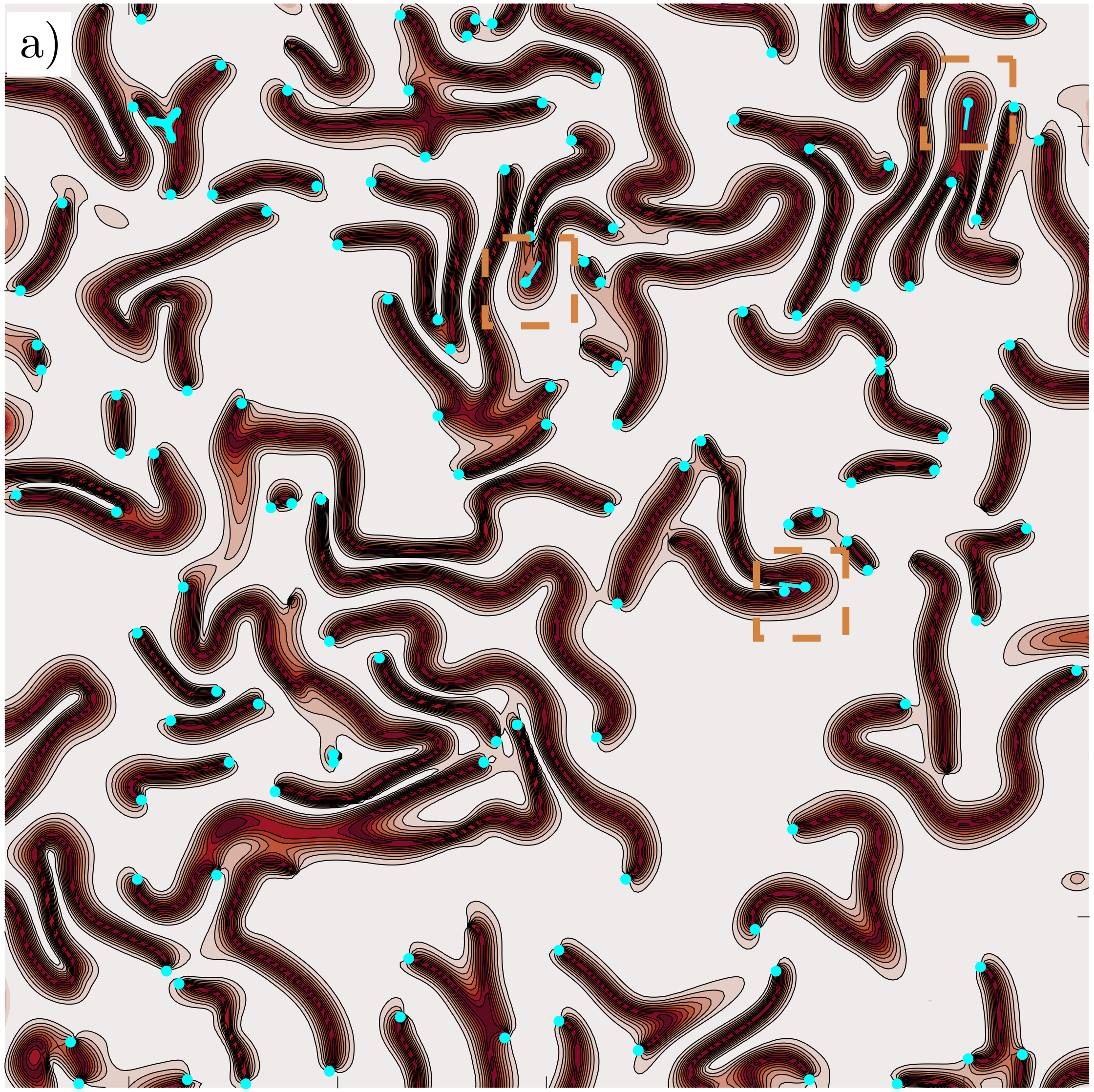
linear stability analysis:

$$\omega_{in} = \frac{3\zeta}{4\eta} \cos 2\theta - \frac{K}{\gamma} q^2$$

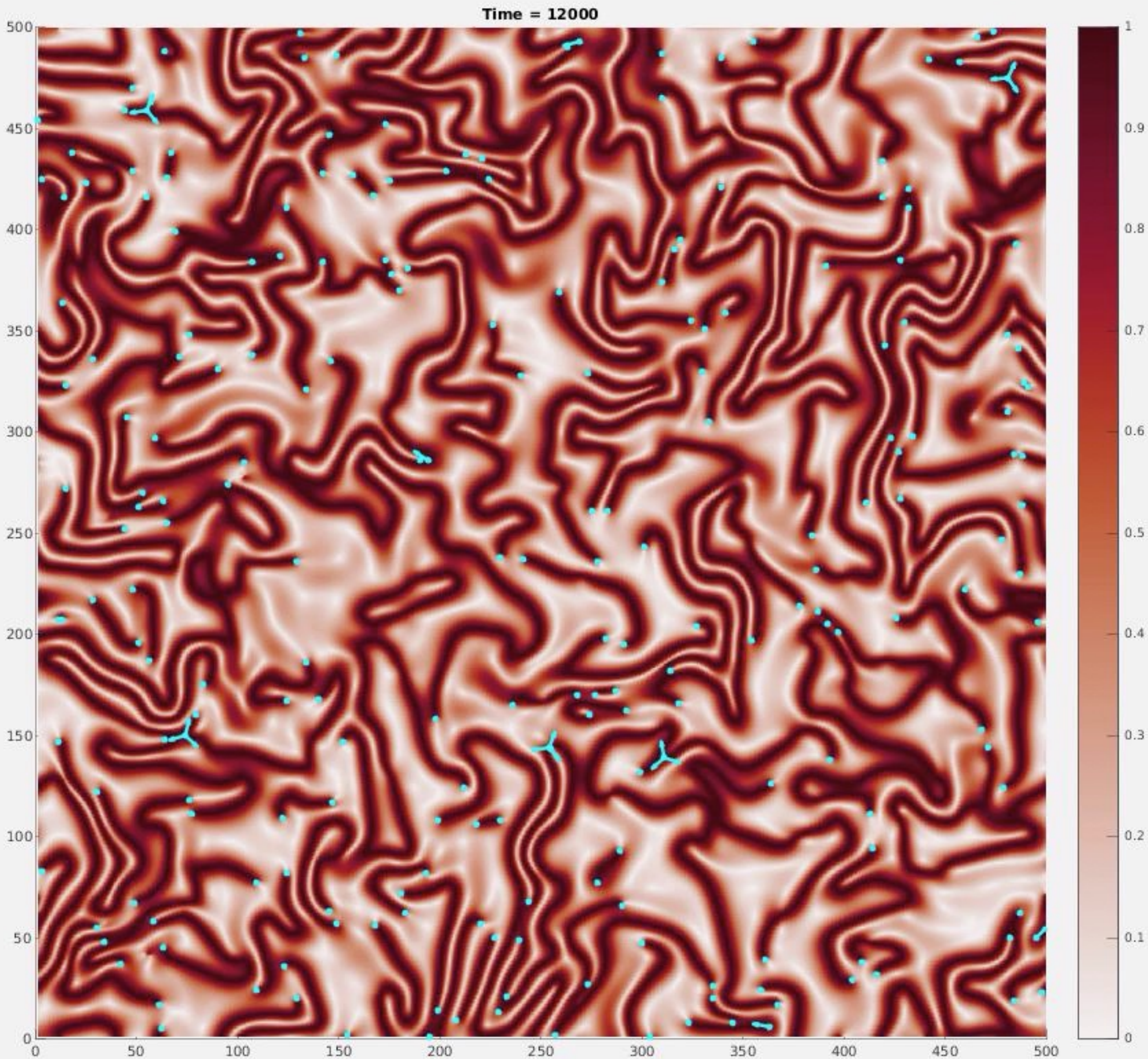
$$\omega_{out} = \frac{3\zeta}{4\eta} \cos^2 \theta - \frac{K}{\gamma} q^2$$

From 2D to 3D





From 2D to 3D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100
150
200
250
300
350
400
450
500
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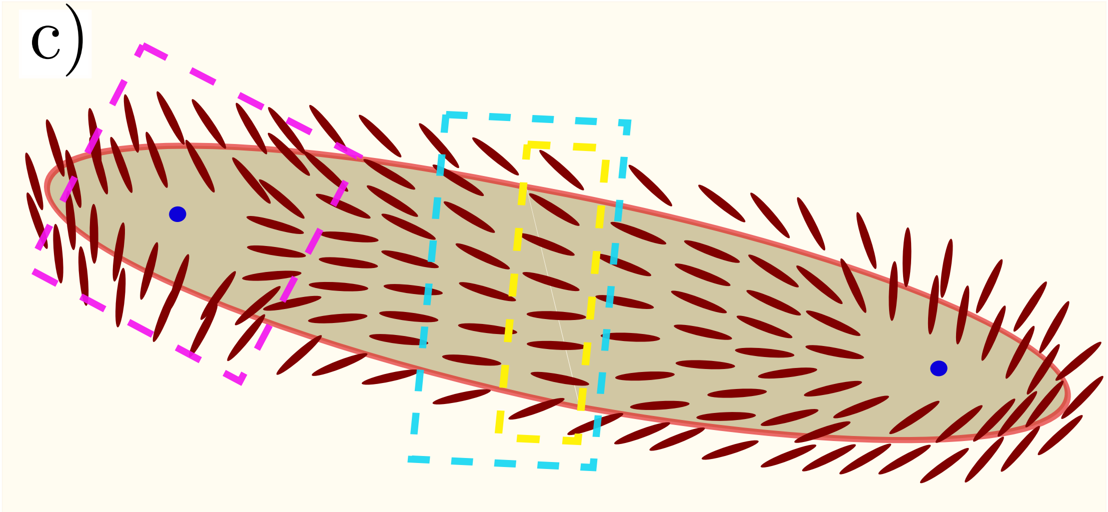
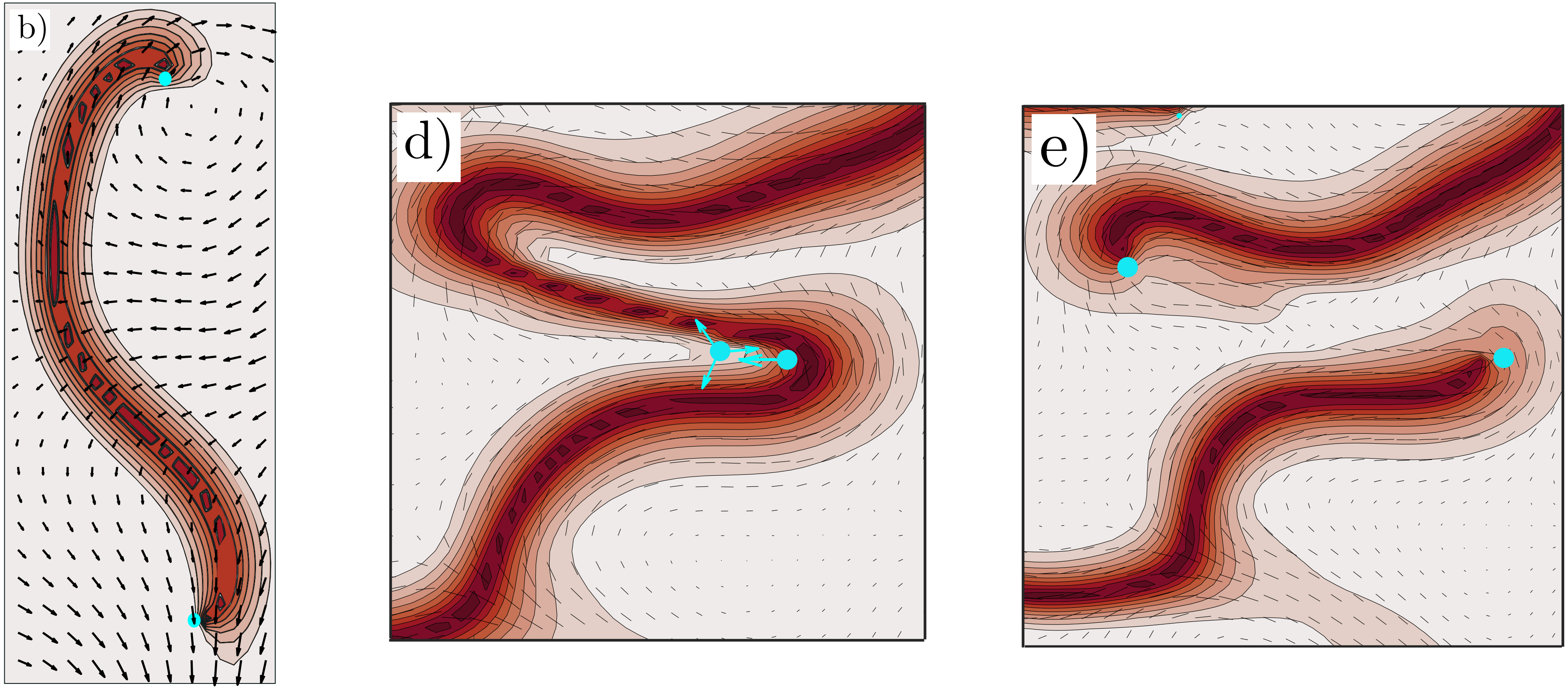
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

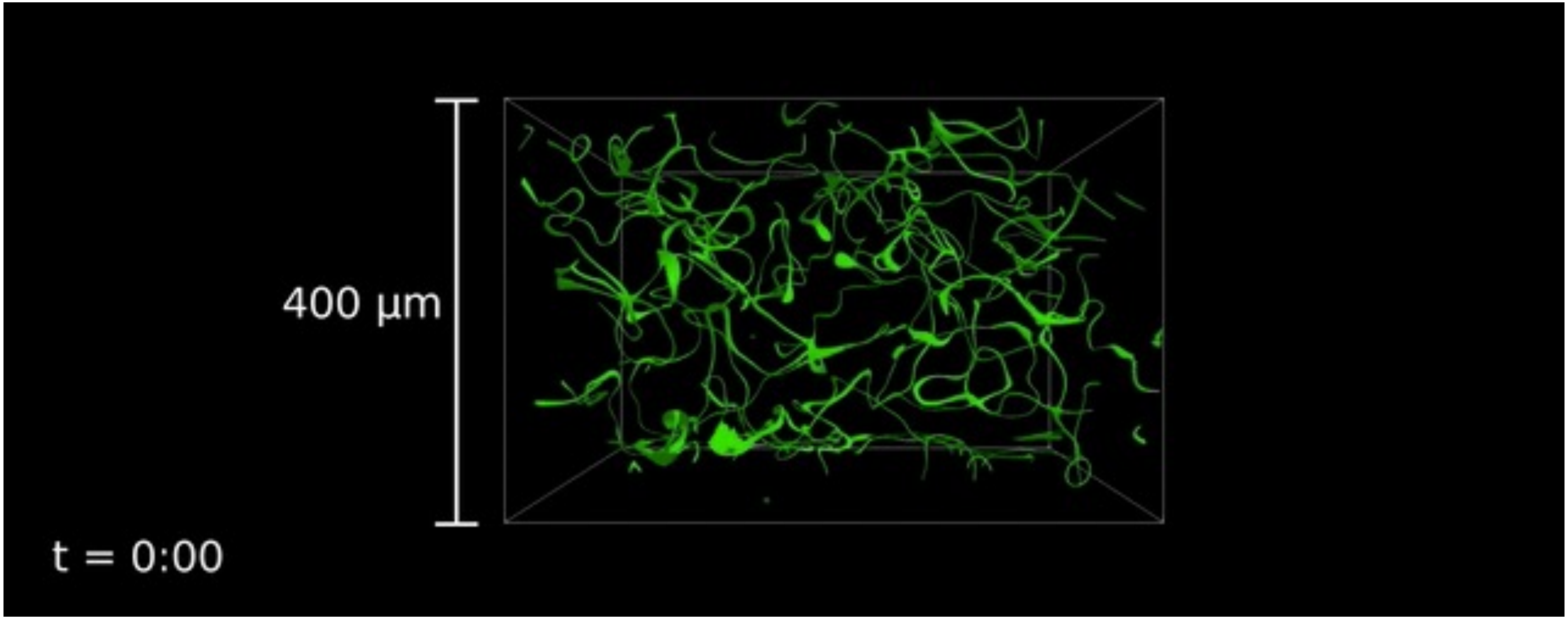


snake director field

snake dynamics



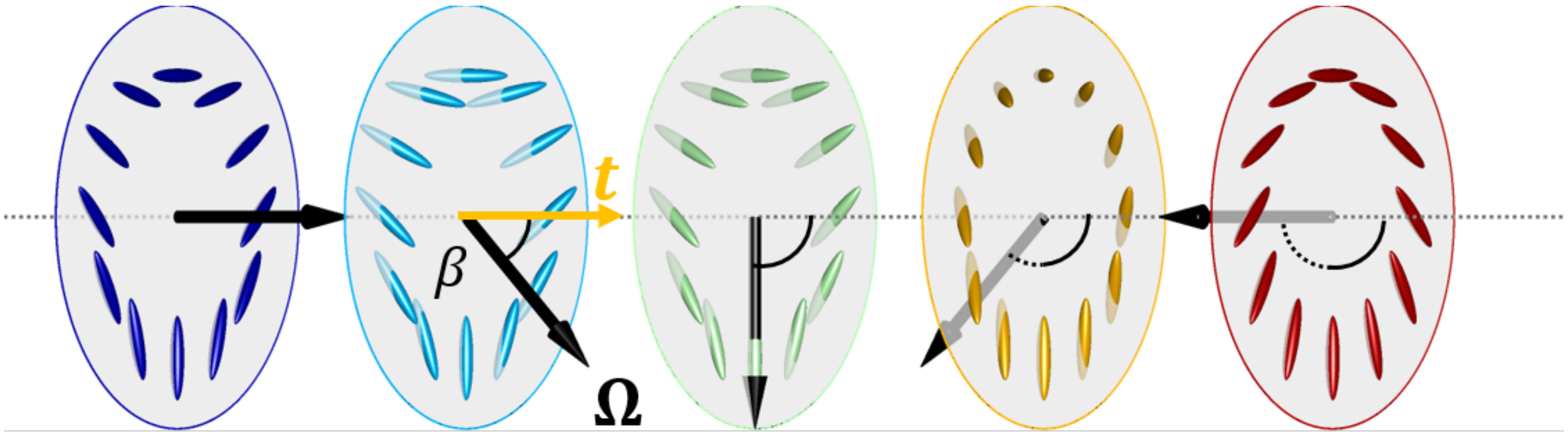
active microtubule bundles in a background of nematic colloids



Duclos et al Science 2020

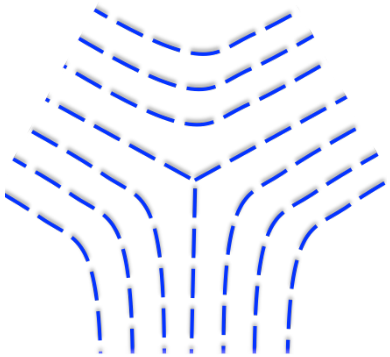
3D: Disclination Lines

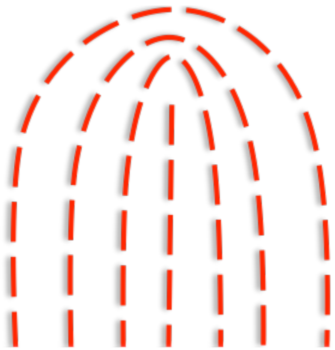
cross section of disclination lines



−1/2 Wedge | Twist | +1/2 Wedge

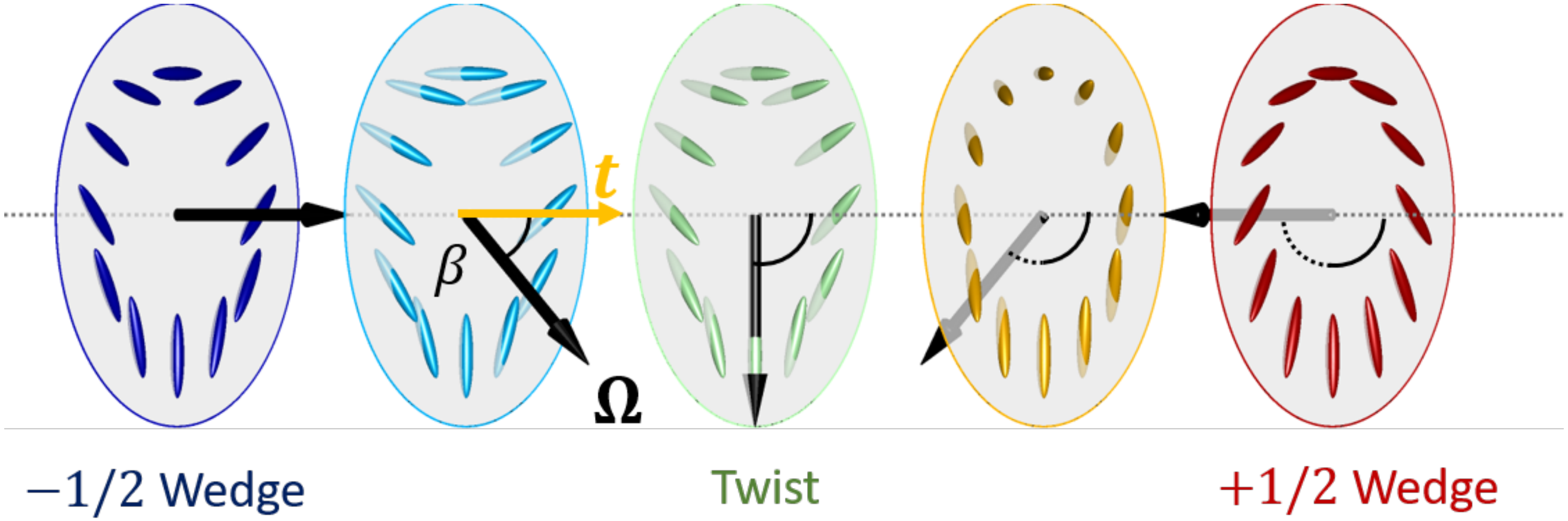
Twist angle: 0 | $\pi/2$ | π

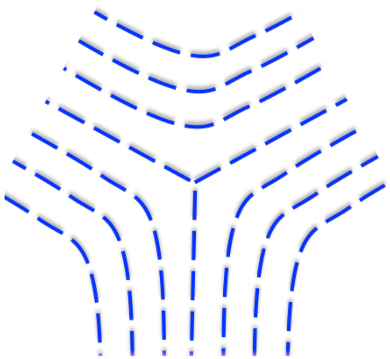


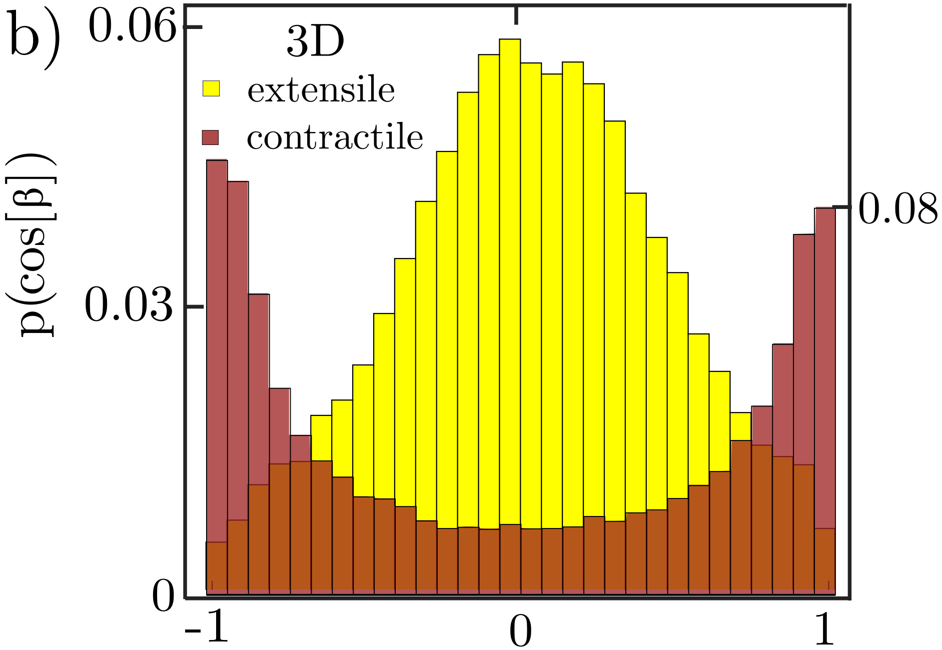


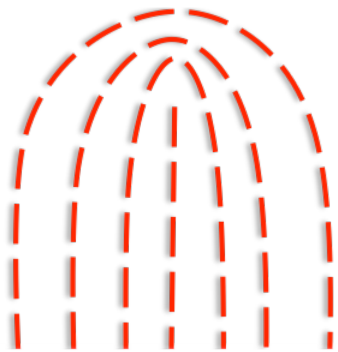
3D: Disclination Lines

cross section of disclination lines

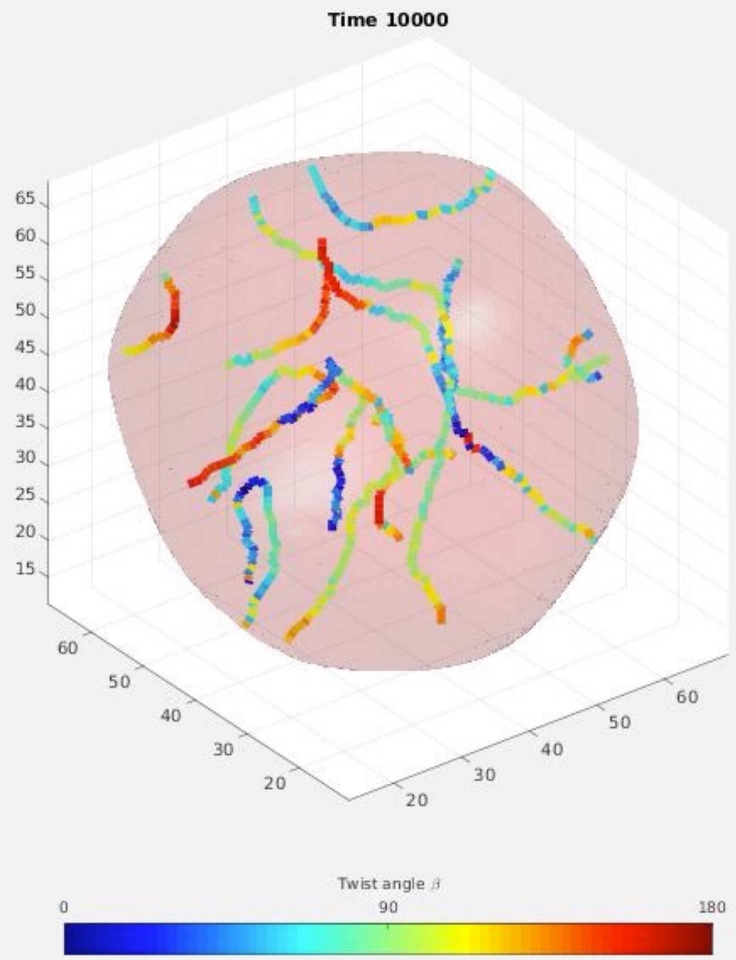


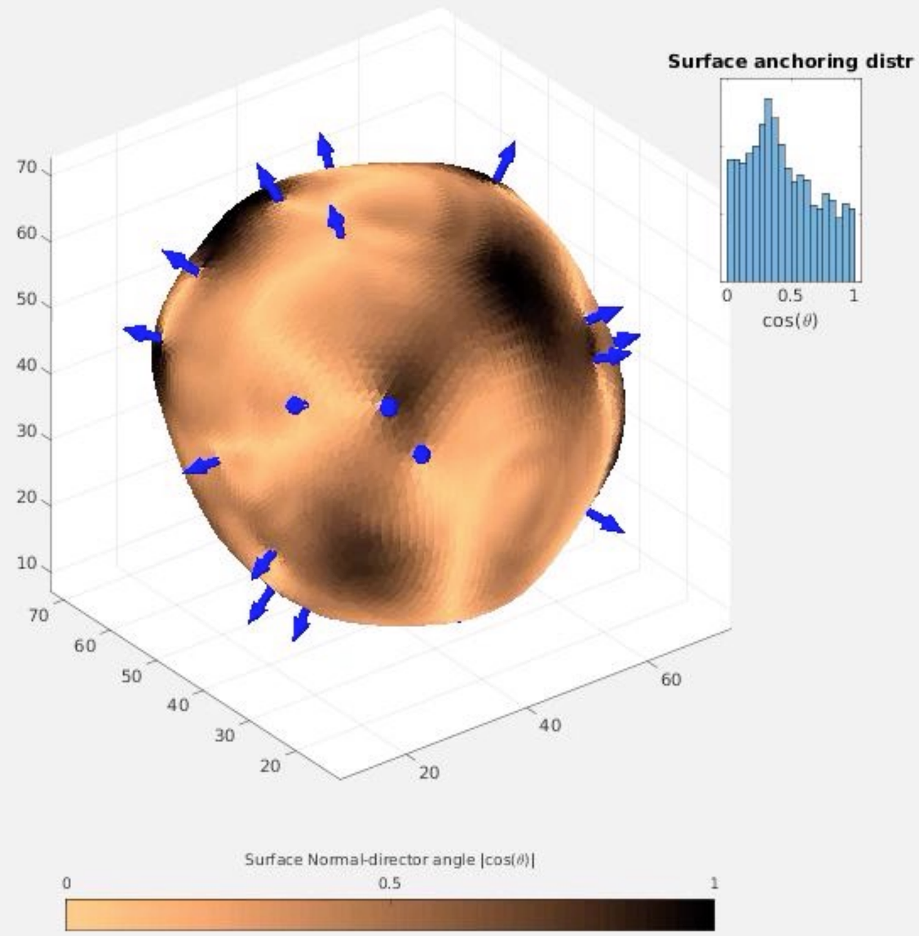




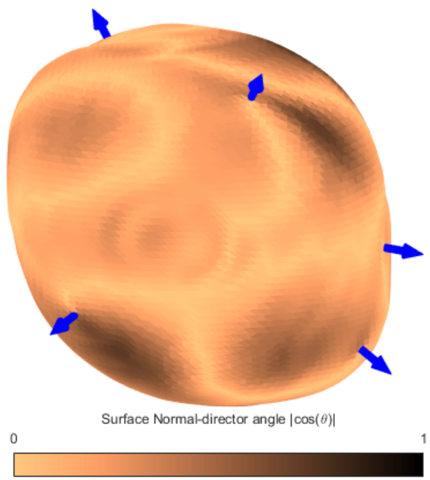


Disclination lines in an active droplet

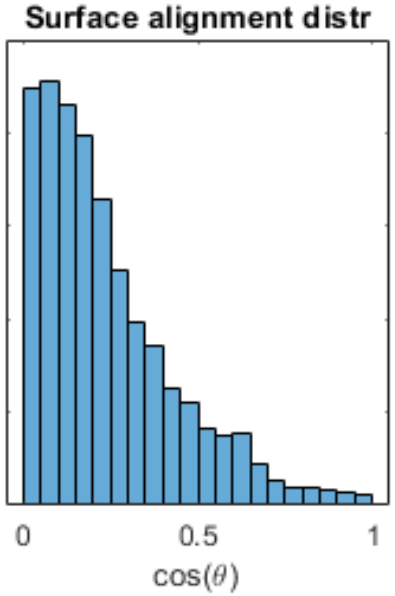


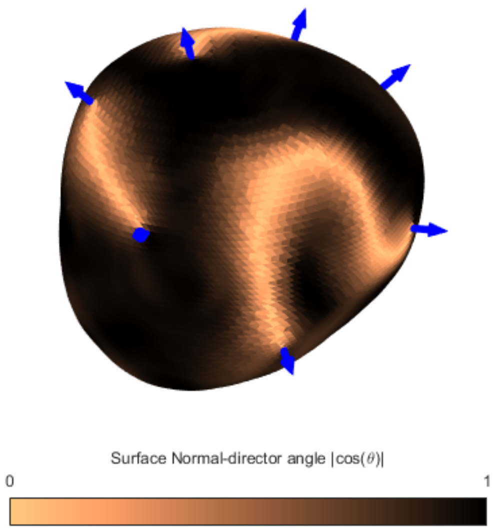


Active anchoring

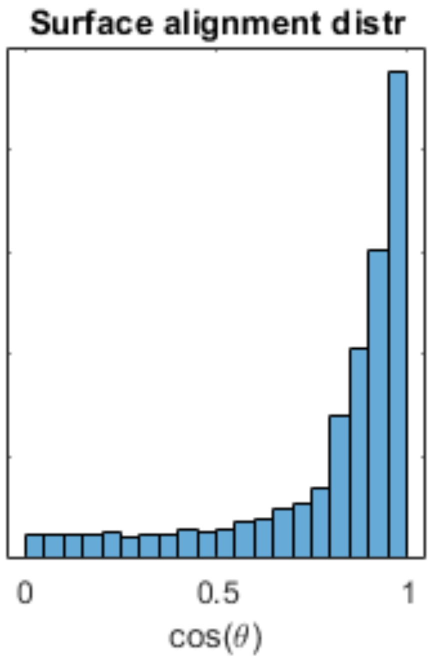


extensile flows =>
In-plane surface
anchoring
(light brown)

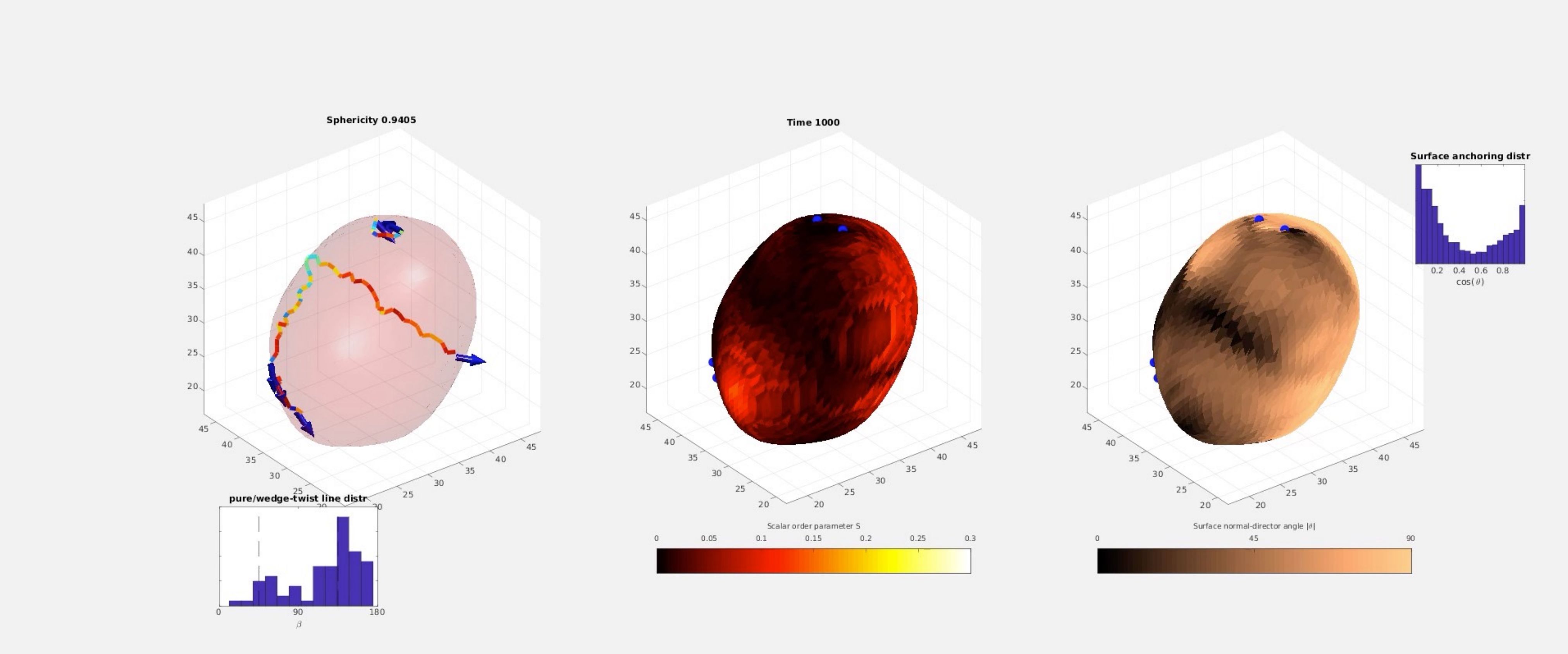




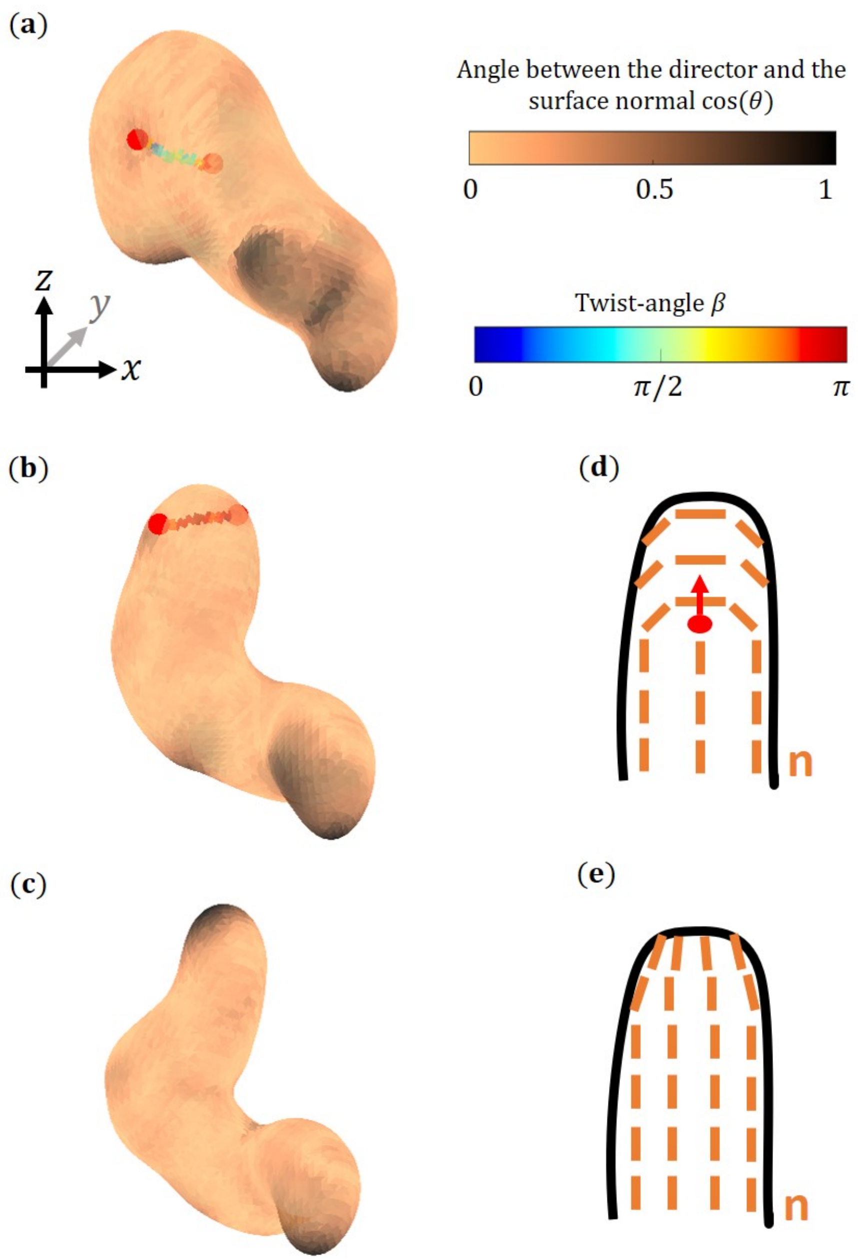
contractile flows =>
normal surface
anchoring
(dark brown)



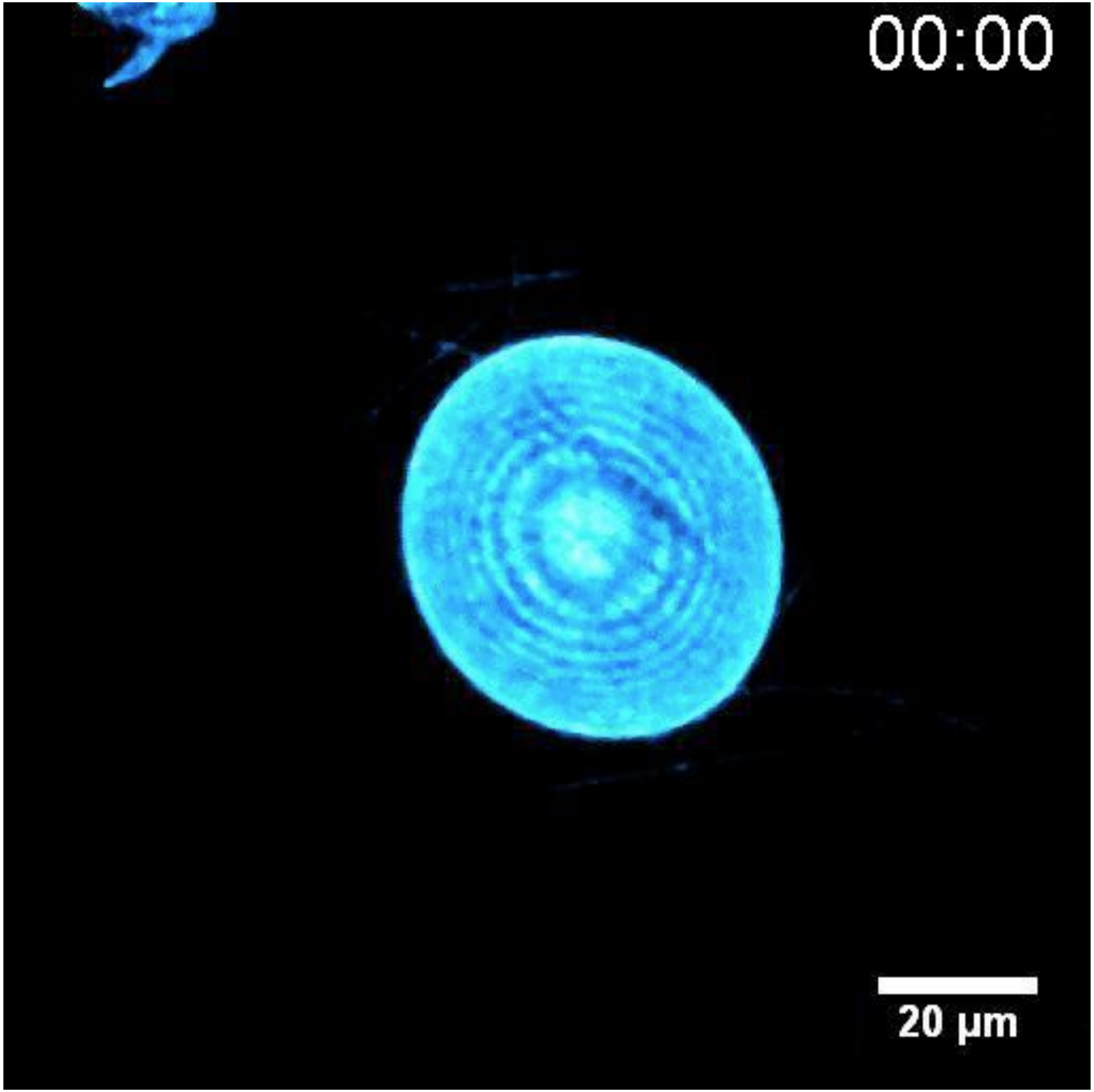
1. Extensile: in-plane anchoring



1. Extensile: protrusions form where disclination lines meet the surface

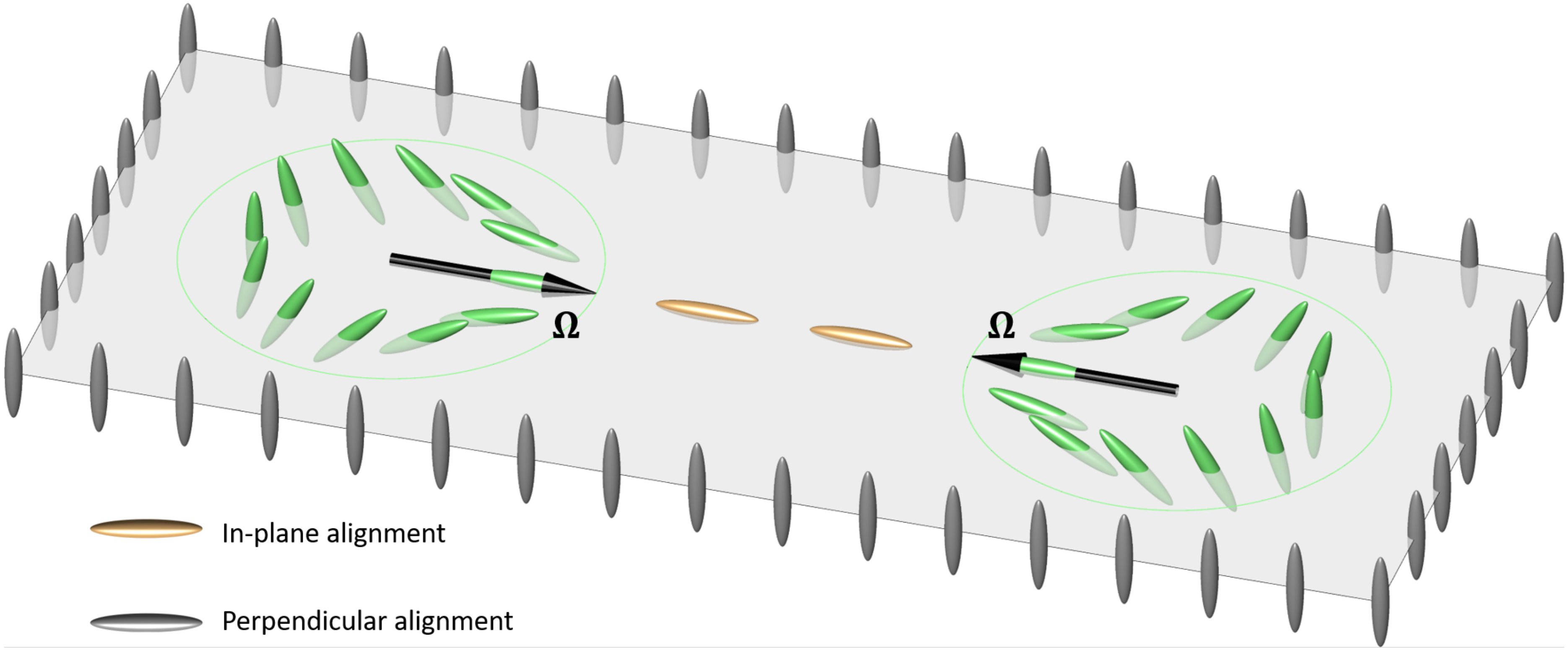


disclination lines tend to line up across protrusions

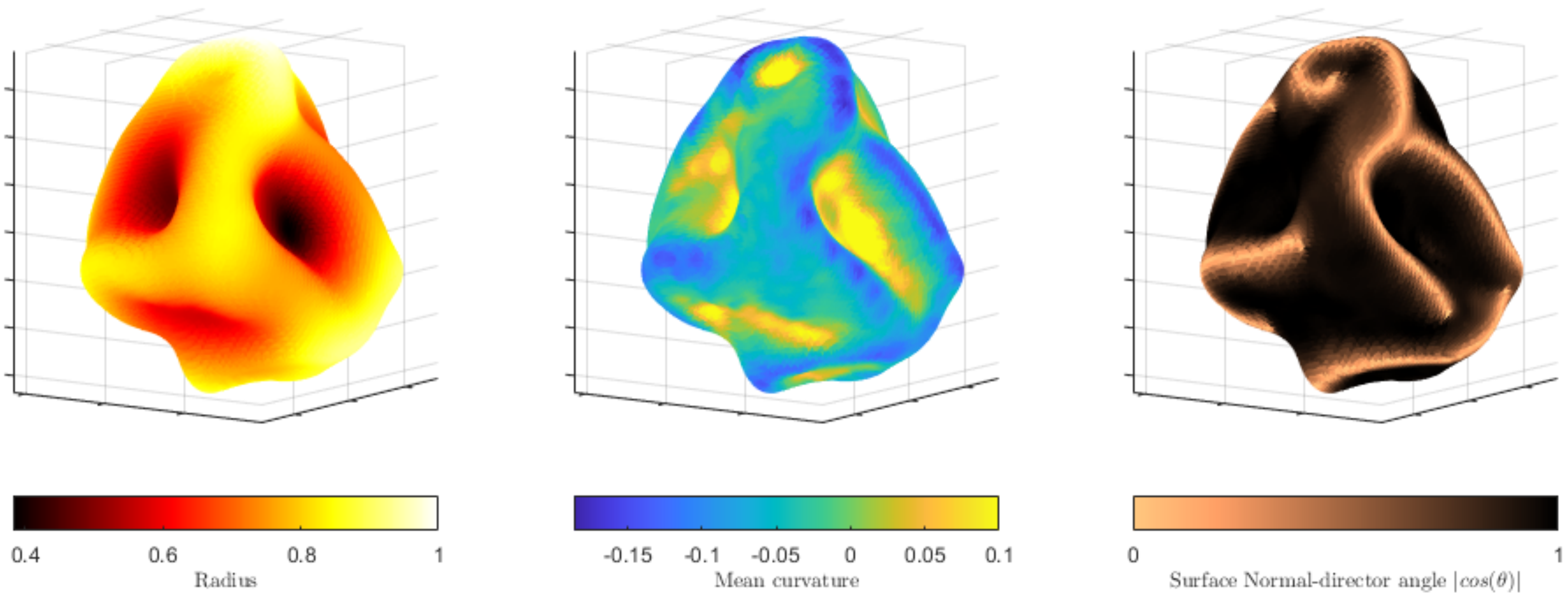


Keber et al
Science 2014

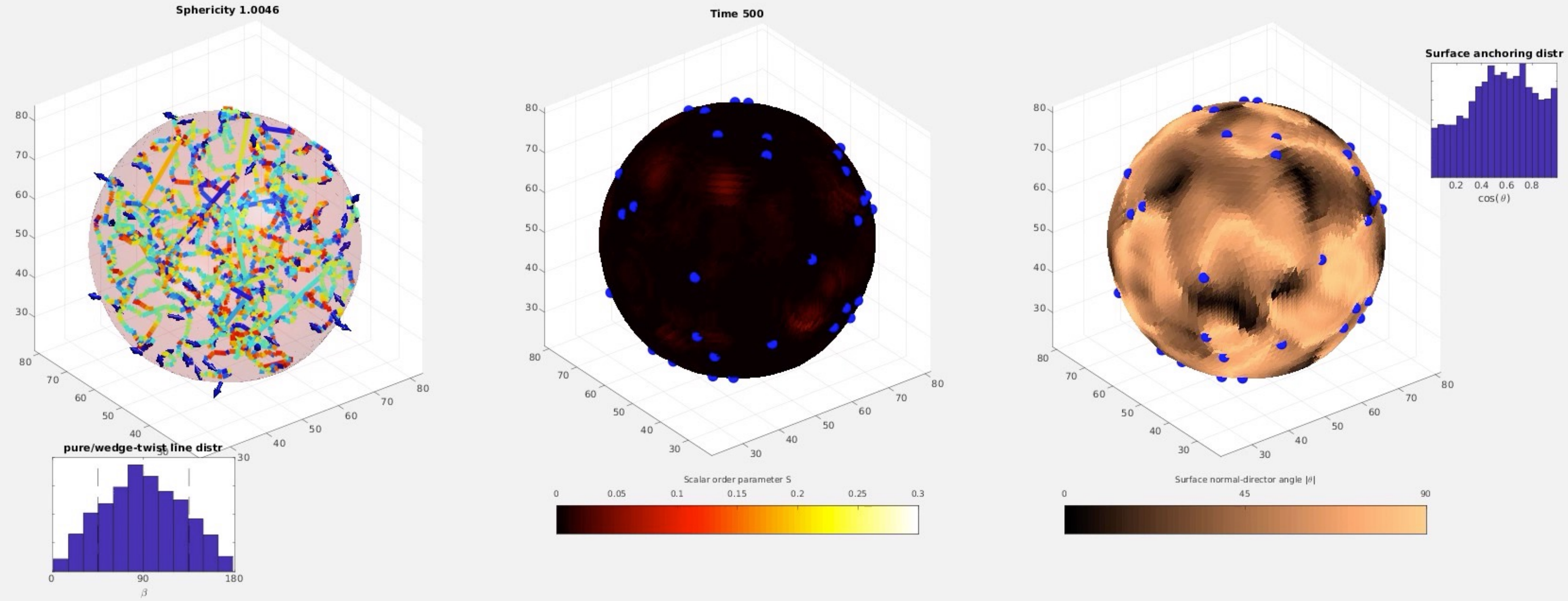
2. Contractile: lines of in-plane alignment at surface



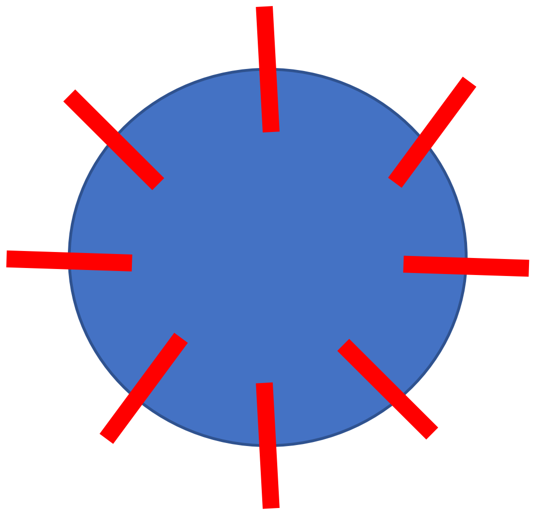
Contractile: surface wrinkles



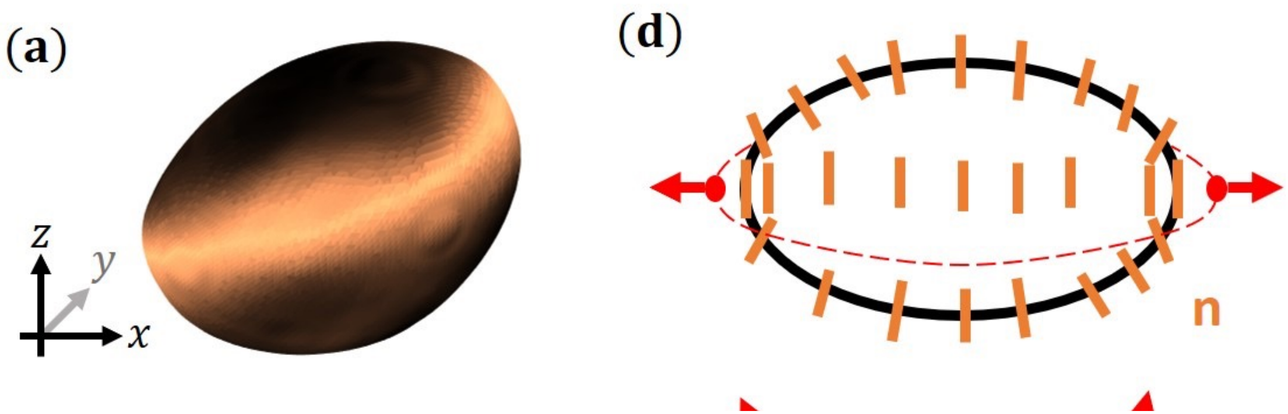
Contractile: surface wrinkles

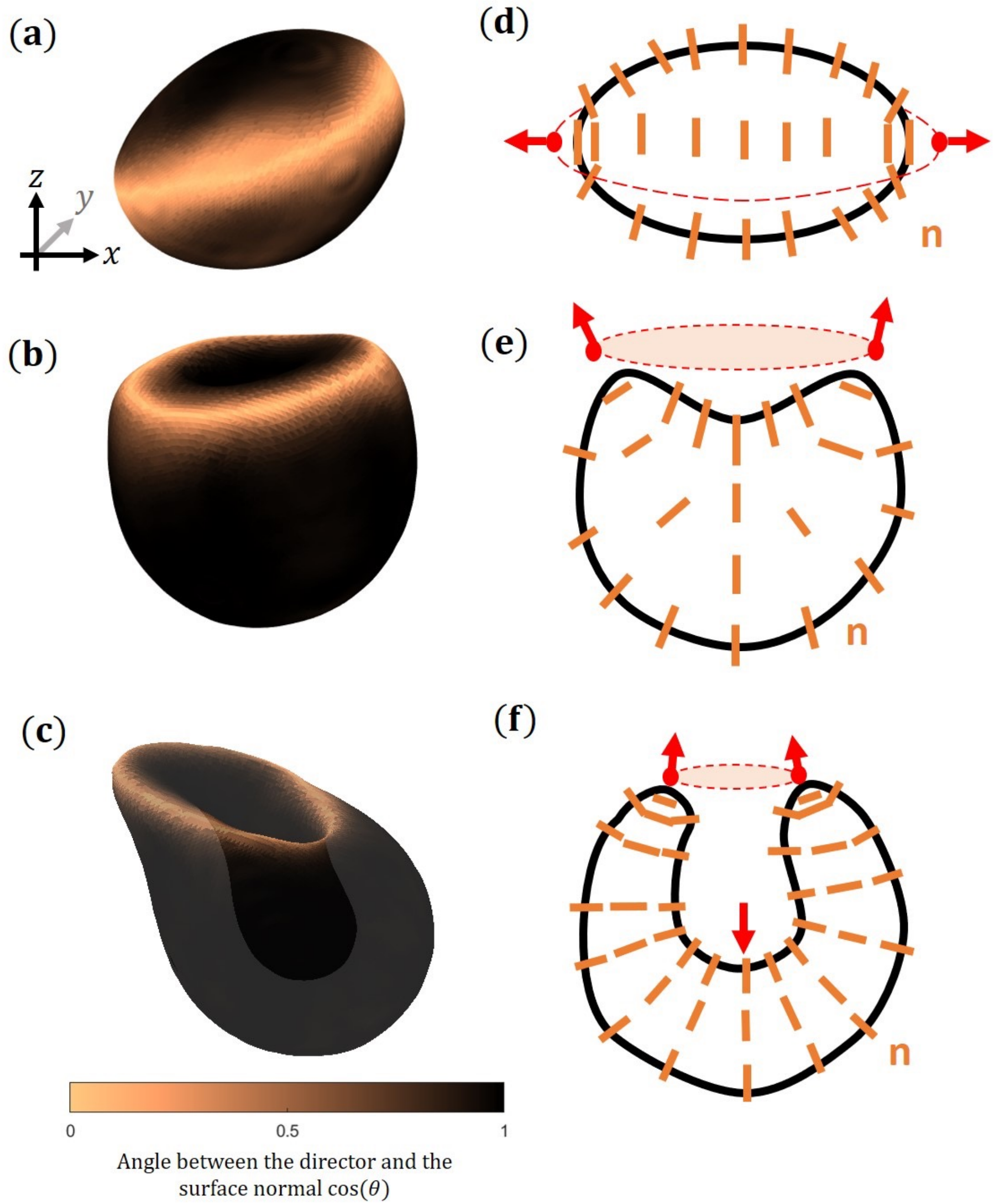


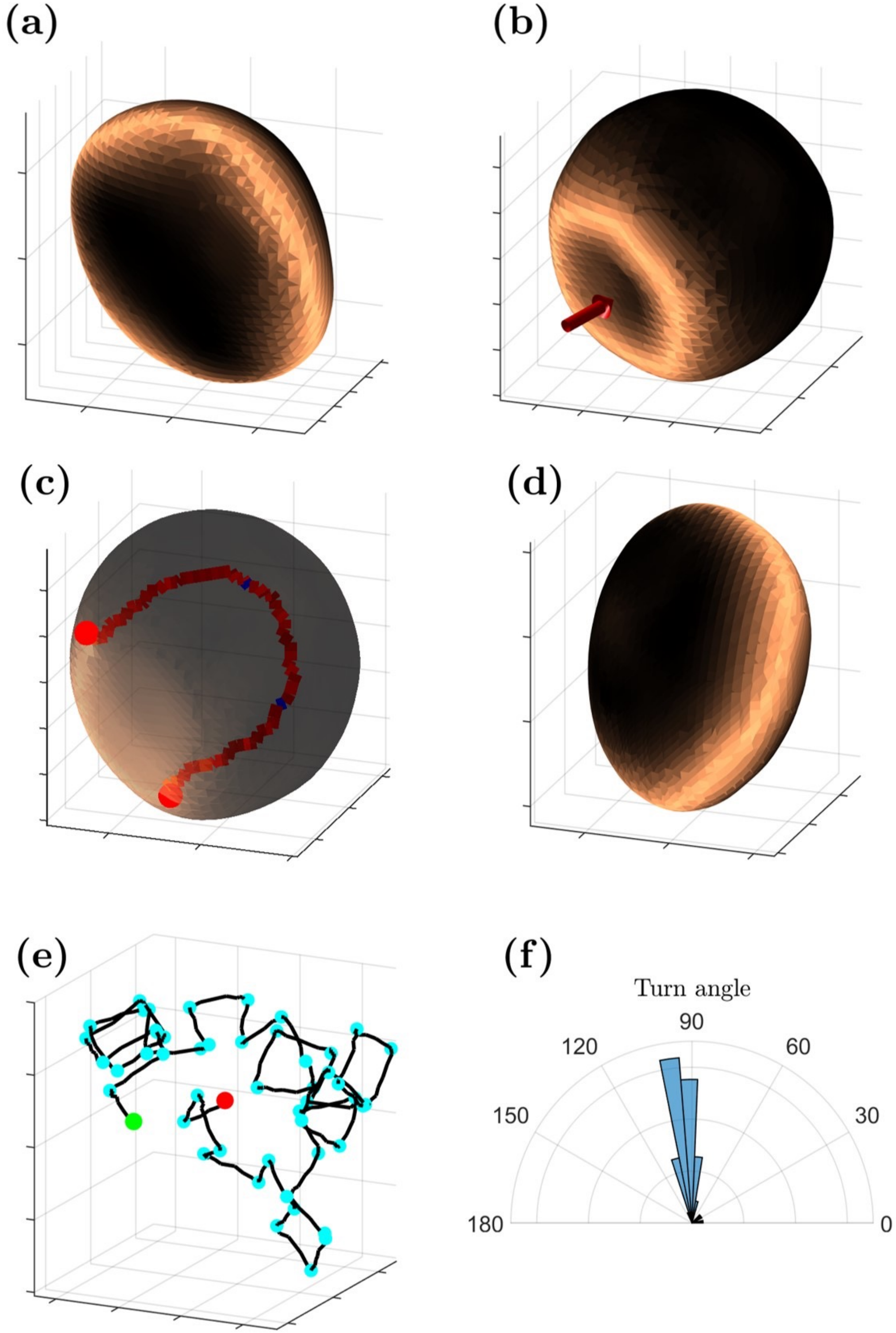
3. Contractile (small droplets):invagination



10

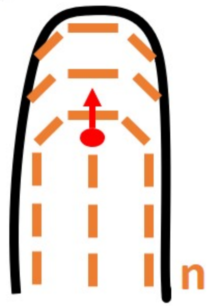



(a)
(b)
(c)
(d)
(e)
(f)
z
y
x
n
n
n
0
0.5
1
Angle between the director and the surface normal cos(θ)


(a)
(b)
(c)
(d)
(e)
(f)
Turn angle
90
120
60
150
30
180
0

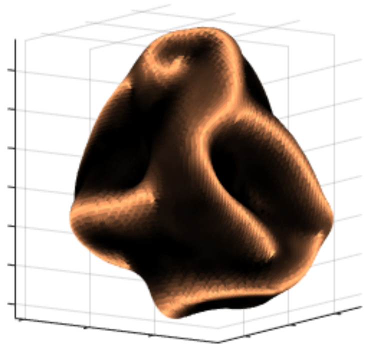
3D active droplet: behaviour depends on active anchoring

(d)



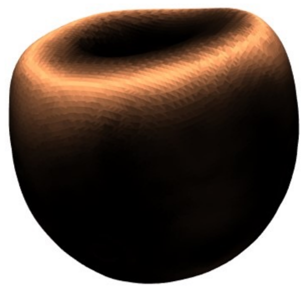
Extensile: protrusions at +1/2 surface defects

Contractile: lines of in-plane anchoring joining surface twist defects => wrinked drops



surface bend ring => invagination, random walk

(b)



Active nematics

- Active turbulence
- Self propelled topological defects

review: Doostmohammadi et al Nature Comms. **9** 3246 (2018)

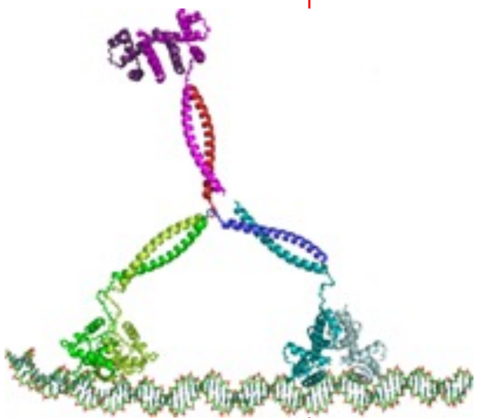
Topological defects in biological shape changes

- from 2D to 3D
- the morphologies of active droplets

Ruske and Yeomans, PRX **11** 021001 (2021)
Nejad and Yeomans, arxiv 2105.10812

Active topological defects in channels

- from laminar flow to active turbulence



Chandragiri et al. , Physical Review Letters **125** 148002 (2020)