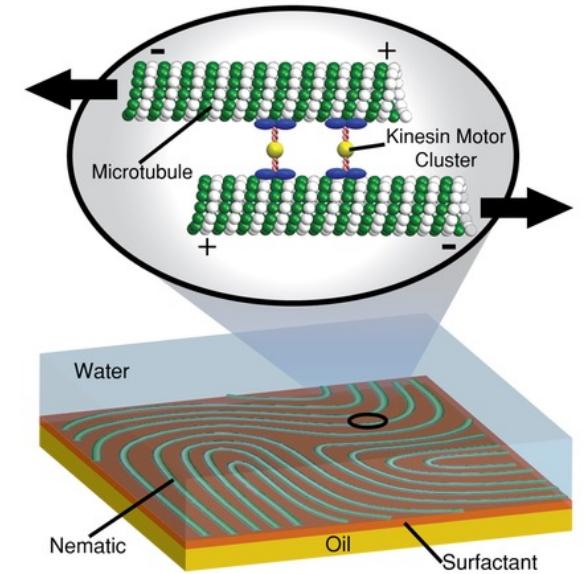
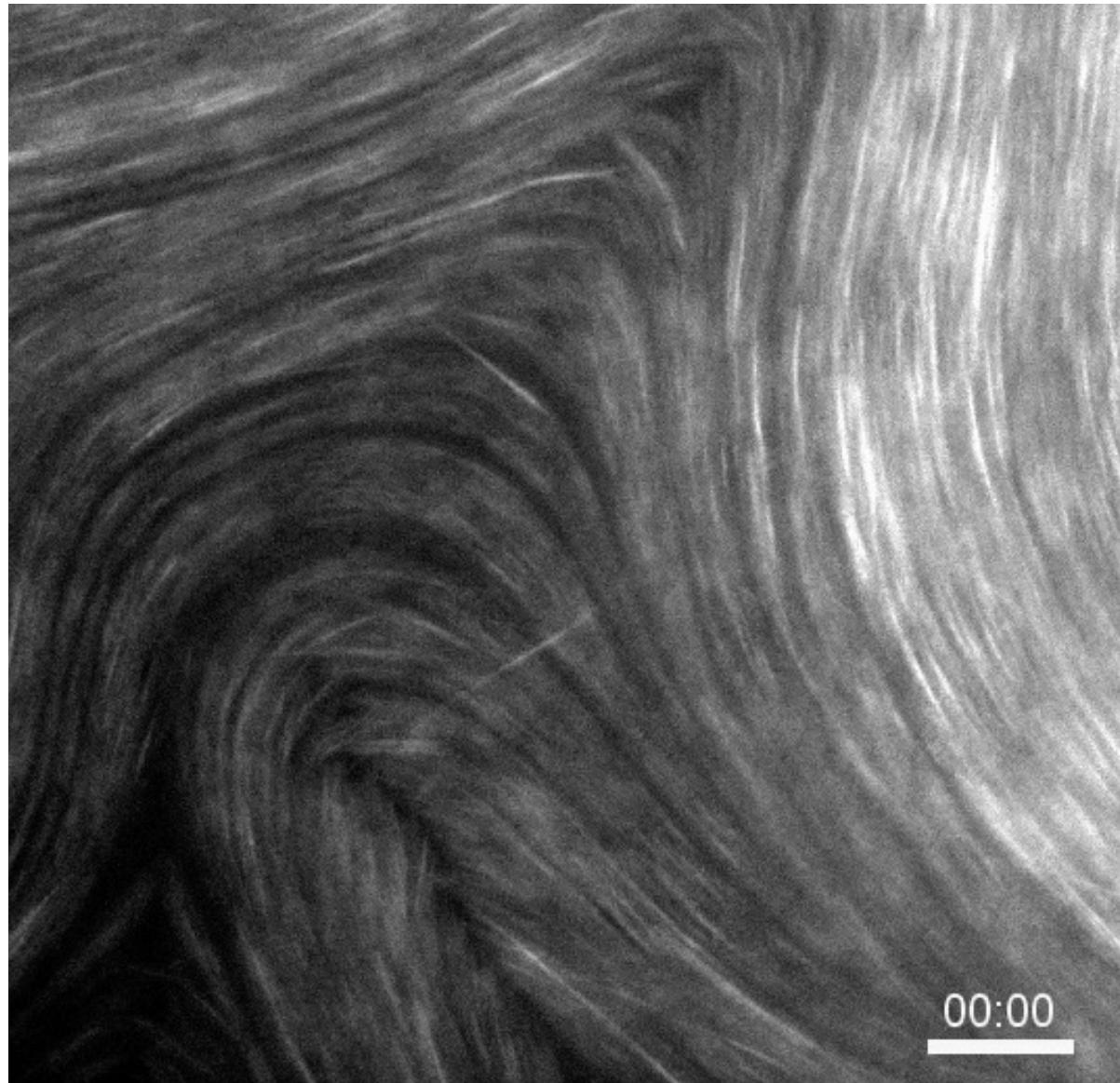


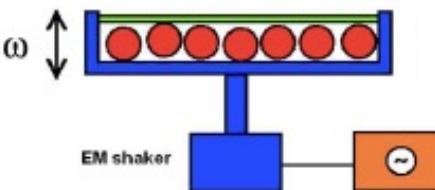
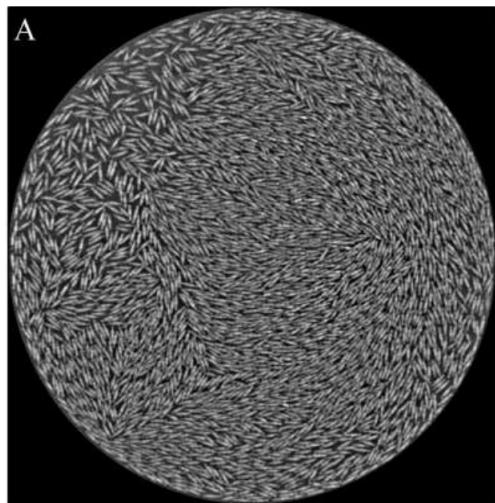
Active nematic liquid crystal: spatiotemporal chaotic flows and topological defects



Tim Sanchez *et al.*
Nature 2012

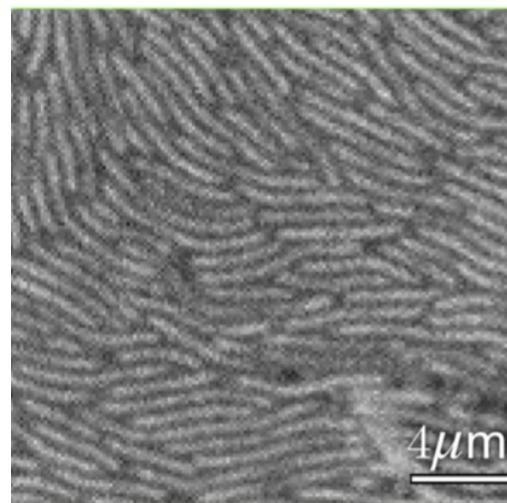
Nematic Order Ubiquitous in Active Systems

Vibrated rods



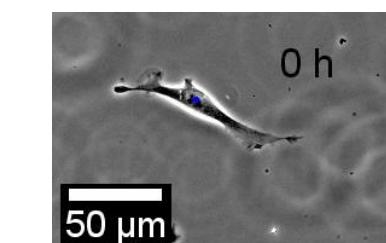
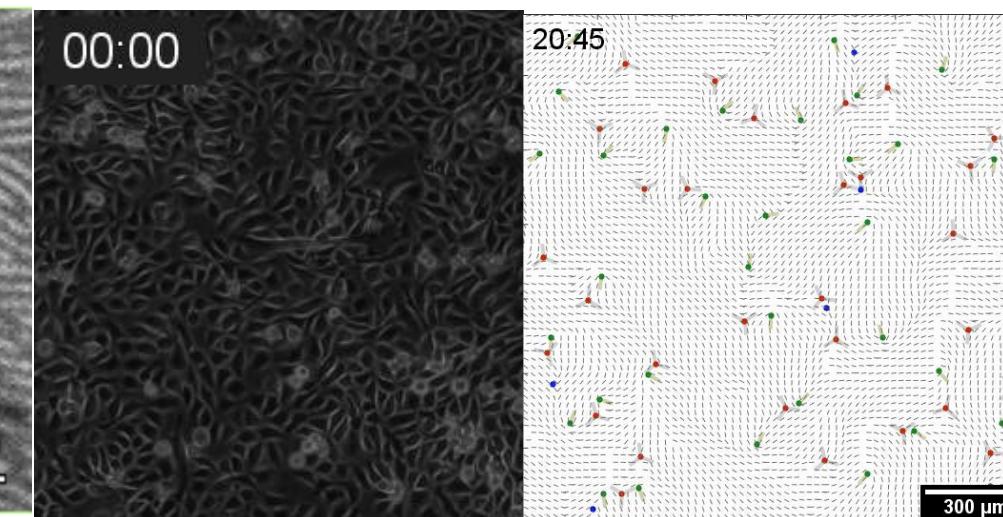
Narayan *et al.*
Science 2007

Myxococcus Xanthus



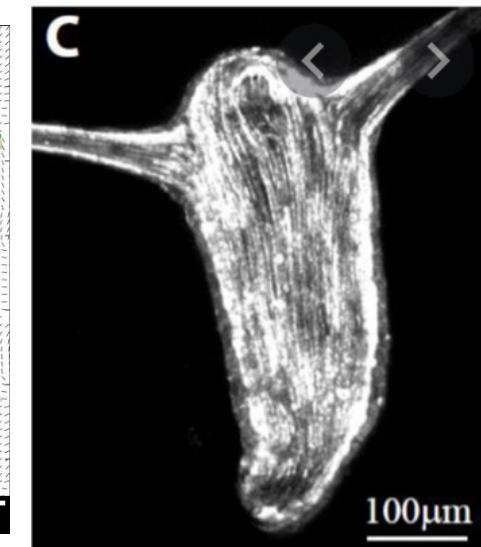
Copehangen *et al.*
Nat Phys 2020

Cell sheets



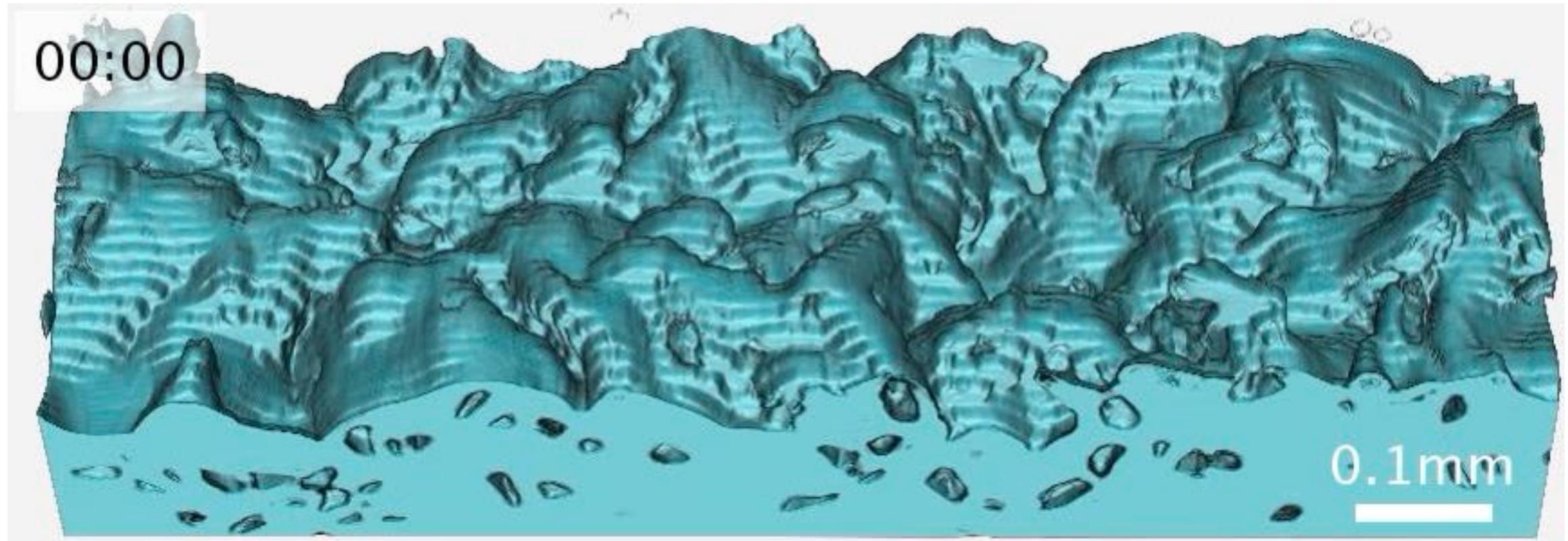
Blanch-Mercader *et al.*
PRL 2018

Hydra



Maroudas-Sacks *et al.*
Nat Phys 2020

3D realization



Liang Zhao, UCSB

- Nematic liquid crystals
- Quantifying order: Q-tensor
- Landau-de Gennes free energy
- Excitation and Topological defects
- Nematic Hydrodynamics
- Active stresses and Active nematic hydrodynamics
- Motile topological defects
- Some directions of current research



Passive nematics

Orientational Order in Active Matter

Active units are often elongated and can align due to a variety of interactions, organizing in states with orientational order.

Two types { direction ≠ orientation }

1) polar/ferromagnetic $\uparrow \uparrow \uparrow \vec{p}$ unit vector

order of polar particles

Order parameter is a vector field

I could represent the probability distribution of molecular direction w/ a function of \vec{p} , $\Psi(\vec{p})$

$$\int d\vec{p} \Psi(\vec{p}) = 1 \quad \text{isotropic state } \Psi = \frac{1}{Z_N} - 2d$$

First moment

$$\int d\vec{p} \vec{p} \Psi(\vec{p}) = \vec{m} \quad \text{order vanishes in isotropic state}$$

2) apolar

/ still use a unit vector \vec{p} to identify orientation, by $\vec{p} = -\vec{p}$

$$\Psi(\vec{p}) \text{ must satisfy } \Psi(\vec{p}) = \Psi(-\vec{p})$$

The first moment that will be $\neq 0$ is

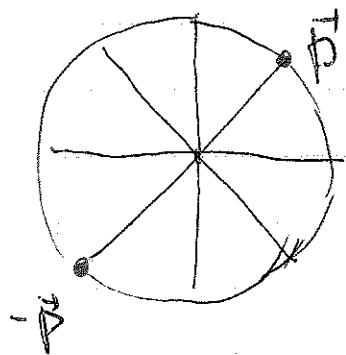
$$M_{ij} = \int d\vec{p} \vec{p}_i \vec{p}_j \Psi(\vec{p}) \quad \text{isotropic state } M_{ij} = \frac{1}{2} \delta_{ij}$$

$$Q_{ij} = \int d\vec{p} (\vec{p}_i \vec{p}_j - \frac{1}{d} \delta_{ij}) \Psi \quad \text{de Gennes Q-tensor}$$

More geometrically:

in 2d the space of orientations are lines through the origin — but points separated by π must be identified

of length 1

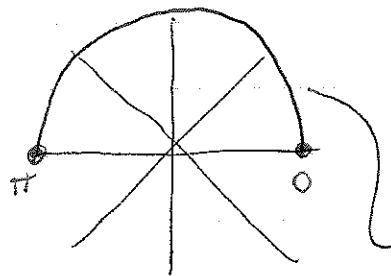


Need a quantity quadratic in \vec{p}
invariant for $\vec{p}, -\vec{p}$

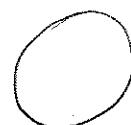
$\vec{p} \otimes \vec{p}$ a matrix

($\vec{p} \cdot \vec{p}$ is invariant but does
not identify orientation)

The space of possible \vec{p} values is $1/2$ circle



but the two red points are the same
→ topology of a circle

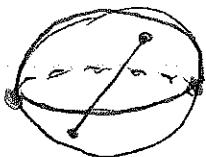


S^1/\mathbb{Z}_2

S^1 circle

$\mathbb{Z}_2 = (+1, -1)$ inversion

3d antipodal identified



but all opposite point on equator
are the same

S^2/\mathbb{Z}_2

ACTIVE NEMATIC LIQUID CRYSTALS

Nematic order is seen ^{many} in biological systems, from chromosome territories to cell monolayers (epithelia, stem cells) to entire organisms.

First a brief introduction to the physics and dynamics of nematic liquid crystals, then move on to active systems.

For reviews w/ experimental references

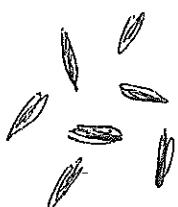
- MCM et al RMP (2013) 85, 1143
- A Doostmohammadi et al Nat Comm 9, 3246 (2018)
- Bowcock et al PRX 12, 010501 (2022)
- Shukar et al Nat Phys Revews 4, 380 (2022)

Crystals have both translational (T) and orientational (O) order (long-ranged in 3d)

Liquids have neither

Liquid crystals are fluid of rod-like molecules that can exist in states with O order, but no T order

isotropic liquid

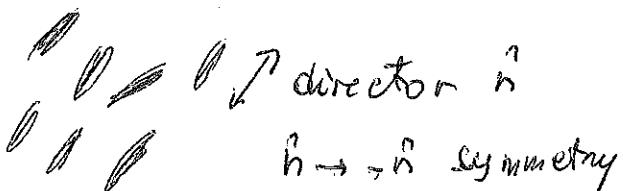


increase density

or

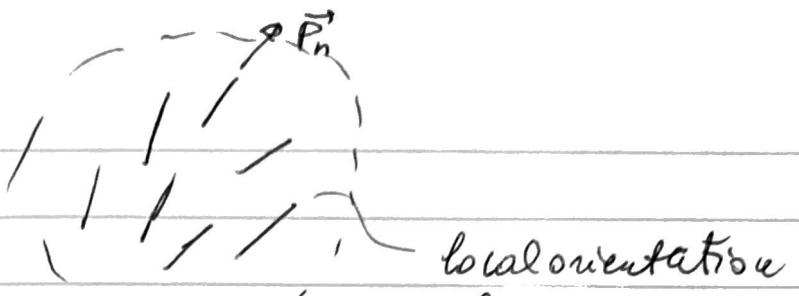
lower T

nematic LC



The transition occurs in systems of purely repulsive hard rod - Onsager 1949
steric effects vs entropy

Coarse-graining



$$Q_{ij} = \left\langle \frac{1}{N} \sum_n \left(P_n : P_{nj} - \frac{1}{2} \delta_{ij} \right) \right\rangle$$

symmetric traceless

$$\text{uniaxial liquid crystal } Q_{ij}(r) = S(r) \left(n_i n_j - \frac{1}{2} \delta_{ij} \right)$$

$$Q = \frac{S}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}$$

S = magnitude of nematic order

$$Q \rightarrow S e^{2i\theta}$$

$$\vec{n}(r) \text{ director } |\vec{n}| = 1$$

Onsager 1949 isotropic-nematic transition
in hard twin repulsive rods.

Gain entropy and lower free energy by aligning

$$S = k_B \ln (\# \text{ states})$$

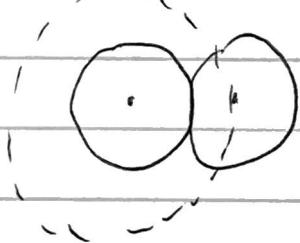
ideal gas

$$S \sim k_B \ln V^N$$

excluded volume

$$S \sim k_B \ln (V - N_{\text{ex}})^N$$

S increases as N_{ex} decreases



aligned rods have smaller N_{ex}

Continuum level:

Order Parameter field of a uniaxial nematic is a symmetric, traceless, rank-2 tensor

$$Q_{ij}(\vec{r}, t) = S(\vec{r}, t) \left[n_i(\vec{r}, t) n_j(\vec{r}, t) - \frac{1}{d} \delta_{ij} \right]$$

magnitude of
order

$S = 0$ disordered

$S = 1$ ordered

$\vec{n}(\vec{r}, t)$ director
 $|\vec{n}| = 1$

direction of
spontaneously
broken symmetry

Energy and dynamics must respect $\vec{n} \rightarrow -\vec{n}$
symmetry

→ Landau - de Gennes
free energy

Landau - de Gennes free energy

describes ground states and excitations

invariants

$$\text{Tr } Q^2 \sim S^2, \text{ Tr } Q^3 \sim S^3, (\text{Tr } Q^2)^2 \sim S^4$$

$$2d \quad \text{Tr } Q^3 = 0$$

$$F_{GL} = \int d\vec{r} \left\{ \frac{A(g)}{2} \text{Tr } Q^2 + \frac{B}{4} (\text{Tr } Q^2)^2 + \frac{K}{2} (\partial_i Q_{jk})^2 \right\}$$

$A(g) < 0$ ordered state

\uparrow
different
elastic

$$S^2 = -A/B \rightarrow 1$$

$\vec{n} = (\cos \theta, \sin \theta)$ spontaneously
broken symmetry

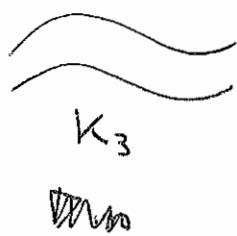
constants

We will work deep in the nematic state
where $S \approx 1$

Free energy of director distortions (Frank)

$$F = \frac{1}{2} \int d\vec{r} \oint K (\nabla \cdot \vec{n})^2$$

bend



splay



3d

twist

K_2

Topology describes properties that are conserved under continuous deformations of shape

Ground state Compare to ferromagnetic polar g.s.

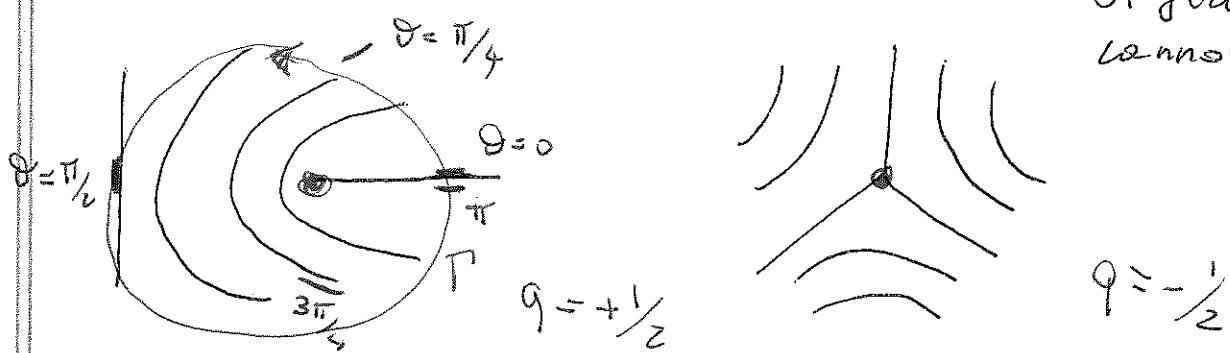
We will work deep in the ordered state where $S=1$ and only consider deformations of the director field. This is just to simplify our life and work with vectors instead of tensors.

Also for simplicity we consider 2d line

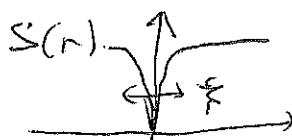
Smooth deformations "spin waves"



Singular distortions : topological defects - a tear in the OP field that cannot be patched



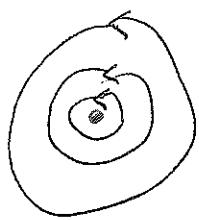
At the core (red dot) the director does not know where to point (and $S \rightarrow 0$)



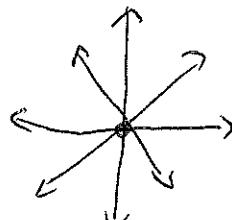
charge or winding number $q = \frac{1}{2\pi} \oint d\theta$ net angle through which the op rotates as one circles the defect

$q = \pm \frac{1}{2}$ defects \rightarrow disclinations Γ

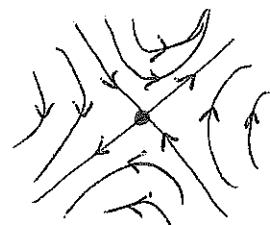
Vector field - let us compare. cannot have $\pm \frac{1}{2}$ defects



$$q = +1$$



$$q = +1$$



$$q = -1$$

A nematic can have charge $q = \pm 1$ defects

But the energy cost for creating a defect $\sim q^2$

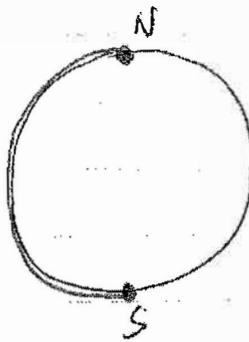
Hence ± 1 defects cost 4 time more energy $\sim q + 1$ will decay in $2 + \frac{1}{2}$.

- Topological charge is conserved
 - Blasius' theorem Net topological charge is zero in the plane, +2 on a sphere, +1 in a disc
 - In 3d defects are lines and loop.
 - global excitations
 - quaniparticles : in 2d the stat phys of defects can be mapped out that of Coulomb charges
- $$V(r) = 2\pi k q_i q_j \ln\left(\frac{|r_{ij}|}{a}\right)$$
- like repel
unlike attract

- fingerprint of broken symmetry

Topological defects are noncontractible paths that windings of the order parameter in the OP space

on a sphere
a closed loop
from the N
to the S pole
is contractible



but in a magnetic
N and South are
the same point
so the red path
is a closed loop

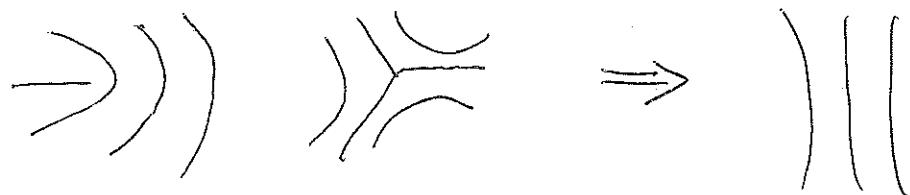
but it is not contractible

It cannot be shrunk to zero without by
a continuous deformation \rightarrow must cut

Due to inversion symmetry the basic defects
in 2d nematics are 180° windings
 \rightarrow defined as charge $\frac{1}{2}$

topological invariant
handles \leftrightarrow topological defects

2d order/disorder transitions as defect unbinding
BKT



Well established description of passive LC in terms of Landau - de Gennes free energy.

To describe active LC we need dynamics.

First dynamics of passive liquid crystals.

Fluid dynamics \rightarrow Hydrodynamics (more general)

$$g \text{ density field} \quad \partial_t g + \vec{\nabla} \cdot g \vec{v} = 0$$

\vec{v} flow velocity \rightarrow NS equation

[E energy density] will not consider

incompressible flows $g = \text{const}$, $\vec{\nabla} \cdot \vec{v} = 0$

Navier-Stokes equation (essentially $m \frac{d\vec{v}}{dt} = \vec{F}$)

$$g(\partial_t \vec{v} + \vec{v} \cdot \vec{\nabla}) \vec{v} = -\vec{\nabla} p + \underbrace{2 \eta \vec{\nabla}^2 \vec{v}}$$

Force density on fluid element

When inertia is negligible* \rightarrow just force balance

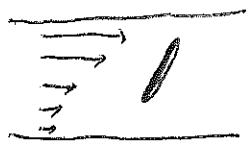
$$0 = -\vec{\nabla} p + 2 \eta \vec{\nabla}^2 \vec{v} \quad \text{Stokes equation}$$

* low Re number

$$\text{Re} \sim \frac{\text{inertia}}{\text{viscous dissipation}} \sim \frac{N^2 g / L}{\eta v / L^2}$$

$$\text{Re} \sim \frac{NLg}{\eta}$$

LC HYDRODYNAMICS



shear and vortical flows
rotate LC molecules
→ deform director

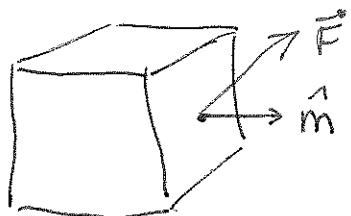
coupling of orientation and flow

Coupled dynamics of \vec{v} and \hat{n}

$$g \partial_t \vec{v} = \eta \nabla^2 \vec{v} - \vec{\sigma} p + \vec{\sigma} \cdot \vec{\tau}^{el}$$

stress tensor σ force / area
but it is a tensor

↑ elastic stress associated
with energy cost of
deforming order



unit vector denotes
direction of surface area

σ_{ij} i-th component of force
on an area $\perp m_j$

$$\sigma_{ij}^{el} \sim n_i K \nabla^2 n_j \quad \text{we will neglect it below}$$

$$*\partial_t n_i + \vec{v} \cdot \vec{\nabla} n_i + w_{ij} n_j = \lambda u_{ij} n_j + \frac{K}{\eta} \nabla^2 n_i$$

* should enforce

$|n| = 1$ w/Lagrange
multiplier

$$w_{ij} = \frac{1}{2} (\partial_i w_j - \partial_j w_i) \rightarrow \vec{\nabla} \times \vec{v}$$

Vorticity

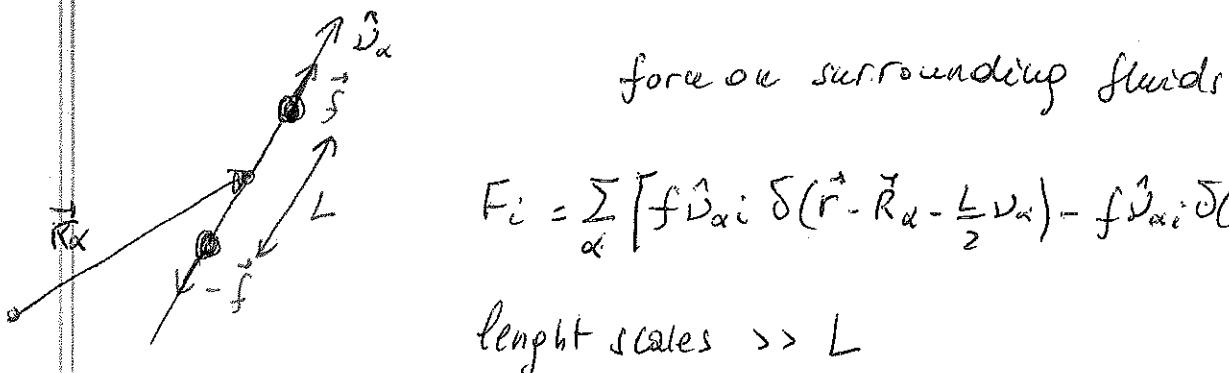
$$u_{ij} = \frac{1}{2} (\partial_i v_j + \partial_j v_i) \quad \text{strain rate}$$

λ : microscopic parameter that depends on molecular shape

K: stiffness

K_s : splay & K_b : bend ($+ K_z$: twist
in 3d)

Active forces \rightarrow ACTIVE STRESS



$$F_i = \sum_{\alpha} \left[f \delta_{\alpha i} \delta(r - \vec{R}_{\alpha} - \frac{L}{2} \nu_{\alpha}) - f \delta_{\alpha i} \delta(r - \vec{R}_{\alpha} + \frac{L}{2} \nu_{\alpha}) \right]$$

$$\begin{aligned} F_i &\approx \sum_{\alpha} f \nu_{\alpha i} \left(-\frac{L}{2} \nu_{\alpha j} \partial_j \delta(r - \vec{R}_{\alpha}) - \frac{L}{2} \nu_{\alpha j} \frac{\partial}{\partial r_j} \delta(r - \vec{R}_{\alpha}) \right) \\ &= -f L \partial_j \sum_{\alpha} \nu_{\alpha i} \nu_{\alpha j} \delta(r - \vec{R}_{\alpha}) \\ &= -f L \partial_j \sum_{\alpha} (\nu_{\alpha i} \nu_{\alpha j} - \frac{1}{d} \delta_{ij}) \delta(r - \vec{R}_{\alpha}) - f L \partial_j \sum_{\alpha} \delta(r - \vec{R}_{\alpha}) \end{aligned}$$

$$F_i(\vec{r}) = + \partial_j \alpha Q_{ij}(r) + \text{active pressure gradient}$$

$$\text{Active stress} \quad \tau_{ij}^a = \alpha Q_{ij} \sim \alpha n_i n_j \quad S \approx 1$$

α dimensions of stress - activity

$\alpha < 0$ extensile

$\alpha > 0$ contractile

Active LC hydrodynamics neglect

$$\rho \partial_t \vec{v} = - \vec{\nabla} p + \eta \nabla^2 \vec{v} + \vec{D} \cdot (\vec{\tau}^a + \vec{\tau}^{el})$$

$$\vec{D} \cdot \vec{N} = 0$$

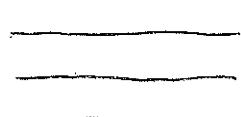
Stokes limit

Irrational part of \vec{w}

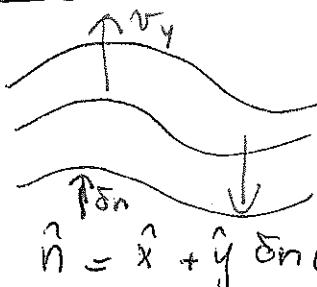
$$\eta \nabla^2 \vec{v} + \vec{v} \cdot \vec{\sigma}^a = 0$$

\uparrow
active stress as
a source of flow

ACTIVE NEMATICS ARE UNSTABLE



$$\hat{n} = \hat{x}$$



bend deformation

$$\hat{n} = \hat{x} + \hat{y} \delta n(x)$$

$$\eta \partial_x^2 v_y = \alpha \partial_x \delta n_y$$

$$\partial_t \delta n_y = \frac{\lambda+1}{2} \partial_x v_y$$

$|\alpha|/\eta$ rate of energy injection

contractile systems are
unstable to splay

Fourier modes

$$v_g = \frac{\alpha}{2} \frac{i q}{q^2} \delta n_y$$

$$\partial_t \delta n_y = \frac{\lambda+1}{2} i q v_g = -\frac{\alpha}{2} \delta n_y$$

unstable growth

for $\alpha < 0$ extensile
any $|\alpha|$

inclusion of elasticity reveals a length scale for
most unstable modes

$$\frac{K}{\ell^2} \sim |\alpha| \Rightarrow l_c = \sqrt{\frac{K}{|\alpha|}} \sim 100 \mu m$$

can be stabilized below α_c by

- ① substrate
- ② confinement
- ③ viscoelasticity

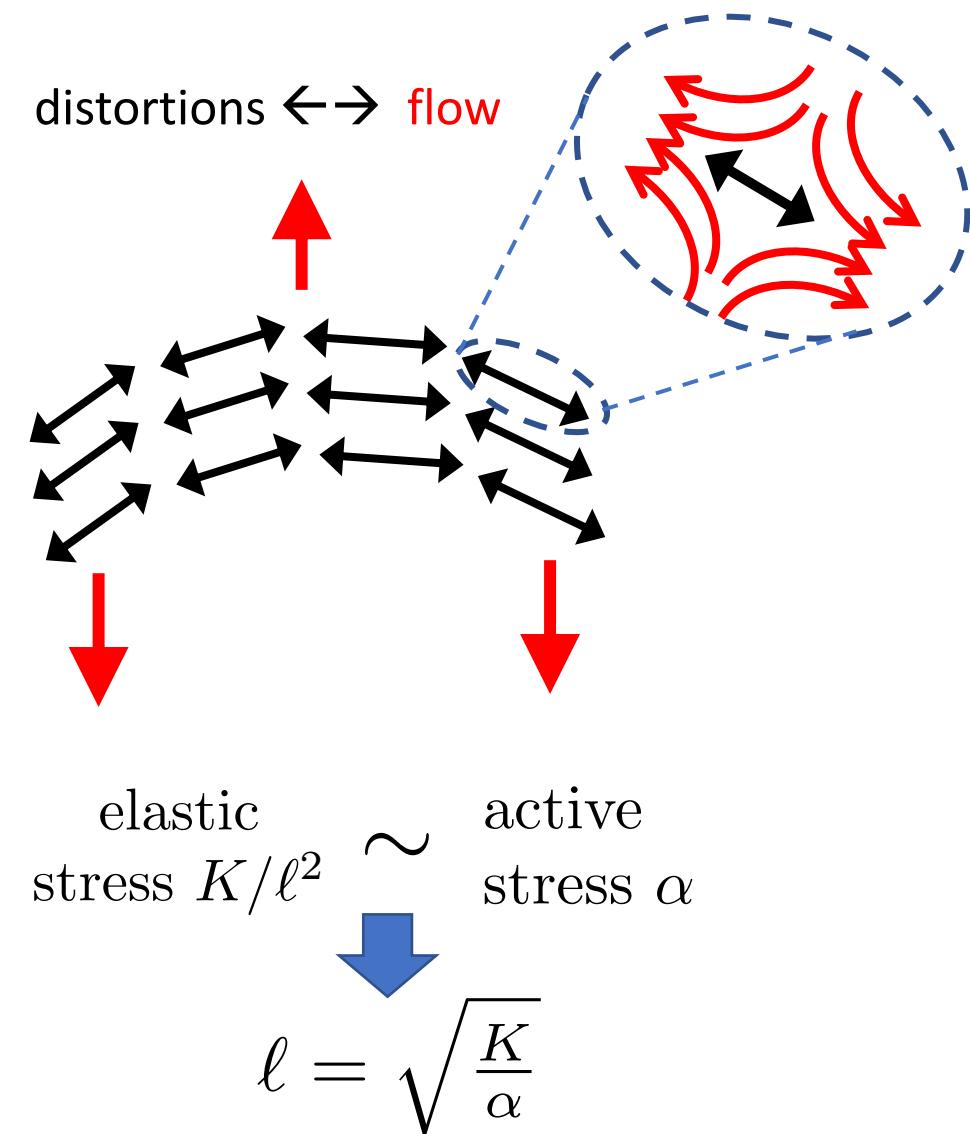
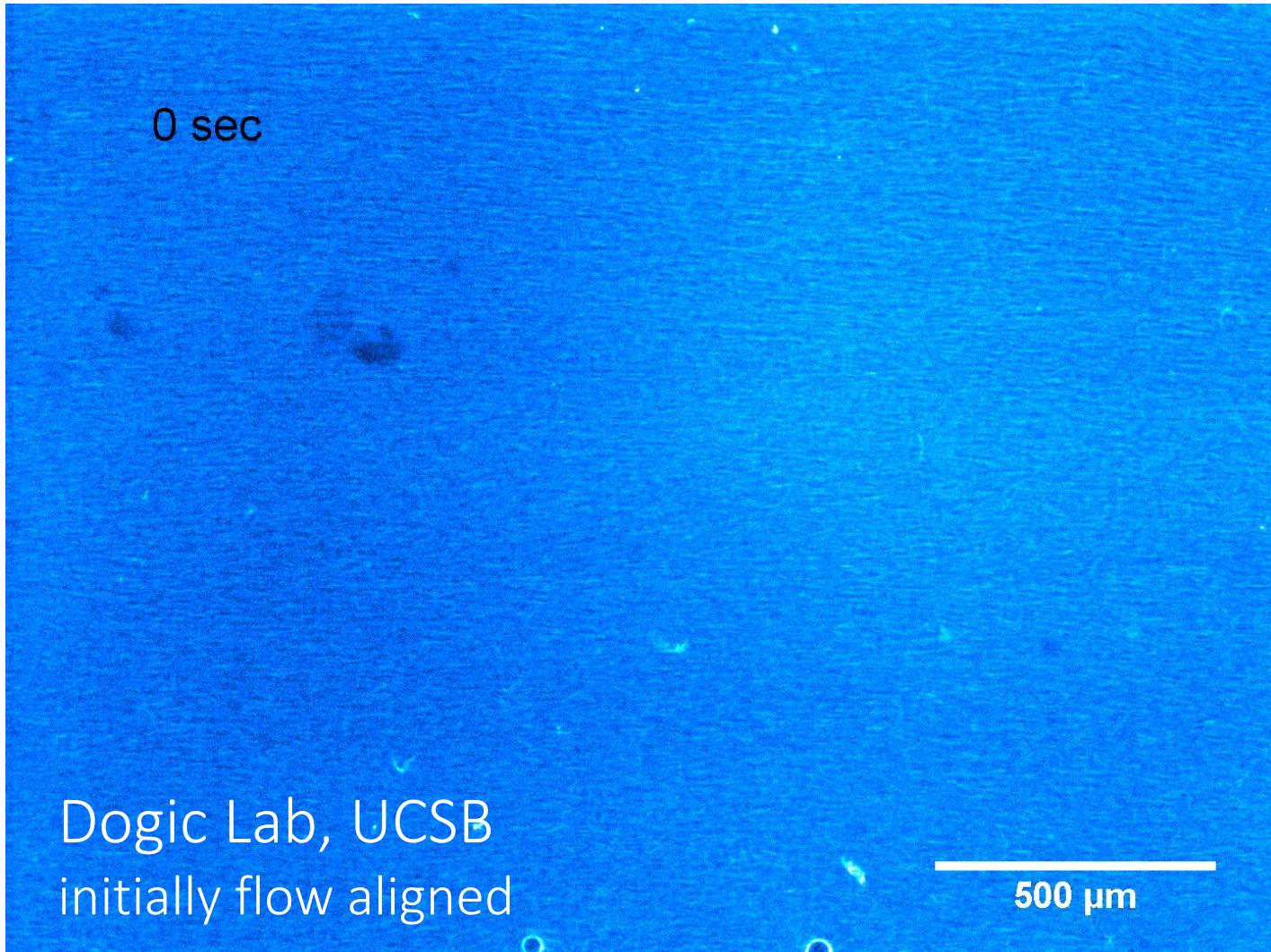
} any mechanism that
screens flows

$$\vec{P} \vec{N} = \eta \nabla^2 \vec{N} + \alpha \nabla \cdot \vec{v}^a \quad l_2 = \sqrt{2/\rho}$$

MT nematics

Active hydrodynamics predicts linear instability

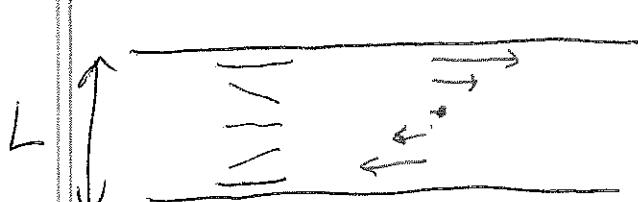
predicted theoretically Simha & Ramaswamy 2002



Active Nematics flow spontaneously

No external forces needed

$$\sigma_{xy} = 0 = \eta \partial_y v_x + \alpha n_x n_y$$



L vs l_α

$$L < l_\alpha$$

anchoring
and elasticity
 $\omega \ll \alpha \rightarrow$ no flow

$$L > l_\alpha$$

spontaneous
turbular flow

$$L \gg l_\alpha$$

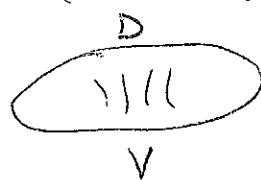
chaotic flow
"active turbulence"
+ topological
defects

seen in MT nematic
cell monolayers } quantitative
comparison

Active stress as source of flow in Drosophila embryo
during gastrulation.

Independently measure pattern of myosin \rightarrow nematic tensor
and cellular flows

Streichen E-life 2019 anisotropic myosin stresses
with nematic alignment dorso-ventral



drives flows during gastrulation
(from 1 layer of cells
to many)

Back to the defects.

Nematic order in fibroblasts : TR Eustace 1968

"patchwork of aligned groups
of parallel cells with narrow
interstices between these that we will term
frontiers"

Now nematic order in many active systems interrupted by topological defects

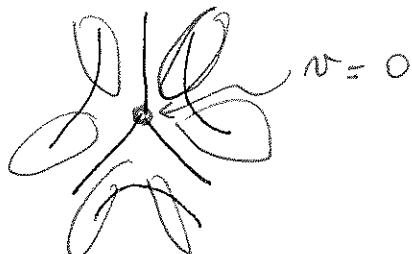
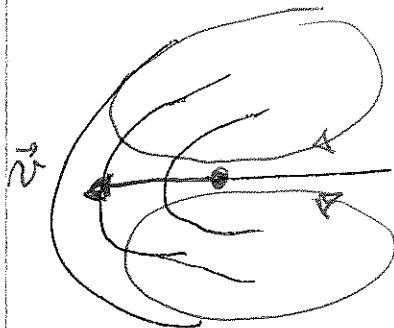
- defects are often mobile
- opposite signs may ~~attract~~ "repel"
- biological function of defects : cell extrusion/death
 - morphogenesis
 - fruiting body

Why are active defects mobile?

We saw that distortions of orientation generate flows

$$\eta \nabla^2 \vec{v} = -\alpha \vec{\nabla} \cdot \hat{n} \hat{n}$$

insert defect texture
and calculate resulting
flow



$$X \text{ } v \sim \alpha / \eta$$

Motility of +1/2 defects

- Order parameter deformations generate flow
- TRS-breaking active stresses + geometric polarity of +1/2 defect → autonomous motility

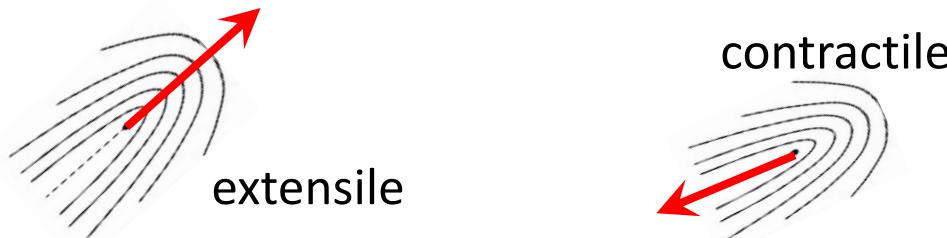
Motility from active flows:

$$\Gamma \mathbf{u} - \eta \nabla^2 \mathbf{u} = \alpha \nabla \cdot \mathbf{Q}$$

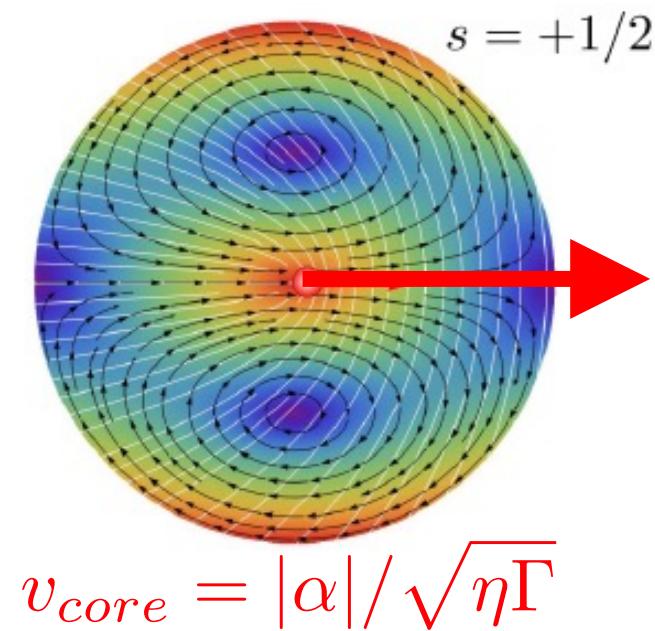
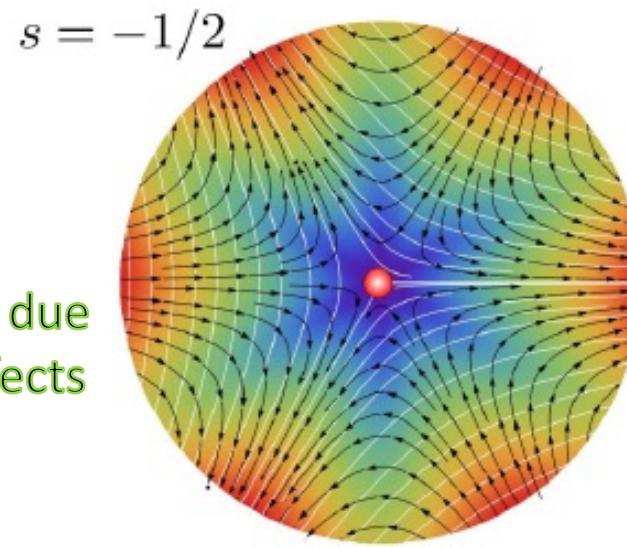
Defect rides with self-generated flow

$$\zeta [\partial_t \mathbf{r} - \mathbf{u}(\mathbf{r})] = \mathbf{F}(\mathbf{r})$$

Elastic force due
to other defects



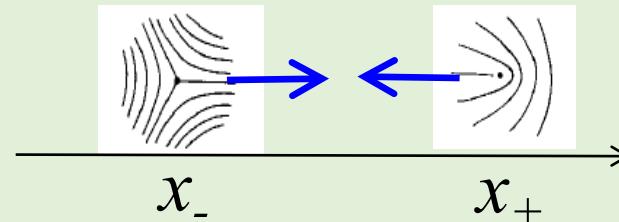
Direction of motion of +1/2 reveals
the nature of active stress



Giomi, Ma, Bowick, MCM, PRL 2013; Pismen, PRE 2013
J Rønning, MCM, MJ Bowick, L Angheluta, Proc R Soc A 2022

Active Defects as ``Self-Propelled'' Particles

In equilibrium defects can be described as ``charged'' particles with known interactions. Opposite-sign defects attract and annihilate

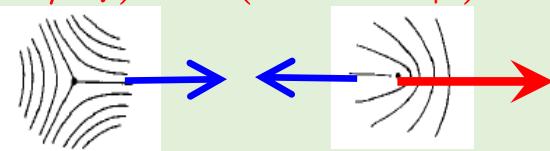


Pair dynamics and annihilation controlled by balance of *friction* and *attraction*

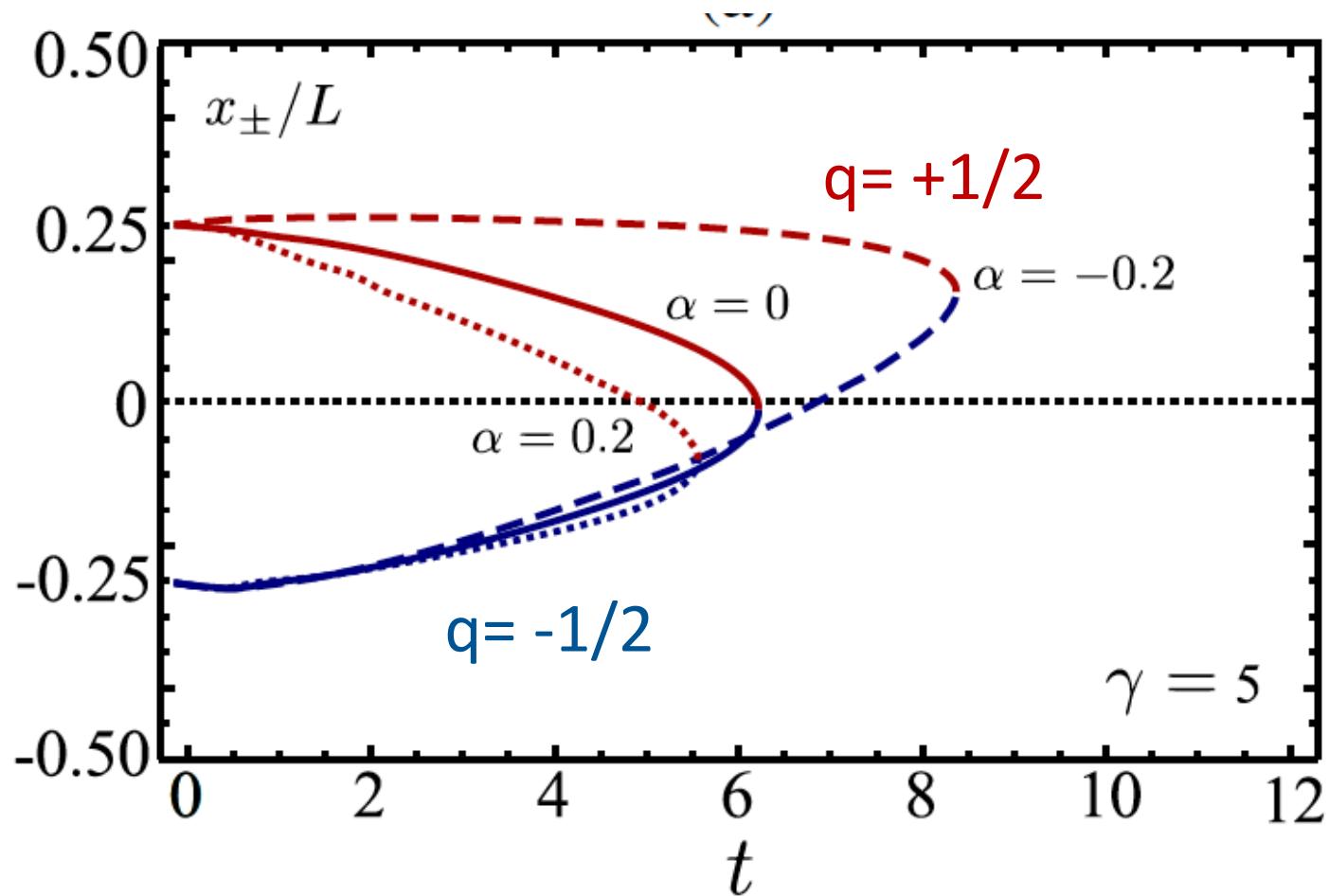
$$x = x_+ - x_- \quad \gamma \dot{x} = -\nabla [K \ln(x/a)]$$

In **active** systems defects ride with the **active backflow** and behave as self-propelled particles.

Activity may overcome attraction



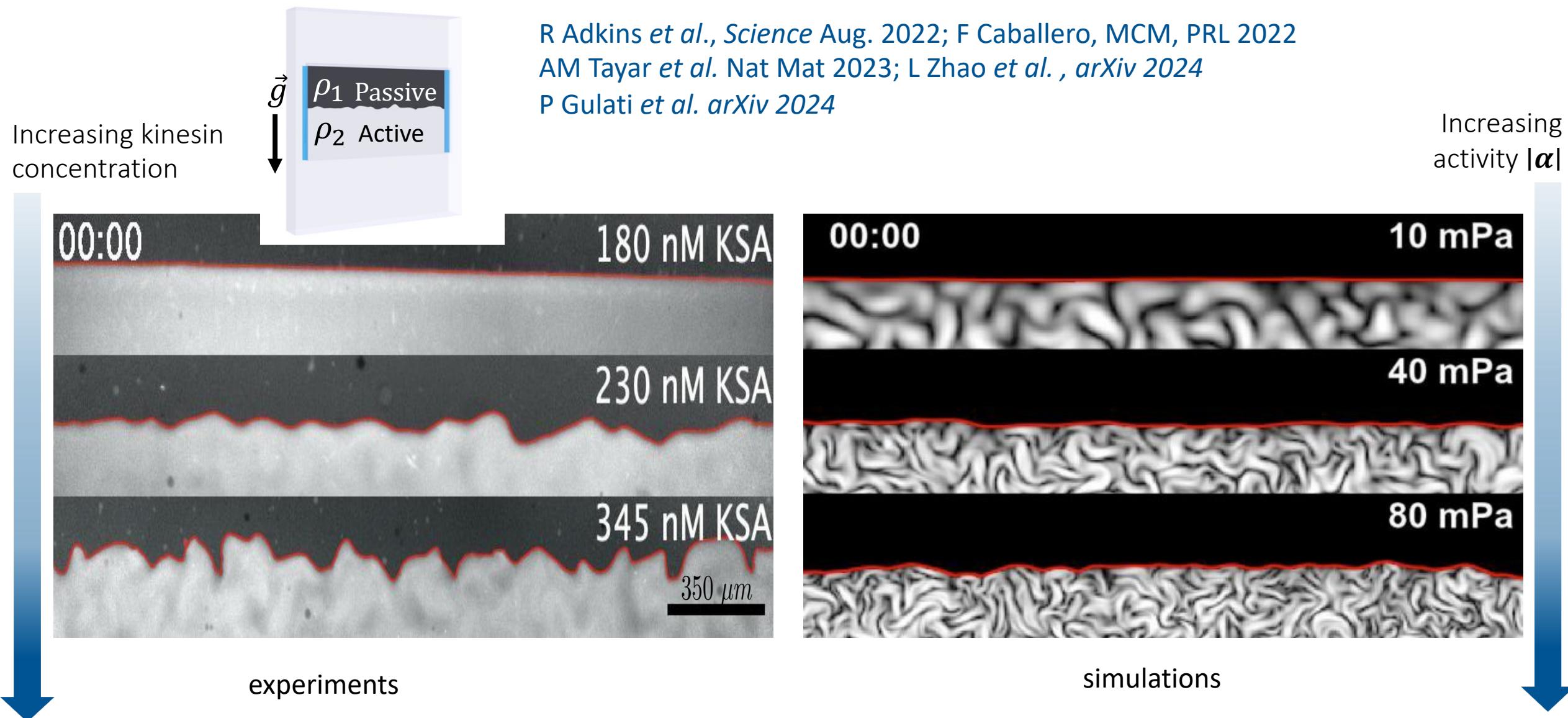
Defect Trajectories



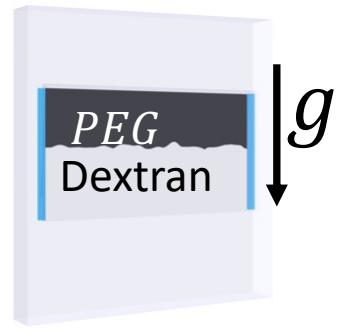
Three directions of current research on active nematics

- Activity as a handle for tuning **interfacial properties**: large fluctuations, wetting, active emulsions (with Zvonimir Dogic)
- Tuning activity in space and time to **control flows** in active fluids and deformations and shape in active gels
- **Active nematic *solids***: defects as centers of stress focusing → *Hydra* development

Giant fluctuations & traveling waves at active/passive interfaces



Active Wetting



Low KSA

180 nM KSA

00:00

High KSA

345 nM KSA

100 μ m

experiments

00:00

10 mPa

20 mPa

30 mPa

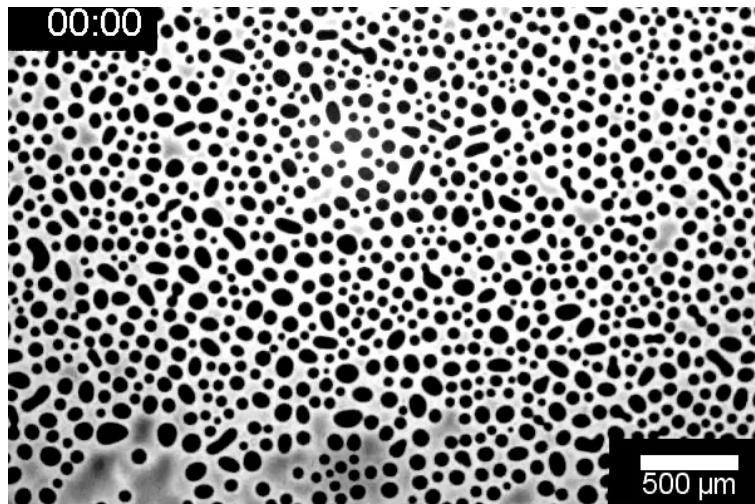
simulations

Active Emulsions: activity speeds up then arrests coarsening

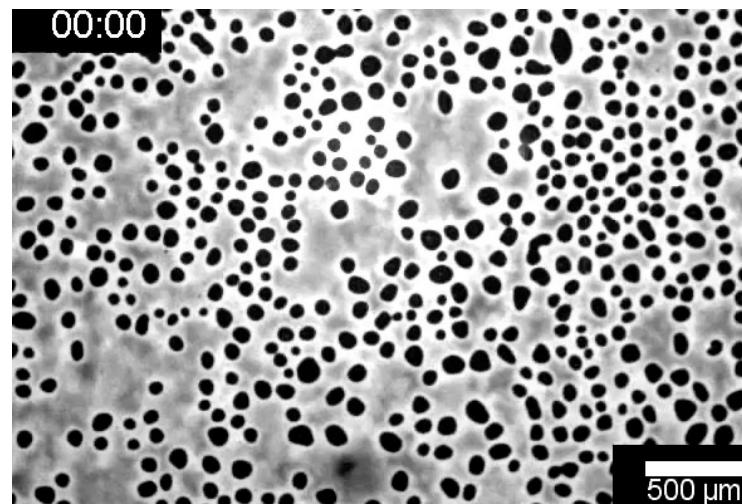


activity

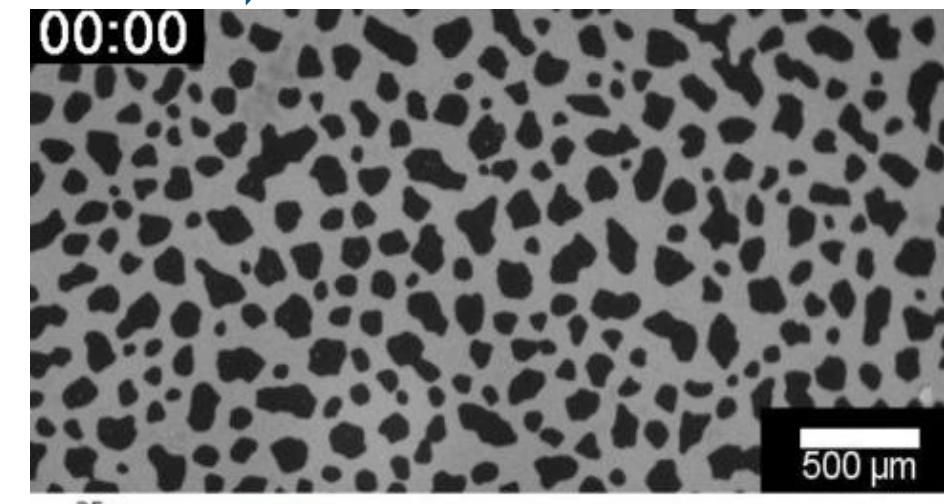
Steady state is an active emulsion



KSA 0 nM

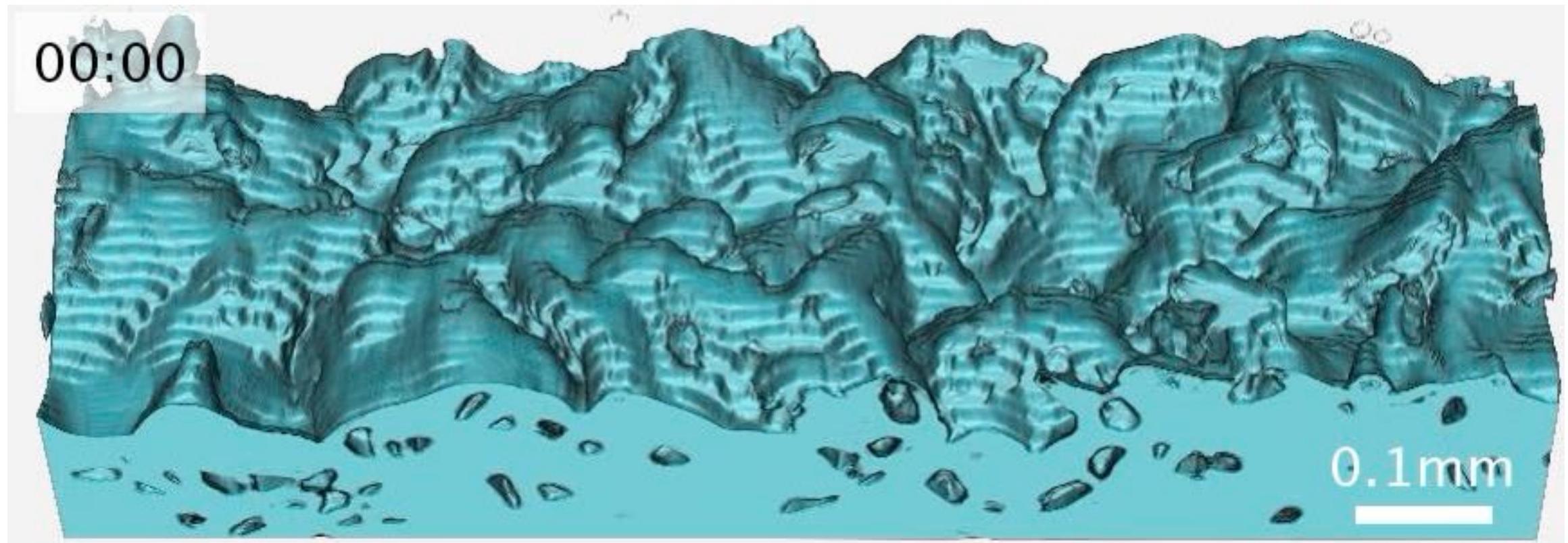


KSA 135 nM



KSA 230 nM

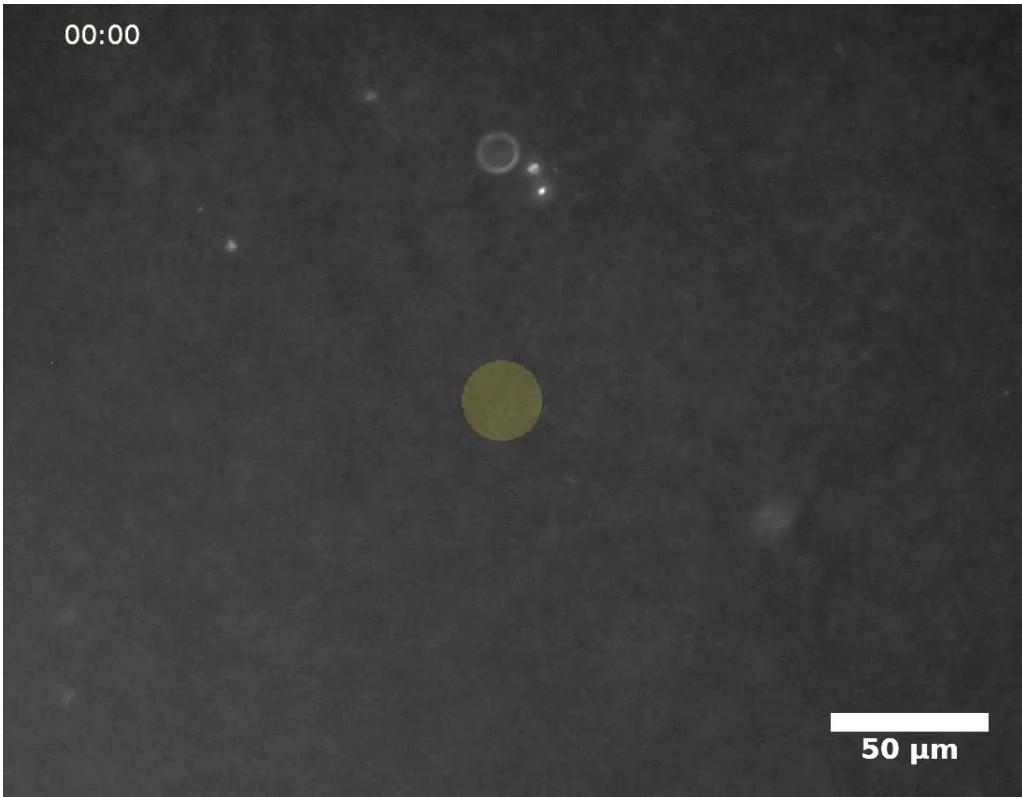
And 2D active interfaces



Liang Zhao, UCSB

Patterning activity to control defects in space & time

Optogenetically modified motor proteins allow spatiotemporal control of activity in cytoskeletal suspensions



Light-sensitive kinesins and microtubules

Asters track the light pattern up to 200 nm/s

Also: R Zhang, Nat Mat 2021,

...

Constructing spatiotemporal profiles of active stresses to achieve a target configuration of active defects and flow



Linearity of Stokes dynamics allows us to construct a symmetry-based additive approach

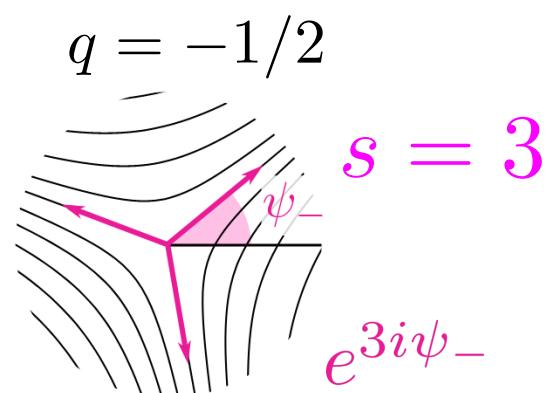
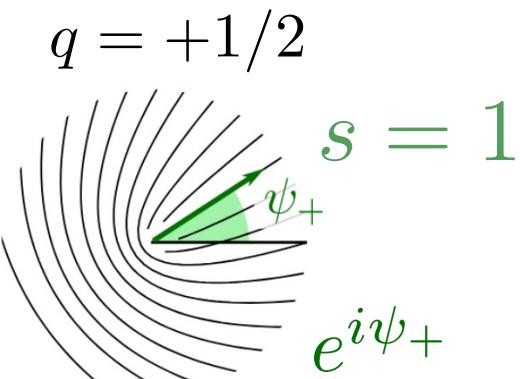
$$\ell_\eta^2 \nabla^2 \mathbf{u} - \mathbf{u} + \Gamma^{-1} \nabla \cdot \underbrace{\alpha(\mathbf{r}, t) \mathbf{Q}}_{\text{Flow structure dictated by combined symmetry of defect texture } \mathbf{Q} \text{ and activity field } \alpha} - \Gamma^{-1} \nabla p = 0 \quad \nabla \cdot \mathbf{u} = 0$$

Flow structure dictated by combined symmetry of defect texture \mathbf{Q} and activity field α

defect velocities

$$\begin{cases} \mathbf{v}_0 = \lim_{r \rightarrow a} \int_0^{2\pi} d\phi \, \mathbf{u}(r, \phi) \\ \boldsymbol{\omega}_0 = \lim_{r \rightarrow a} \int_0^{2\pi} d\phi \, \nabla \times \mathbf{u}(r, \phi) \end{cases}$$

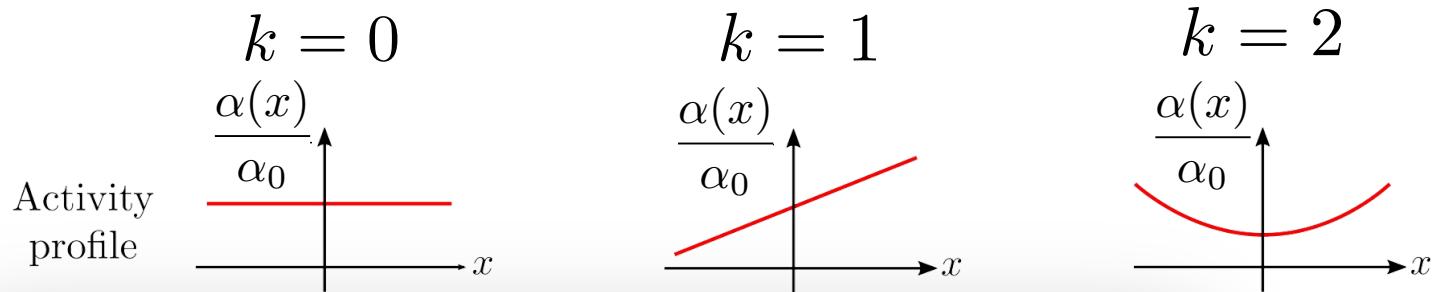
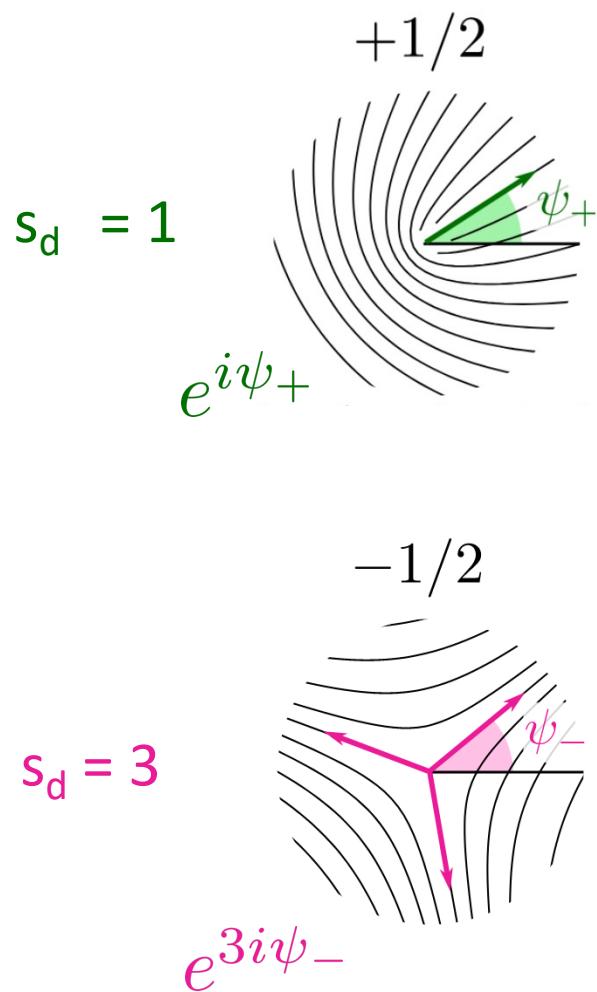
Defect symmetry number $s = 2|1 - q|$



Activity profile decomposed in polar components of defined rotational symmetry:

$$\alpha(\mathbf{r}, t) = \sum_k \alpha_k(r, t) e^{ik\phi}$$

A simple rule for additive control of defects



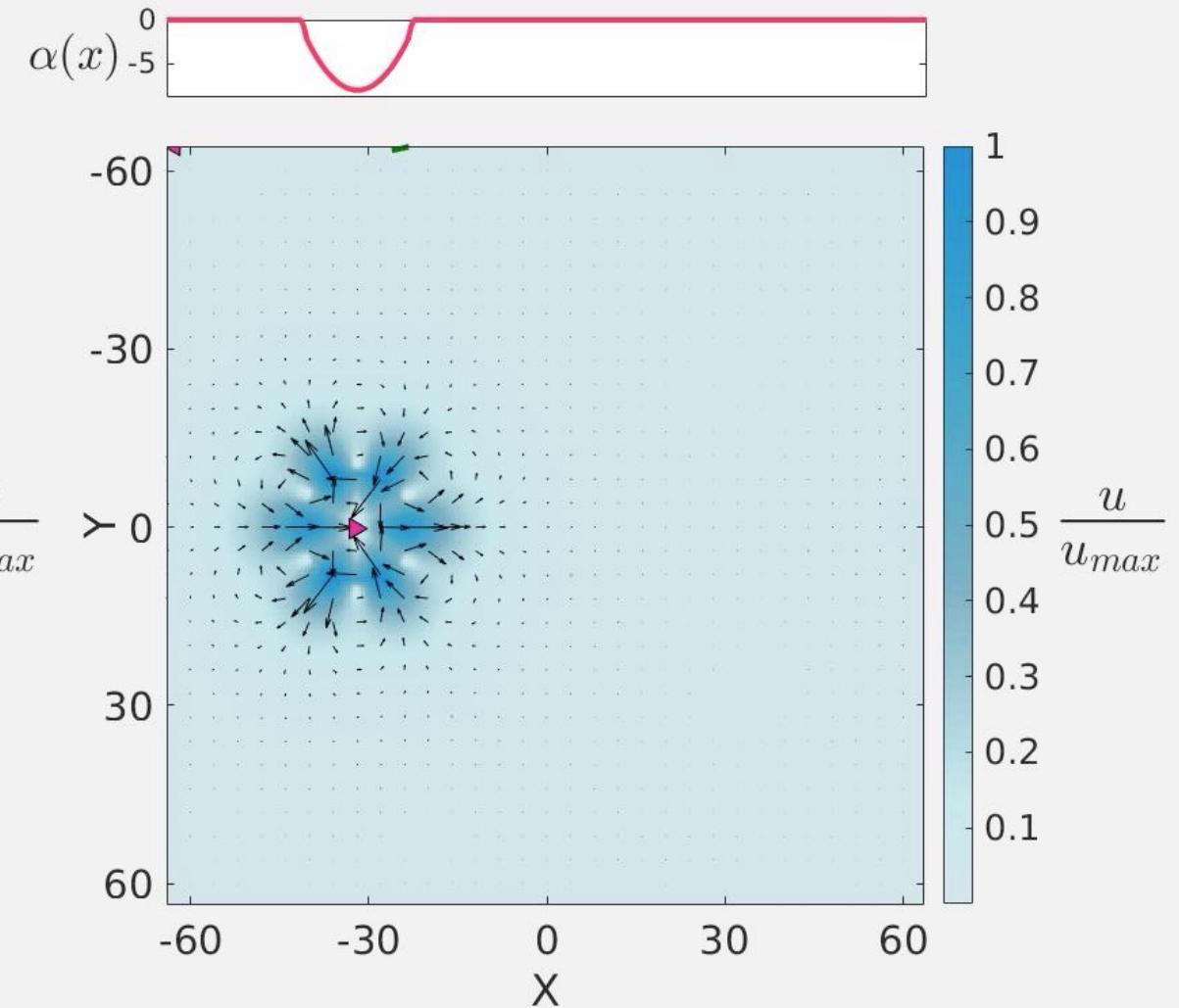
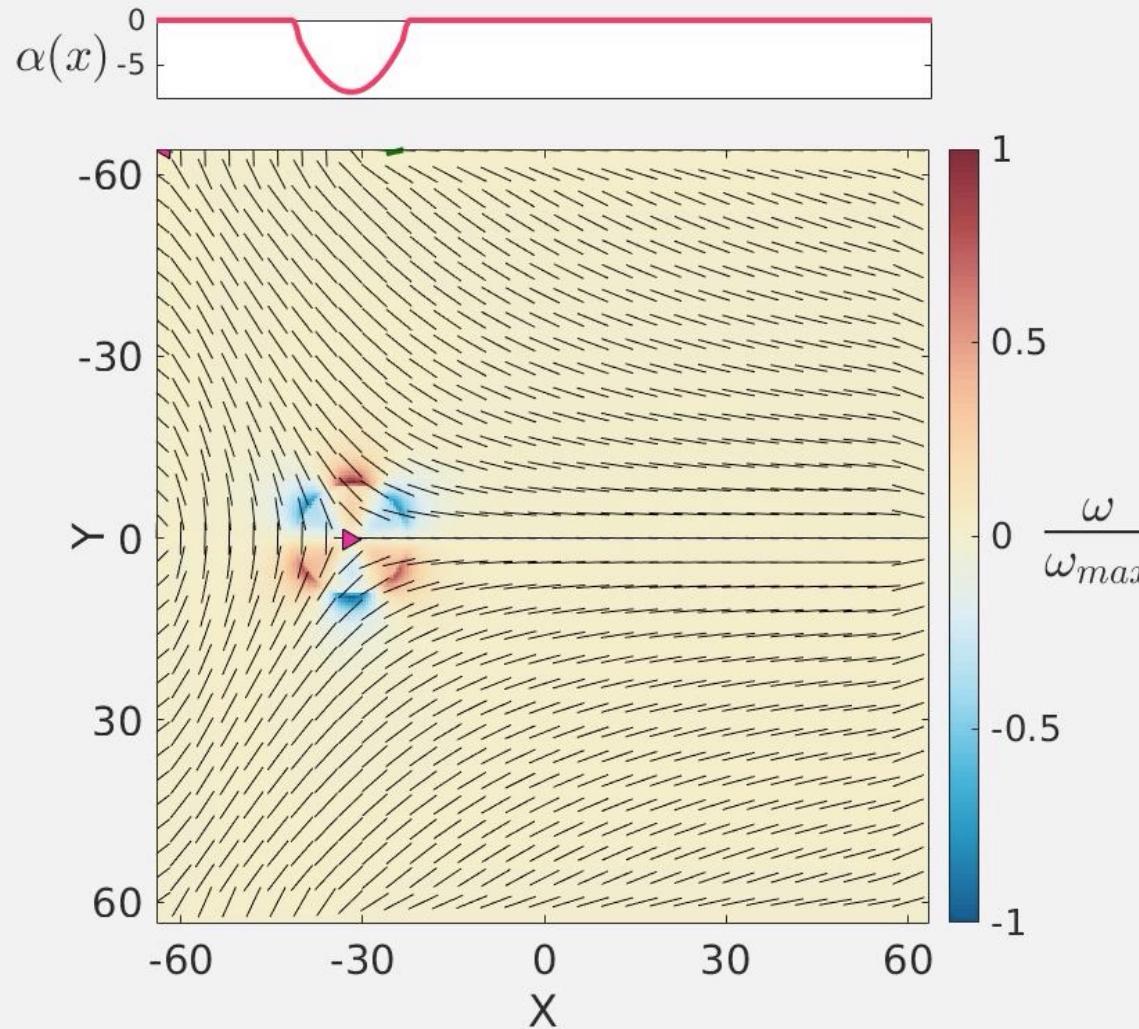
$$\Delta s = s - k$$

$|\Delta s| = 1$ - Nonzero defect velocity

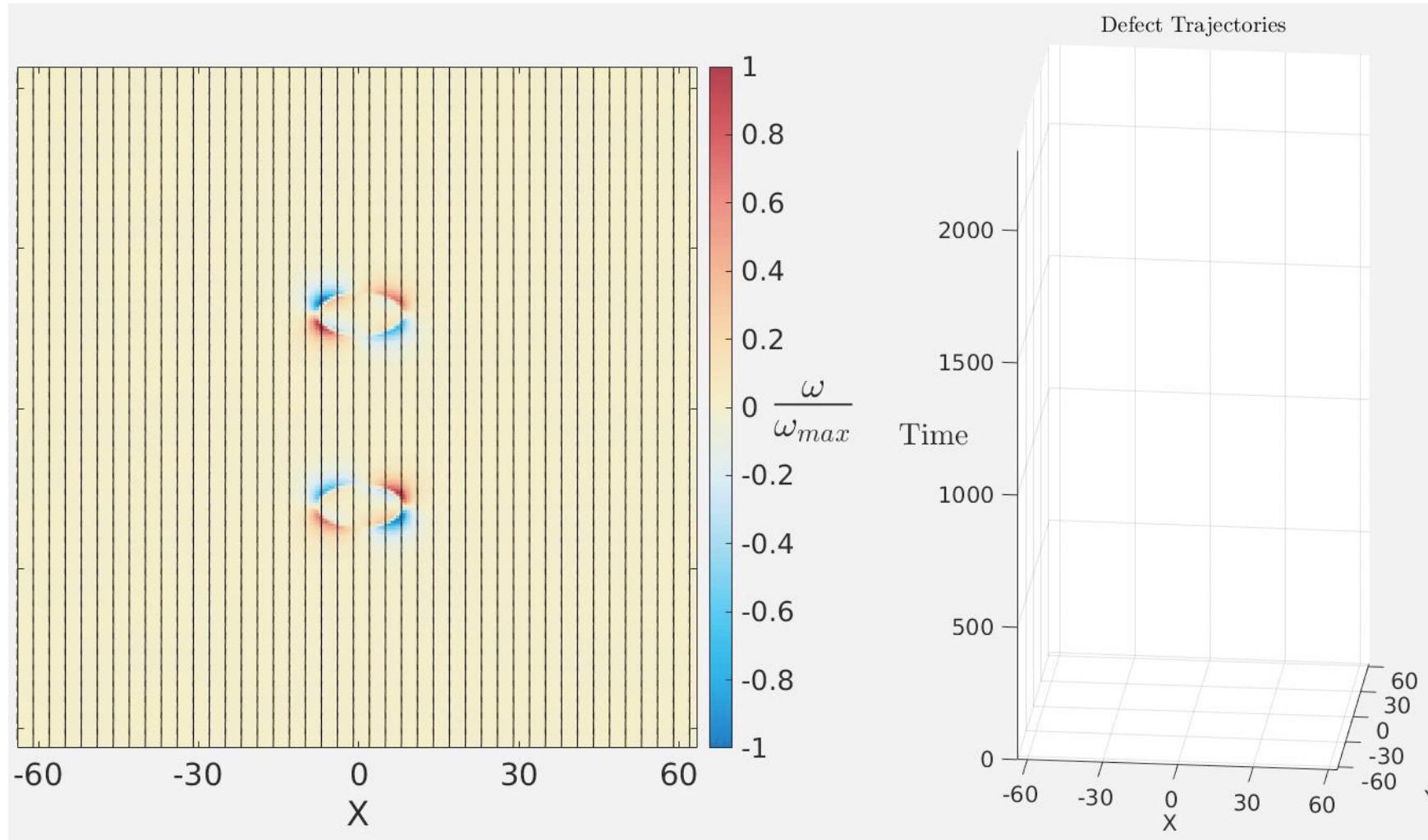
$|\Delta s| = 0$ - Nonzero defect vorticity

Other Δs values leave defects unaffected

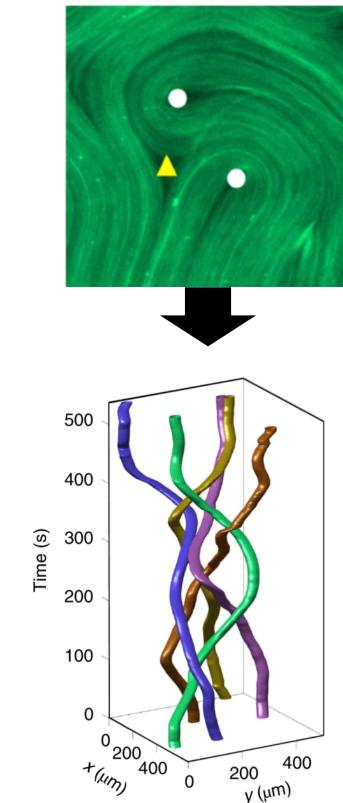
Parabolic activity trap moves -1/2 defect



Defect braiding with active topological tweezers

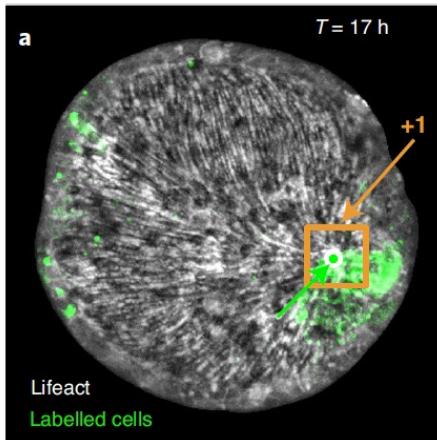
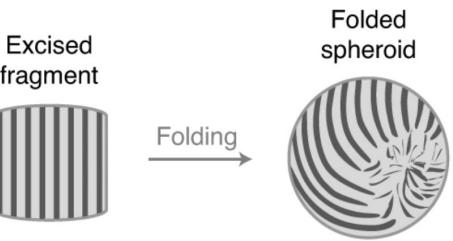


Defect trajectory braiding in chaotic state provides a quantitative measure of fluid mixing → topological entropy [Tan et al. Nat Phys 2019](#)

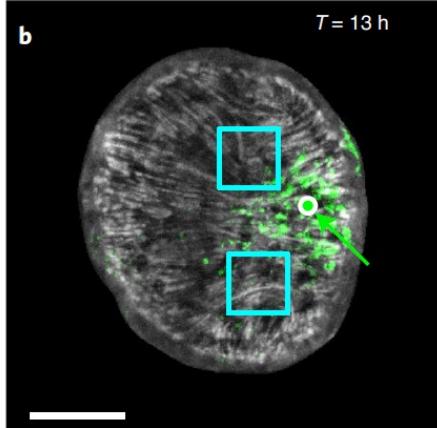


Hydra: defects as organizing centers of morphogenesis

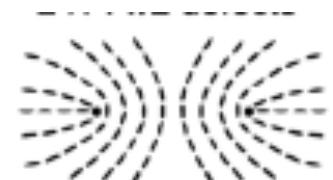
Hydra budding and regeneration *Maroudas-Sacks et al. Nat Phys 2020*



Future head
coincides with
+1 defect

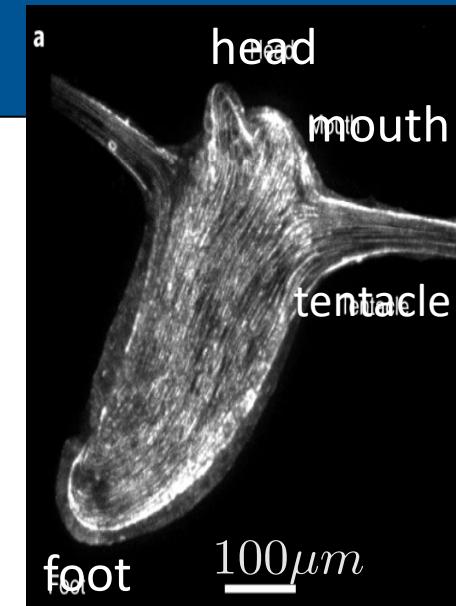


Future foot
coincides with
two -1/2 defects



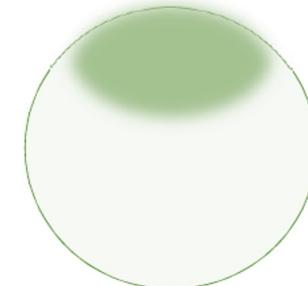
Nematic organization of
supracellular actin controls
morphogenetic processes

Specific defects as organizers of
head, foot, tentacles



Interplay of mechanics, geometry and
biochemical signaling:

- sphere elongates into ellipsoid → coupling between geometry and orientational order
- Strain promotes expression of head morphogen (Wnt)
Ferenc et al. Sci Adv 2021



Defect motility in active nematic solids

Coupling nematic texture to strain $\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ $\epsilon_{kk} \simeq -\delta\rho/\rho_0$

$$\partial_t \mathbf{Q} = (1 + b\epsilon_{kk} - Tr[\mathbf{Q}^2])\mathbf{Q} + K\nabla^2\mathbf{Q} + \chi\tilde{\epsilon}$$

$b > 0 \rightarrow$ compressional strains ($\epsilon_{kk} < 0$)
``melt'' the nematic



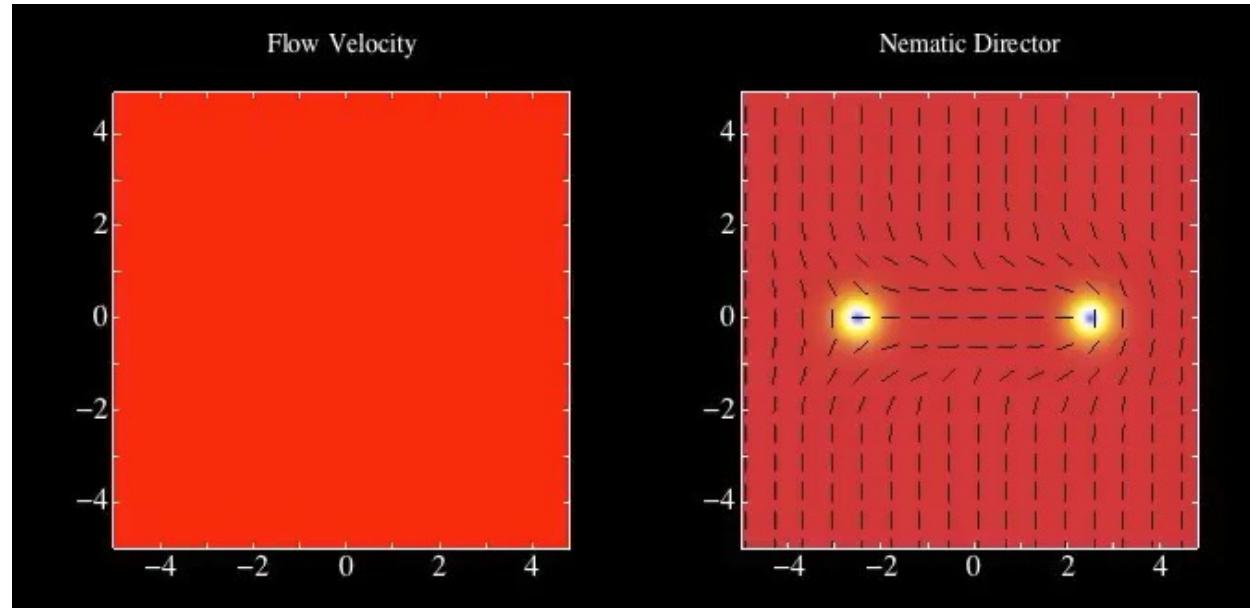
aligns

Force balance $\partial_j[2\mu\epsilon_{ij} + (B + \mu)\delta_{ij}\epsilon_{kk}] + \partial_j[(\alpha_B - b)Tr[\mathbf{Q}]^2\delta_{ij} + (\alpha - \chi)Q_{ij}] = 0$

elastic forces

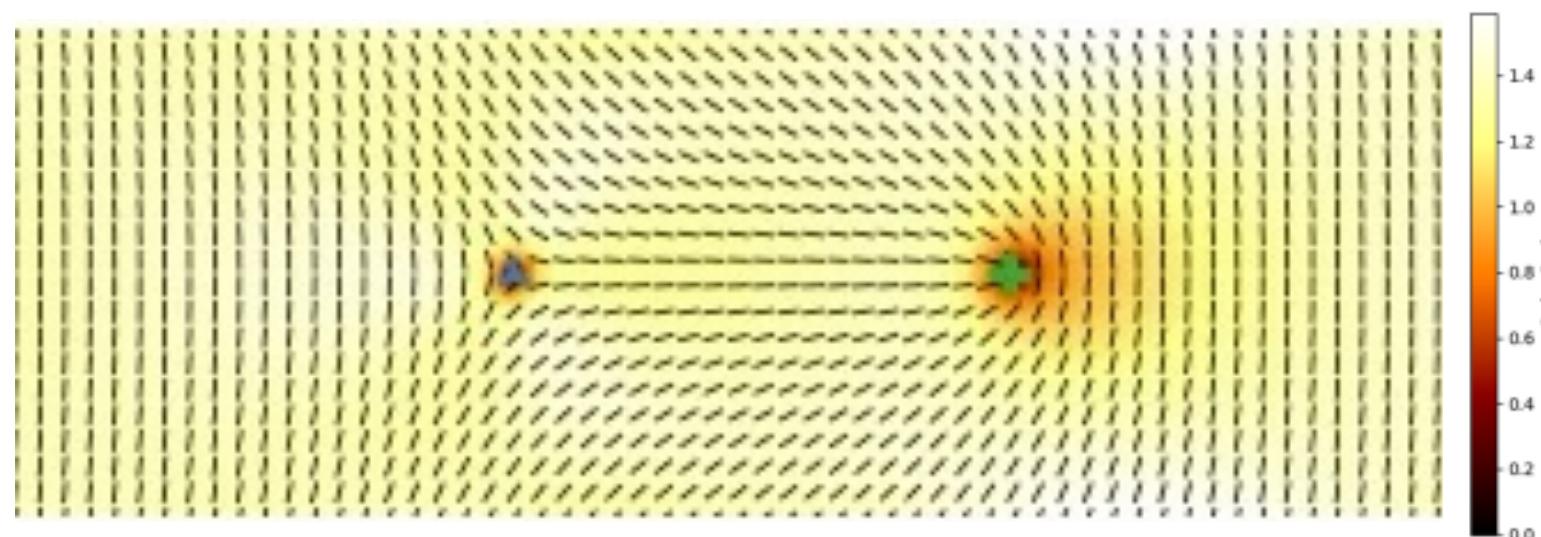
Active stresses can tune and
even suppress instabilities

Nematic fluid
L Giomi, MJ Bowick, X
Ma, MCM, PRL 2013



Defects move
advection by local
flow

Nematic solid
M O'Leary, F Brauns,
MJ Bowick, MCM
2024



Defects move
relative to elastic
material as
nematic texture
remodels

The elasto-nematic coupling can give rise to stable +1 defects that form by merging of two self-propelled $+1/2$ defects.

