Defect Dynamics in Active Nematics

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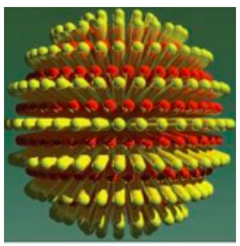
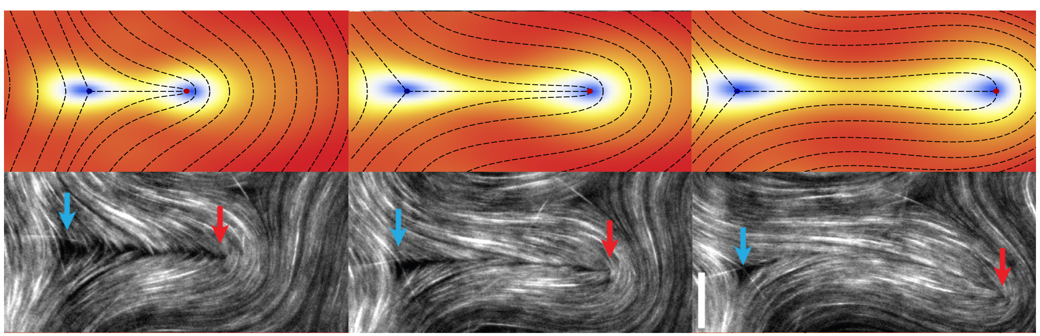
Syracuse University



Soft Matter Program @SU

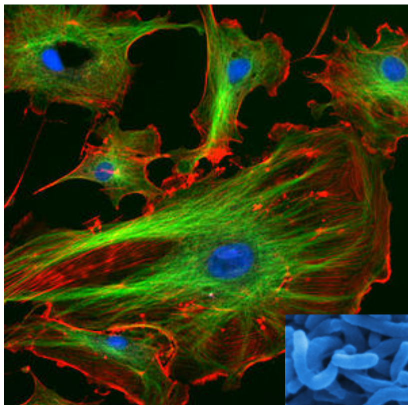


IGERT: Soft Interfaces Bridging the Divide in Graduate Education (iBriD)

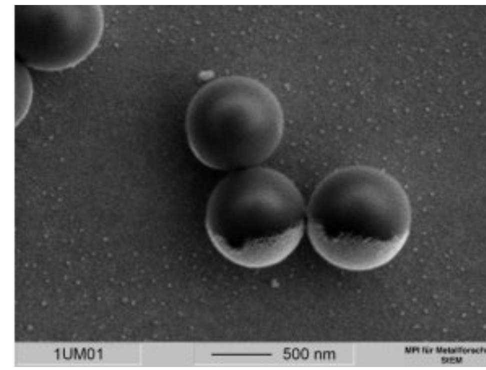
SYRACUSE BIOMATERIALS INSTITUTE

Active Matter on Many Scales

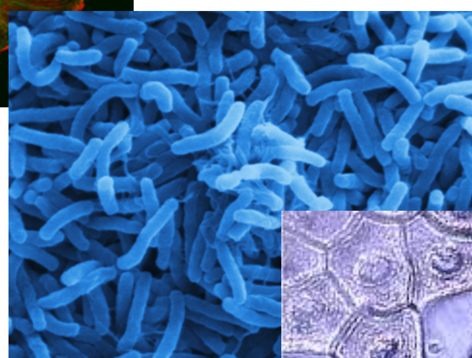
Collection of interacting entities that are individually driven and collectively generate organized motion and function.



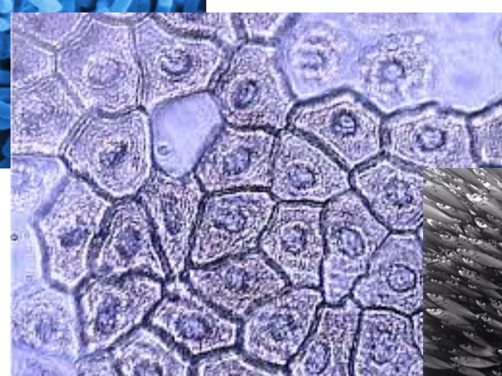
Inside the cell cytoskeleton: actin, microtubules & motor proteins



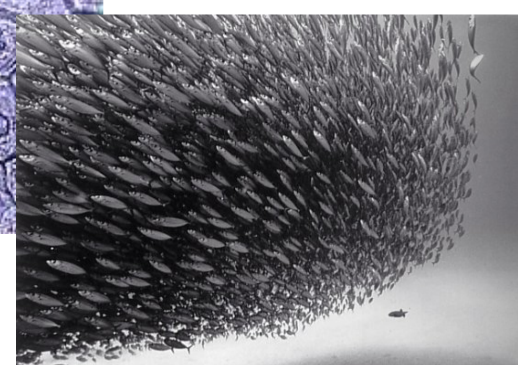
Synthetic microswimmers



Many cells: bacterial colony



Many cells: tissues



Fish schools, bird flocks, …

What defines active matter?

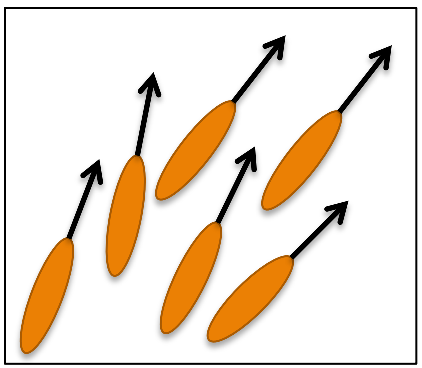
- Nonequilibrium systems where the drive acts on each unit, rather than at the boundary → `` reverse energy cascade''
- Emergent behavior and dynamic self-assembly: coordinated behavior at large scales in the presence of noise without leaders or external cues

→ Can we use statistical mechanics to classify behaviors and identify generic properties?

Review: *Hydrodynamics of Soft Active Matter*, Marchetti et al, Rev. Mod. Phys. **85**, 1143–1189 (2013)

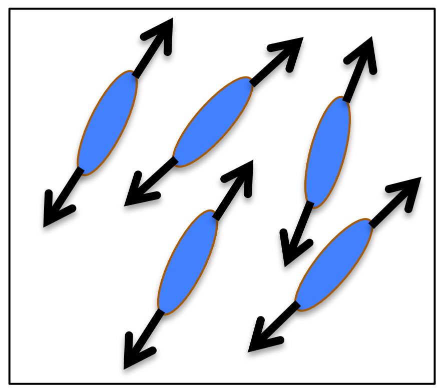
Active Particles, Interactions & Types of Order

Polar particles (bacteria, birds) & **polar** interactions (Vicsek)



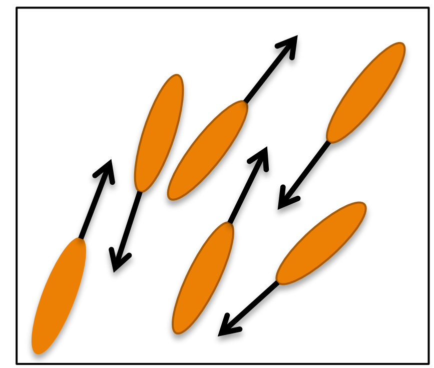
``Ferromagnetic'' order: a moving state or flock

Apolar particles (MT bundles, melanocytes) & **apolar** interactions



Nematic order: no **mean** motion

Polar particles (active rods, myxo) & **apolar** interactions (steric)



Nematic order, but polar flocks ``SP rods''

Continuum models:

Toner & Tu, 1995

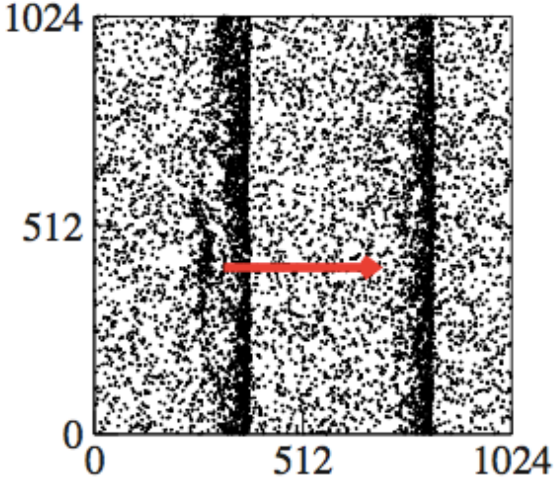
Simha & Ramaswamy, 2002

Baskaran & MCM, 2008

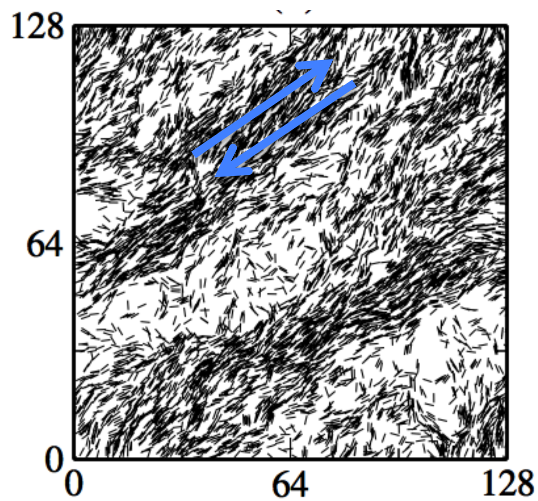
Banded structures

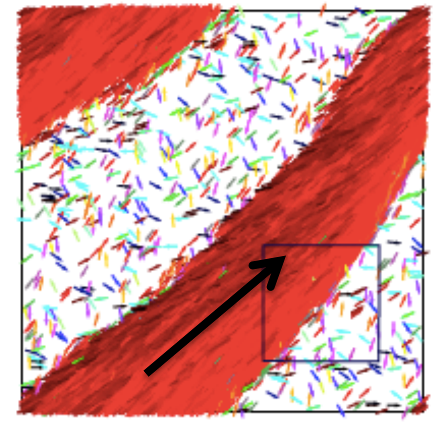
SP Rods

Polar

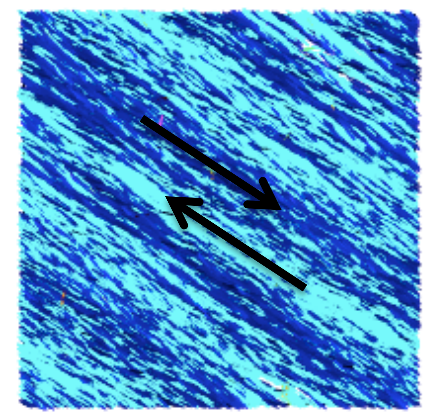


Nematic





(e) $\mathrm{Pe} = 25,\ \rho L_{\mathrm{rod}}^2 = 10.2$



(g) $\mathrm{Pe} = 75,\ \rho L_{\mathrm{rod}}^2 = 25.5$

Vicsek model: polar+ polar Chaté, Ginelli, Grégoire & Raynaud, PRE 2008

Nematic Vicsek apolar +nematic Chaté, Ginelli & Montagne, PRL 2006

SP rods + soft repulsion: polar + apolar Abkenar, Auth & Gompper PRE 2013

See H. Chaté's 2/13 talk

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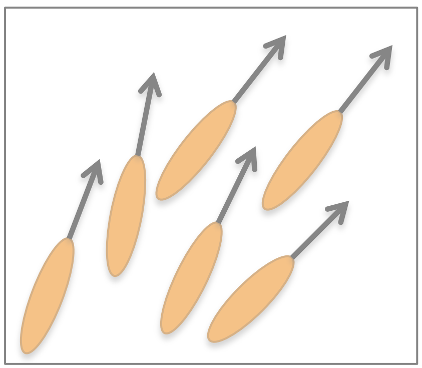

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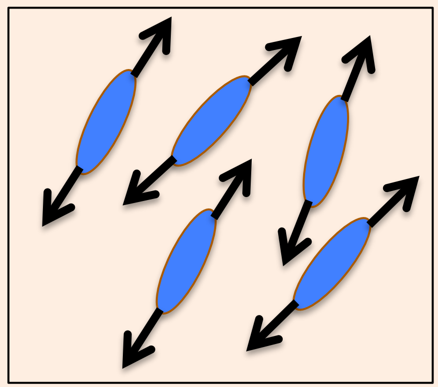

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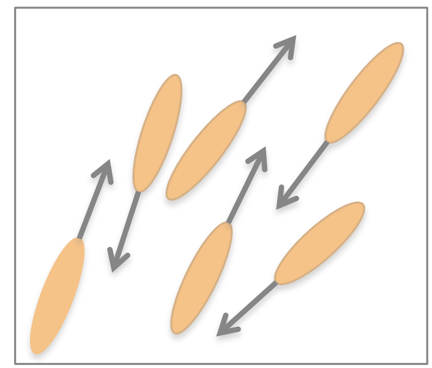
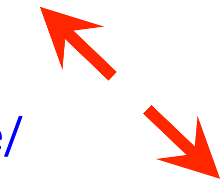
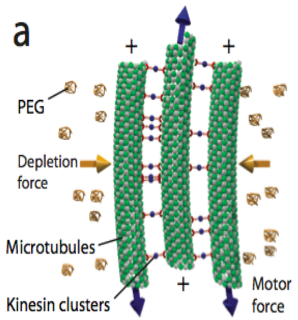


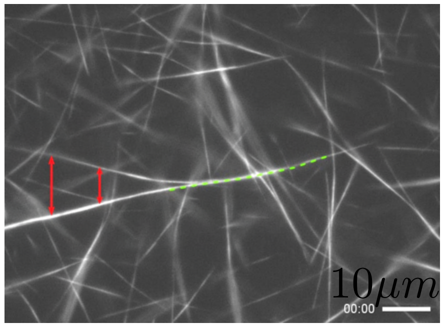
Nematic order, but polar flocks ``SP rods''

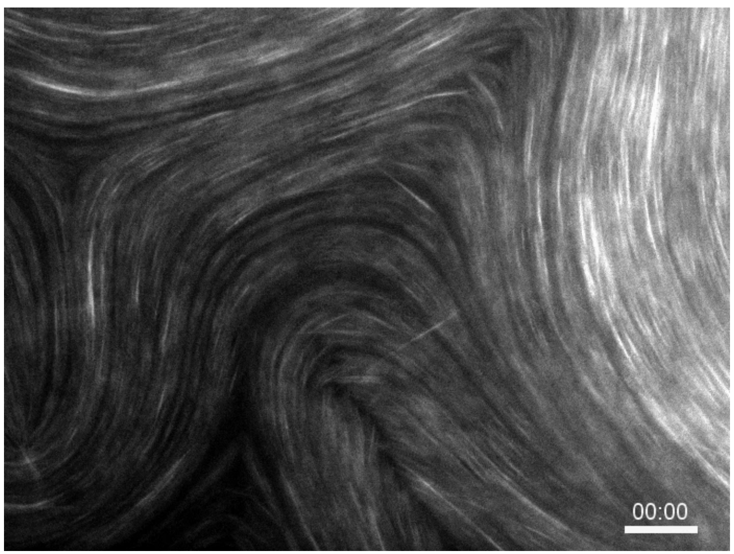
Active Nematics



Extensile/
Pullers

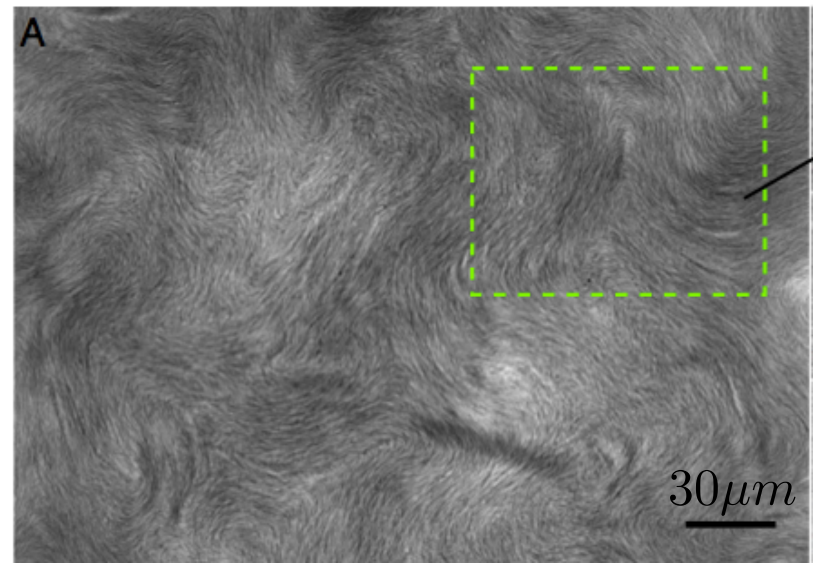






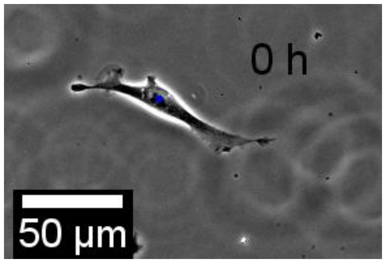
$15\mu m$

Sanchez et al, Nature 2012
2D active fluid at oil/water interface



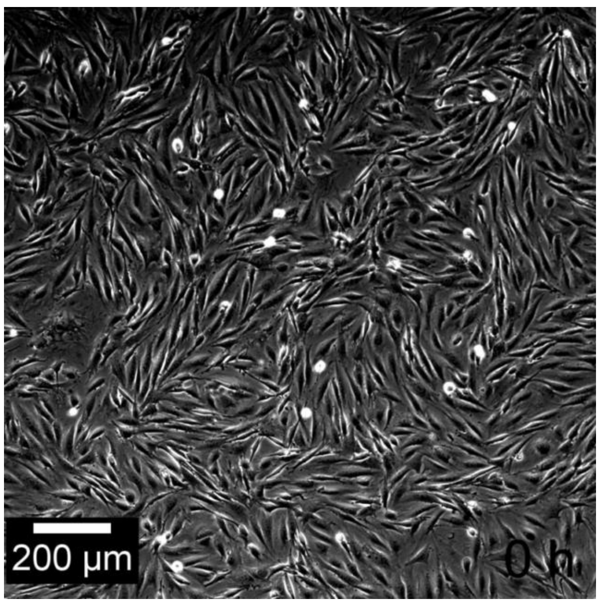
Zhou et al PNAS 2014
E. Coli swimming in chromonic LC

Active Nematics II



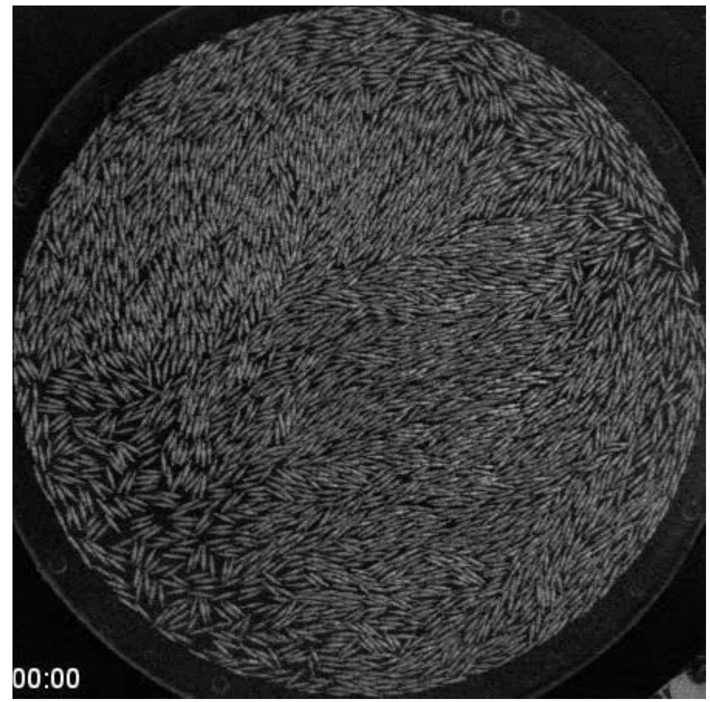
fibroblasts

Contractile/
Pusher



Duclos et al, Soft Matter (2014)

vibrated granular rods



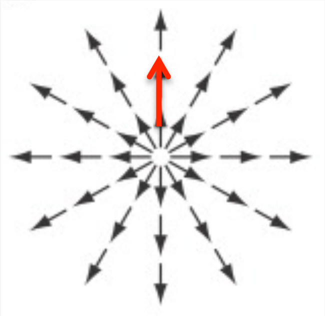
Narayan et al., Science (2007)

Topological Defects

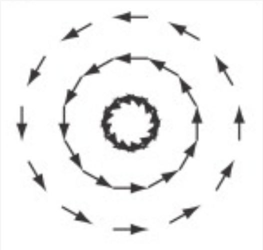
Ordered states contain topological defects that are ``fingerprints'' of the broken symmetry.

Polar: asters & vortices

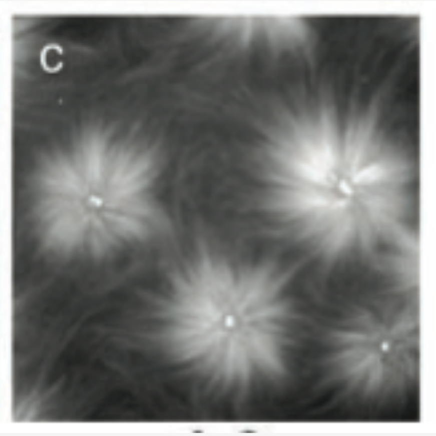
strength +1



aster

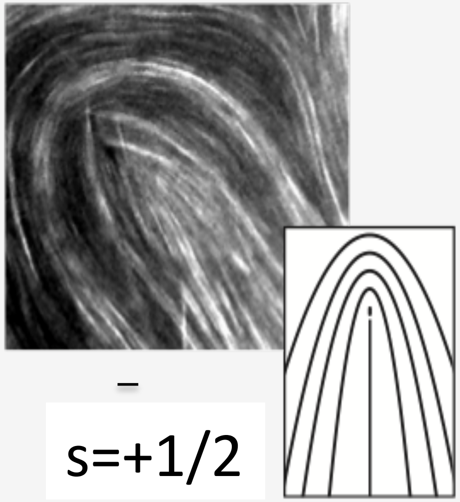


vortex

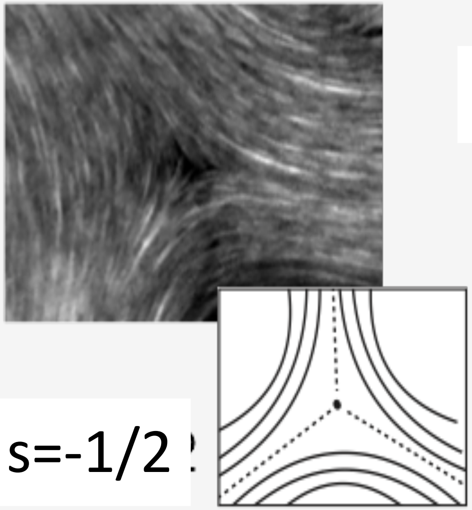


Microtubules & kinesins (Surrey et al 2001)

Nematic: disclinations



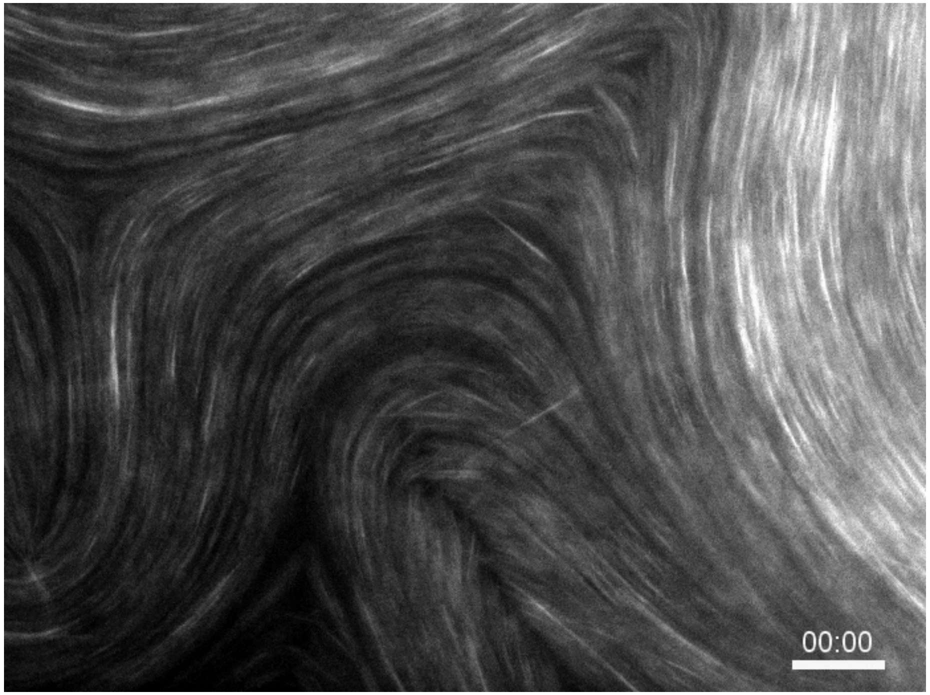
s=+1/2



s=-1/2

Sanchez et al, 2012

In equilibrium **opposite strength defects** are generated upon quench, **attract** & annihilate.



In active systems **opposite strength defects** are continuously generated, may **repel**, and drive the dynamics.

Giomi, Bowick, Ma & MCM, PRL 2013

Outline

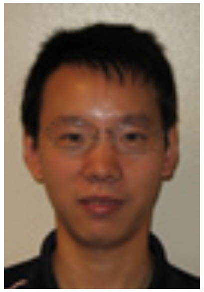
- Active hydrodynamics and defect proliferation in nematic films
  - Giomi, Bowick, Ma & MCM, PRL 110, 228101 (2013); arXiv 1403.5254
  - Thampi, Golestanian & Yeomans, PRL 111, 118101 (2013); EPL 105 (2014); arXiv 1402.0715
  - Gao et al, arXiv 1401.8059

- Active defects as self-propelled particles: opposite can repel!
  - Giomi, Bowick, Ma & MCM, PRL 110, 228101 (2013)
  - Pismen, PRE 88 050502(R) (2013)

- Topological structures in active nematic vesicles
  - Keber, Loiseau, Sanchez, DeCamp, Giomi, Bowick, MCM, Dogic & Bausch, submitted

Theory

Luca Giomi
(SISSA → Leiden)



Xu Ma
SU

Prashant
Mishra
SU

Mark
Bowick
SU

Rastko Sknepnek
Dundee, UK

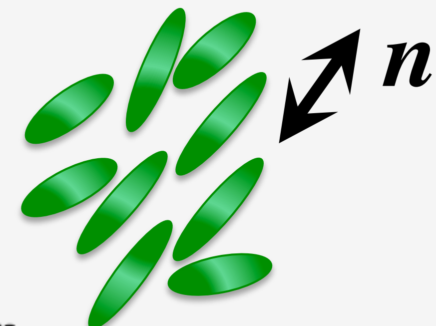
Active Vesicle Experiments

- Felix Keber (TUM)
- Etienne Loiseau (TUM)
- Tim Sanchez (Harvard)
- Stephen deCamp (Brandeis)
- Zvonimir Dogic (Brandeis)
- Andreas Bausch (TUM)

Hydrodynamics of Active Nematic
coupling of orientation and flow

- ρ density of suspension= constant (incompressible)
- ***C*** concentration of active particles: diffusion-convection type equation with active currents

- Order parameter $$Q_{ij} = \langle \sum_{\alpha} \left(n_{\alpha i} n_{\alpha j} - \frac{1}{2} \delta_{ij} \right) \rangle$$



$$\begin{cases} |\mathbf{Q}| \sim \text{order strength} \\ \text{principal axis}: \ \text{orientation of order} \end{cases}$$

- $\mathbf{v}$ flow velocity of suspension

Kruse et al, EPJE 2005; Marenduzzo et al, 2007; Liverpool & MCM 2007; …

Dynamics of Q Tensor

$$[\partial_t + \mathbf{v}\cdot\nabla]\,Q_{ij} = \lambda S u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} + \frac{1}{\gamma}H_{ij}$$

orientation/flow coupling

$$u_{ij} = (\partial_i v_j + \partial_j v_i)/2$$

$$\omega_{ij} = (\partial_i v_j - \partial_j v_i)/2$$

rotational friction

$$H_{ij} = -\frac{\delta F}{\delta Q_{ij}} = -\left[A + B\mathbf{Q}^2\right]Q_{ij} + K\nabla^2 Q_{ij} + \ldots$$

stiffness

$$\tau_p = \gamma \ell^2 / K$$

relaxation of local structure

Flow velocity: Navier-Stokes equation

$$\rho\partial_t v_i = \eta\nabla^2 v_i - \partial_i p + \partial_j\left(\sigma^p_{ij} + \sigma^a_{ij}\right)$$

viscous stress

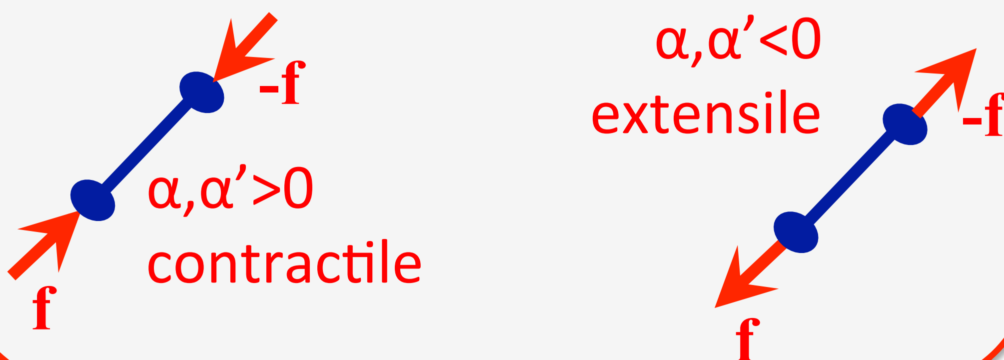
elastic stress

incompressibility
$\nabla\cdot\mathbf{v} = 0$

active stress
$$\sigma^a_{ij} = \alpha'\delta_{ij} + \alpha Q_{ij}$$

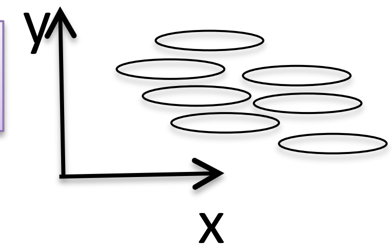
Activity ~ rate of ATP consumption

Active units extert force dipoles on the medium, generating active stresses
(Pedley & Kessler, 1992;…)

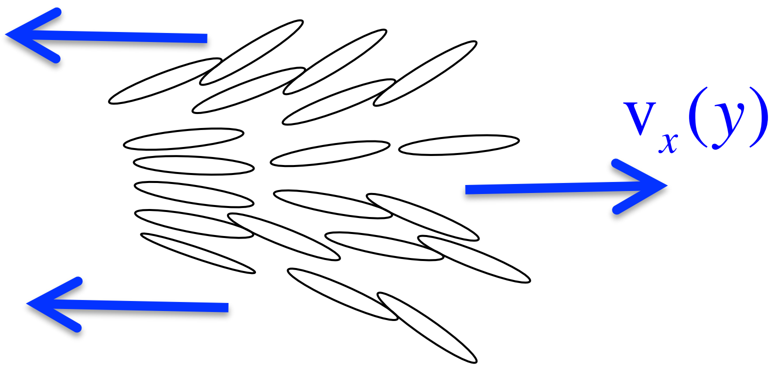


$\tau_a = \eta/|\alpha|$
injection of active stresses

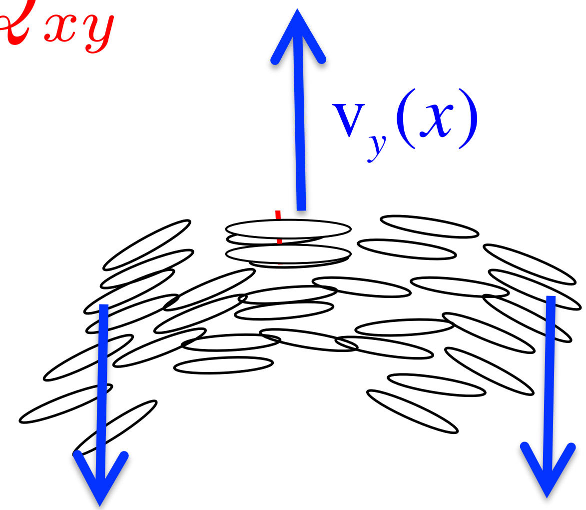
Active stresses generate shear flows



$$\sigma_{xy} = \eta(\partial_x v_y + \partial_y v_x) + \alpha Q_{xy}$$



splay unstable for α>0
(contractile/pullers)

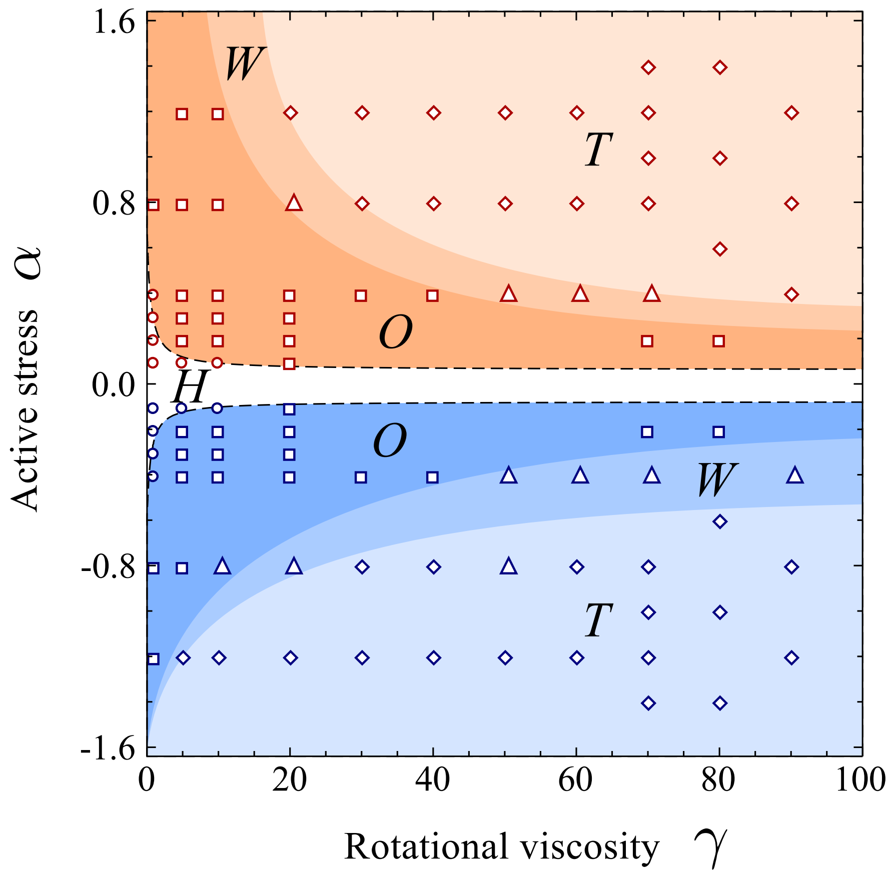


bend unstable for α<0
(extensile/pushers)

$$\text{active stress} \sim \text{elastic stress} \rightarrow \quad \xi_a \sim \sqrt{\frac{K}{|\alpha|}}$$

→ Band formation (cf. spontaneous flow instability of thin films, Voituriez et al., EPL 2005)

Phase diagram



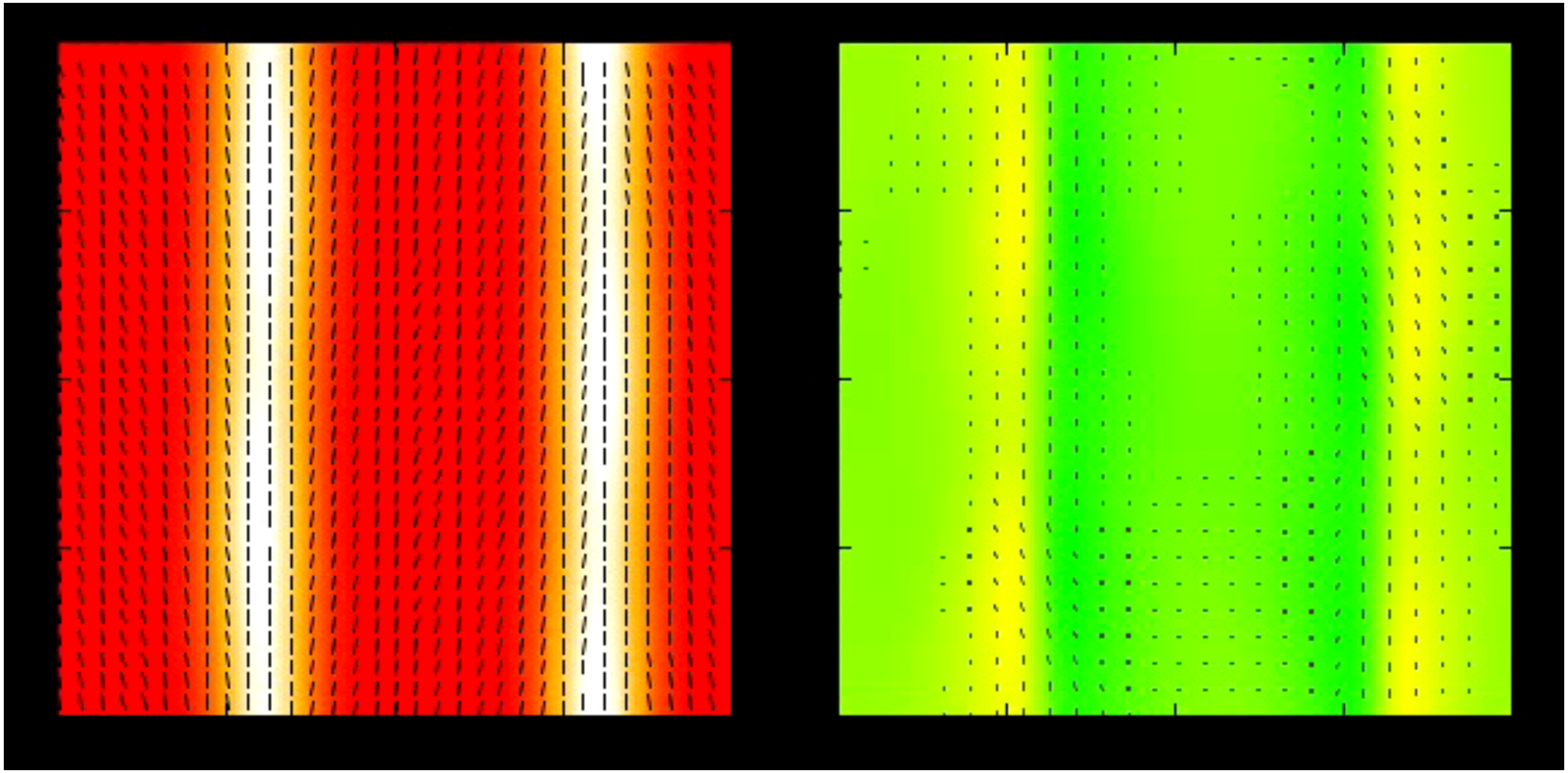
H - homogeneous ordered state

O – Relaxational oscillations (Giomi et al, 2013)

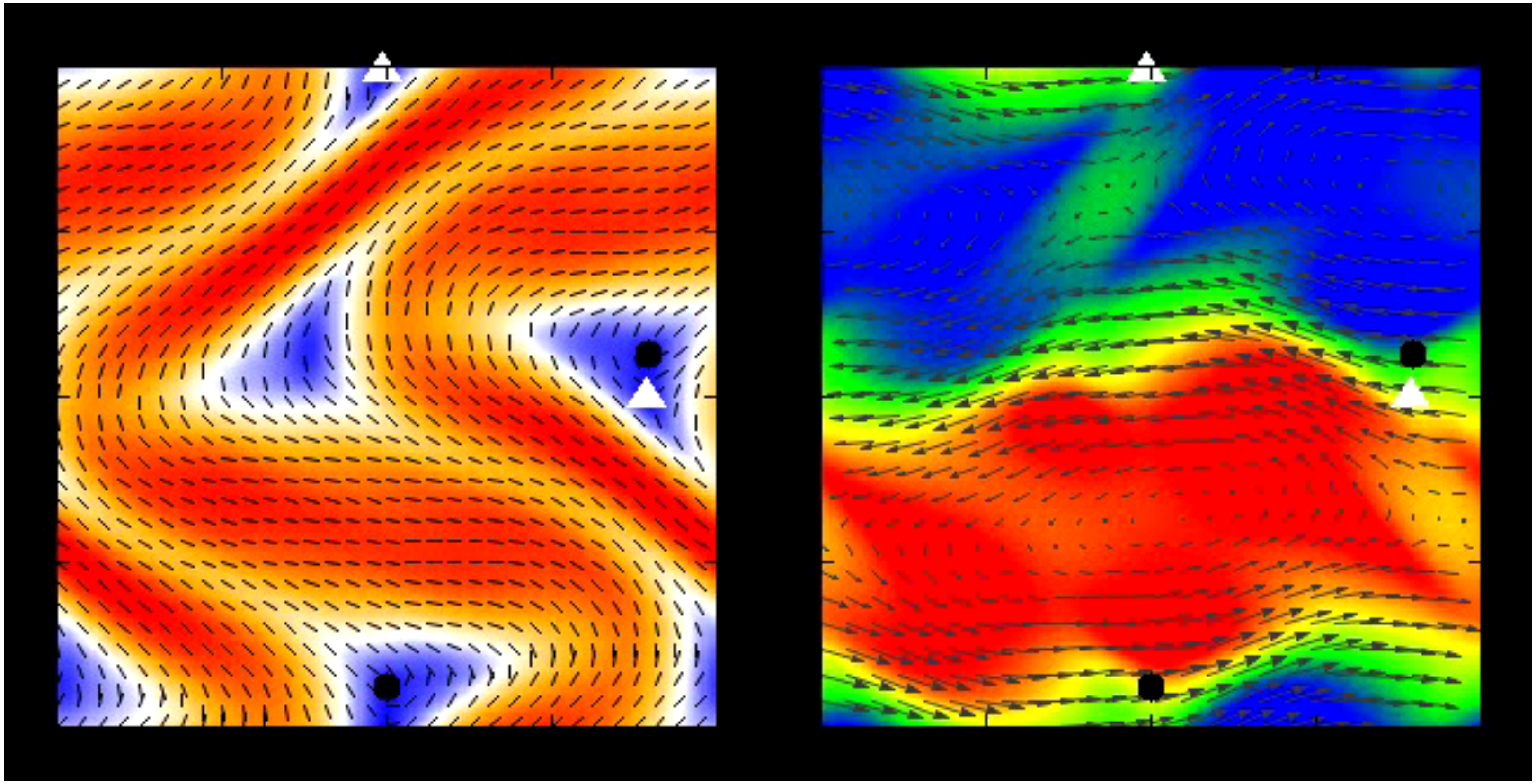
W – Wall formation & unzipping

T - Turbulence

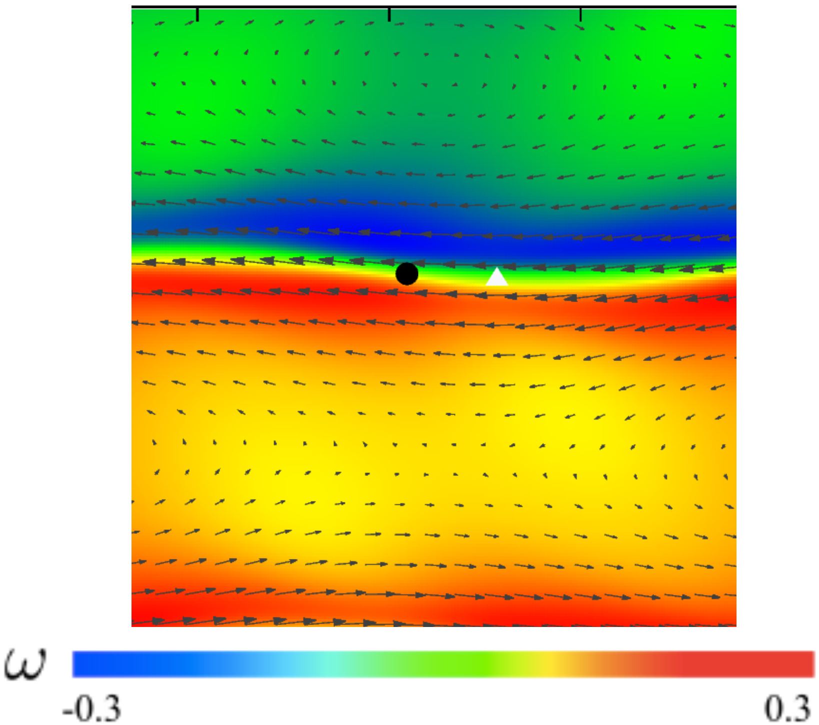
Wall formation (extensile)

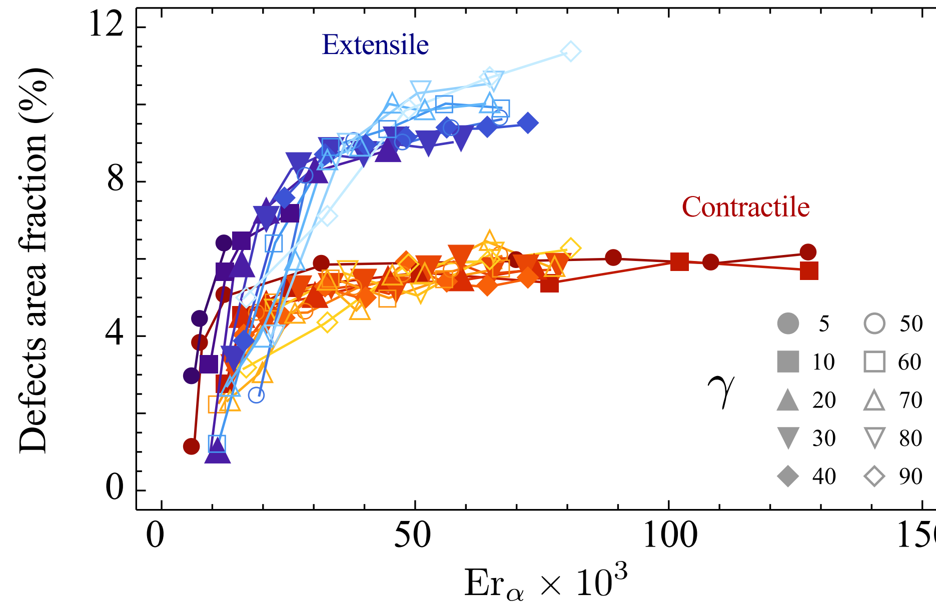


``Turbulence'' (extensile)



Spontaneous Vorticity & Defect Proliferation





defect-antidefect pair creation where vortices of opposite vorticity meet

Ericksen number

$$Er = \frac{\dot{\epsilon}\gamma h^2}{K} \quad \rightarrow \quad Er_\alpha = \frac{\alpha\gamma L^2}{\eta K}$$

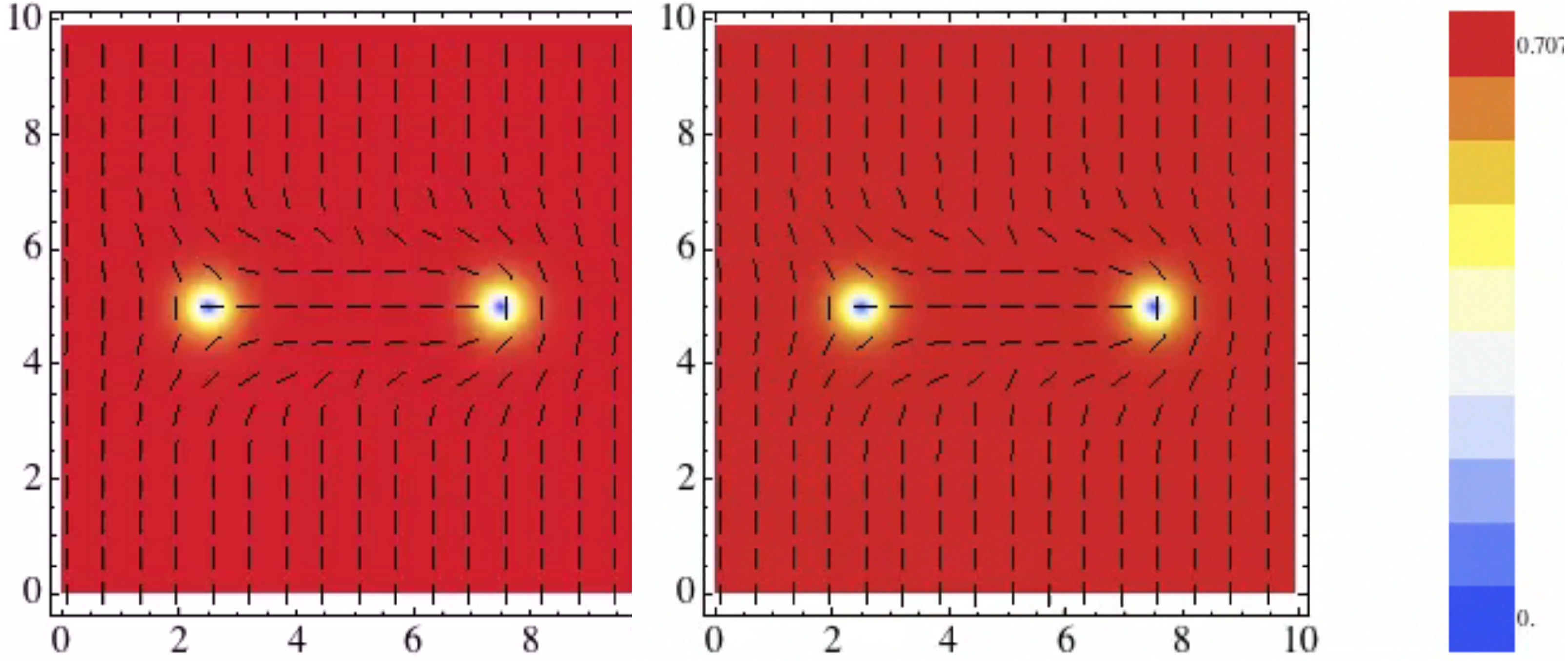
$$\eta\dot{\epsilon} \quad \rightarrow \quad \alpha$$

Also: Thampi *et al*, 2013, 2014; Gao *et al* 2014

Dynamics of defect pairs

from numerical integration of hydrodynamic equations

Giomi, Bowick, Ma & MCM, PRL 2013



passive
α=0

active **contractile** $\alpha>0$

For this configuration, activity yield pair **attraction**, speeds up approach

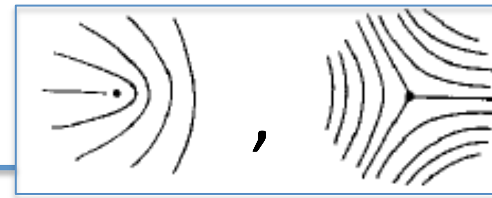
Active Backflow

Giomi, Bowick, Ma & MCM, PRL 2013

Director distortions from disclinations yield active stresses that act as a source for flows → solve for flow in Stokes limit

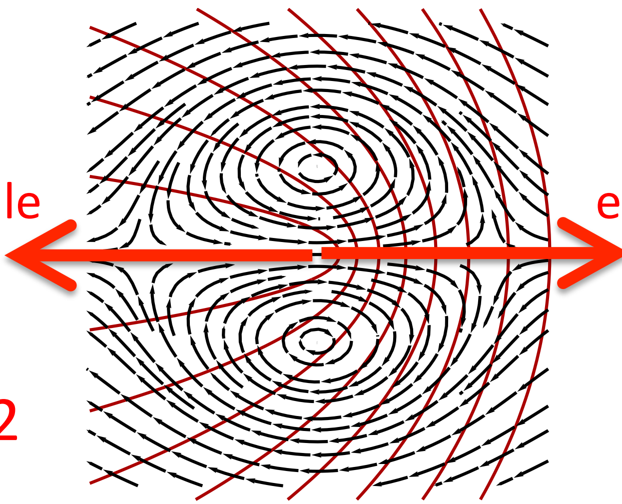
$$\cancel{\partial_t \mathbf{v}} = \eta \nabla^2 \mathbf{v} + \alpha \nabla \cdot \mathbf{Q}$$

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

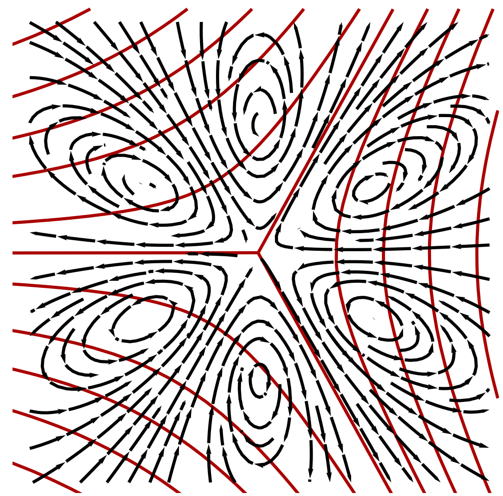


contractile

extensile



+1/2



-1/2

$v_{core} \sim \alpha / \eta$ direction depends on sign of α

$v_{core} = 0$

Pismen, PRE 2014

Active Defects as ``Self-Propelled'' Particles

No backflow → pair dynamics controlled by balance of *friction* and *attraction*

$$x = x_+ - x_-$$

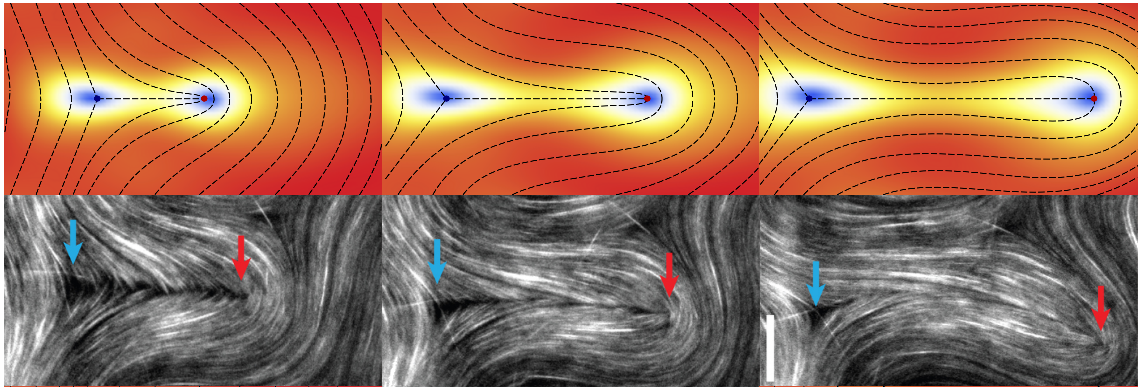
$$\zeta \dot{x} = -\nabla \left[K \ln(x/a) \right]$$

In the presence of active backflow defects ride with the flow

$$\zeta \left[\dot{x}_\pm - v_b(x) \right] = -\nabla \left[K \ln(x/a) \right]$$

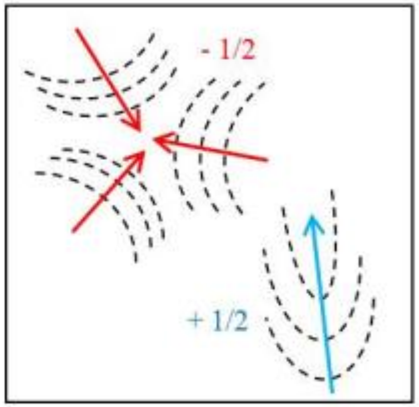
$$v_b(x) \simeq -(\alpha/\eta) R \delta(x - x_+)$$

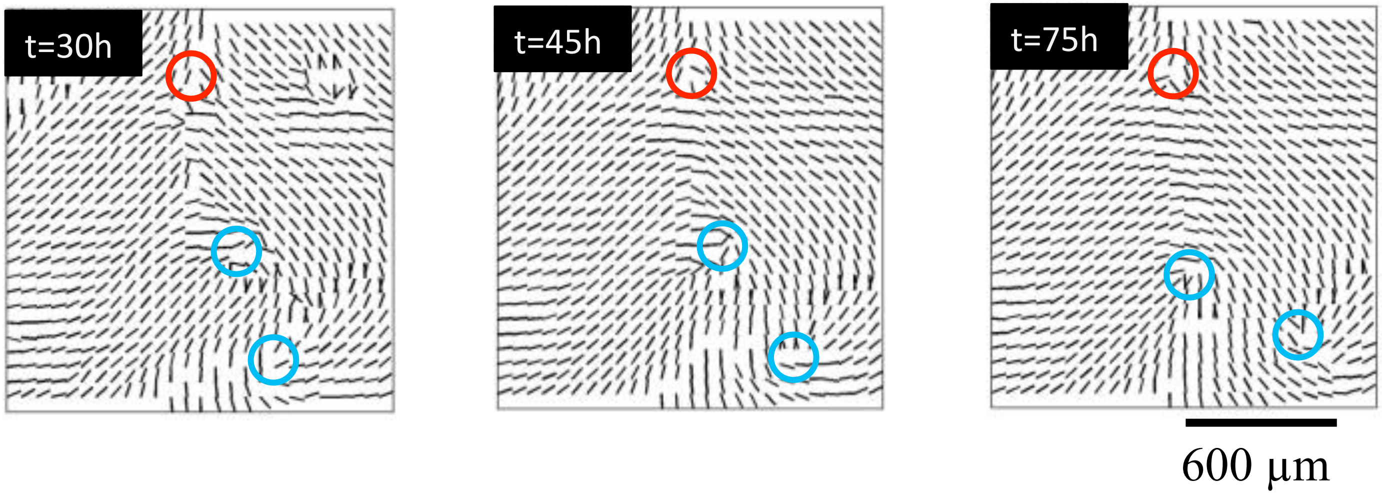
Extensile active nematic



Contractile system: fibroblasts monolayer

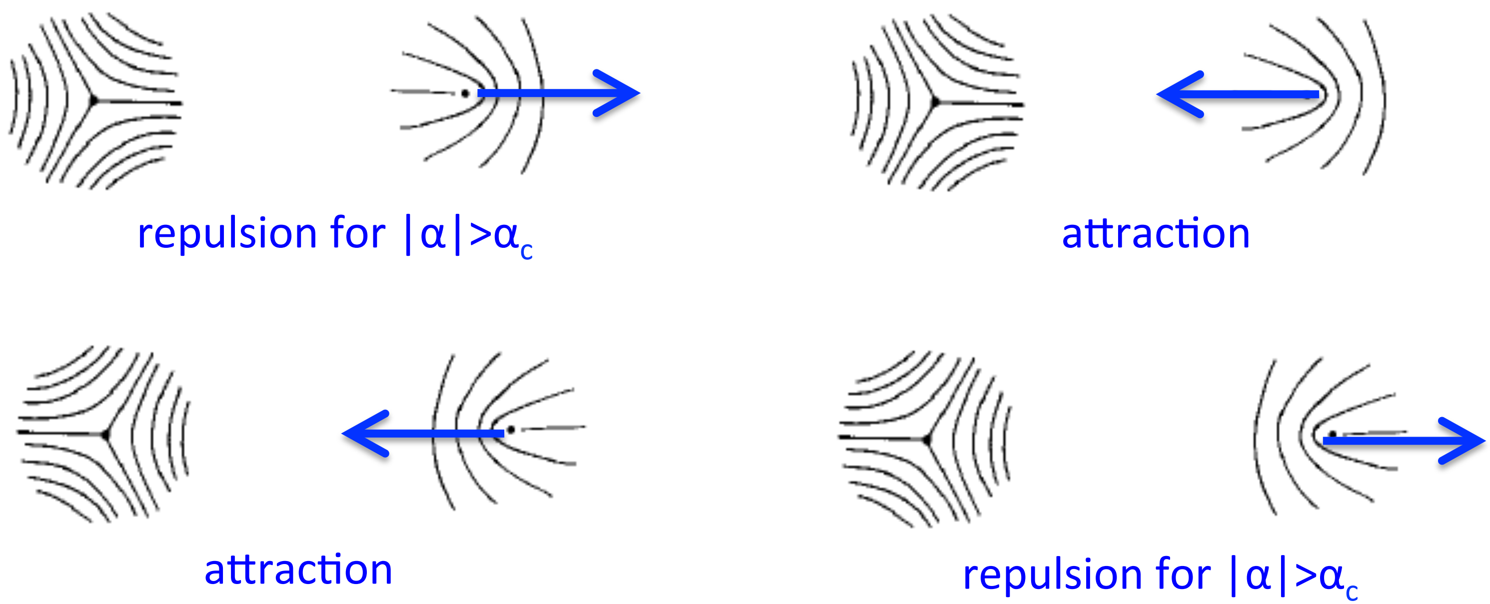
Guillaume Duclos
Silberzan's Lab





Defects as Self-Propelled Particles

Extensile systems | Contractile systems

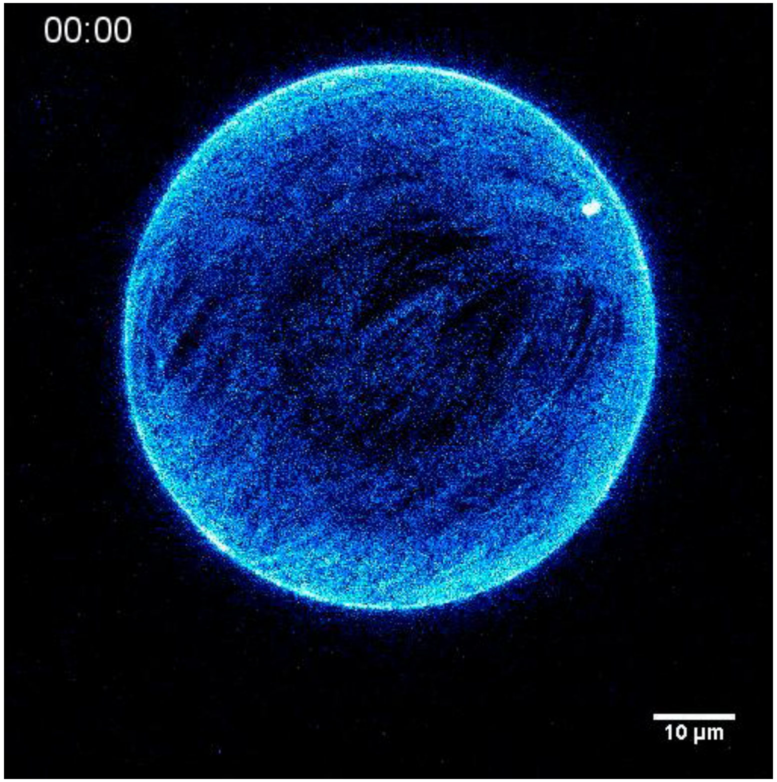


- Topological defects as fingerprints of symmetry (nematic vs polar)
- Direction of motion of +1/2 defect reveals extensile/contractile nature of active stresses

Active vesicles

Keber, Loiseau, Sanchez, DeCamp, Giomi, Bowick, MCM, Dogic & Bausch, submitted

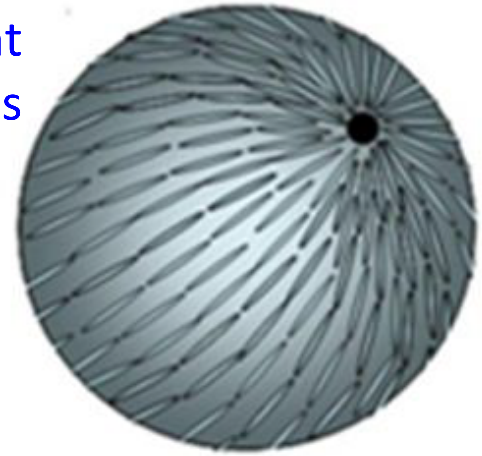
Active MT suspension in a vesicle
→ 2d nematic on the surface of a sphere



Nematic order on a sphere requires a +2 topological charge

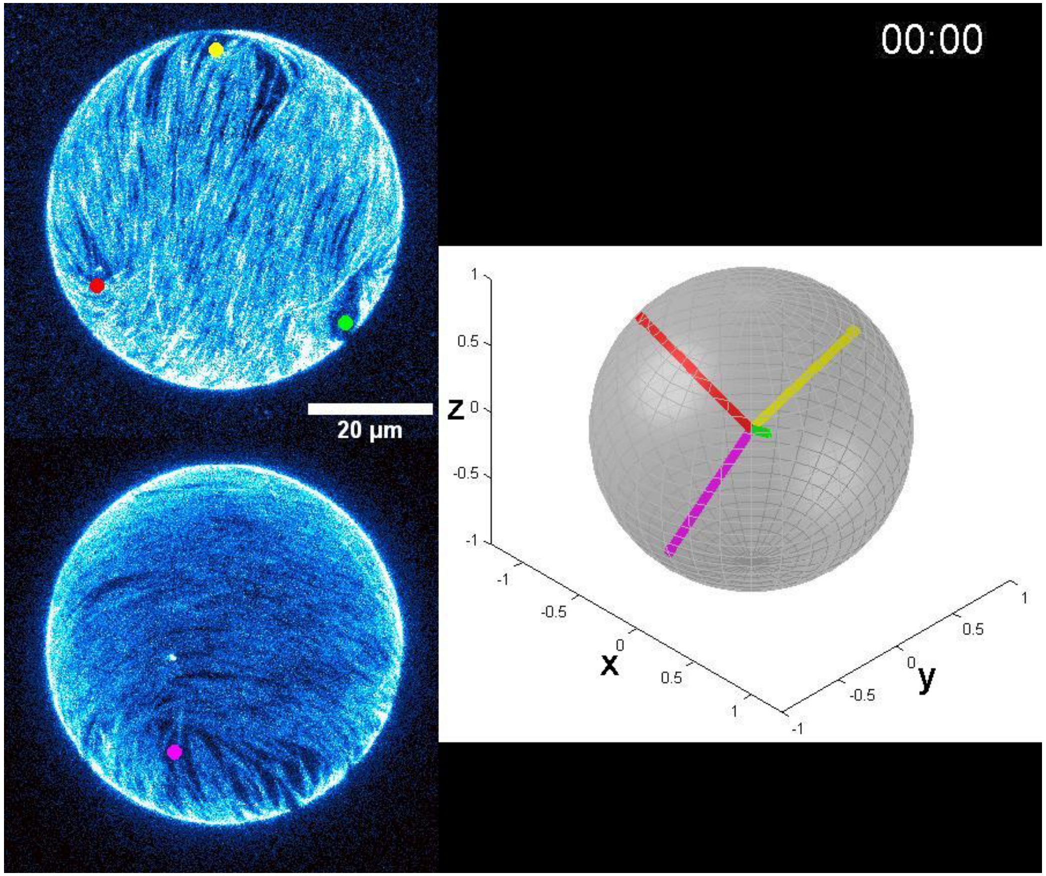
Four +1/2 defects at corner of a tetrahedron

Two +1 defects at the poles

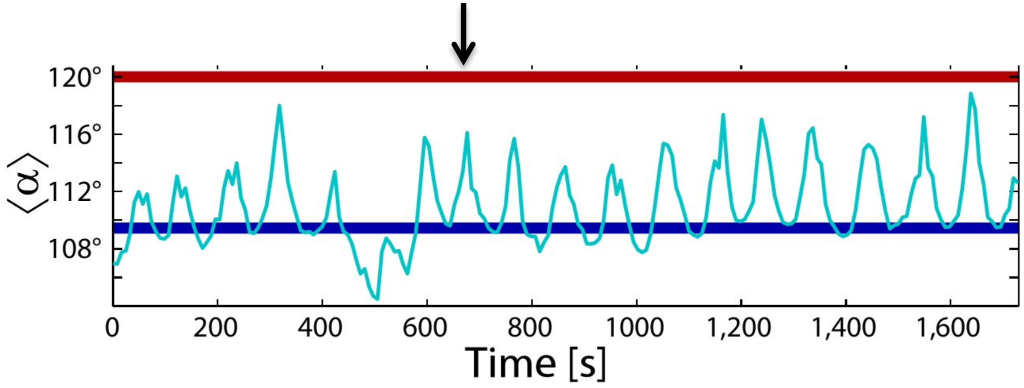


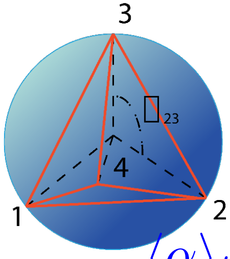
In active nematic defects oscillate between tetrahedral and planar configurations

$$\langle \alpha \rangle = \frac{1}{6} \sum_{i<j} \arccos \left(\frac{\mathbf{r}_i \cdot \mathbf{r}_j}{R^2} \right)$$



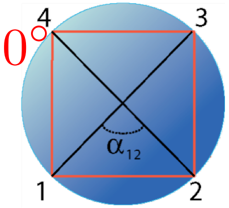
Frequency set by size of sphere and ATP concentration (12 mHz)





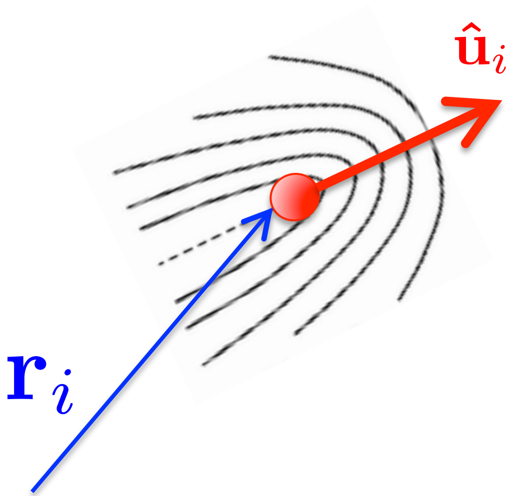
$\langle \alpha \rangle_{tetr} = 109°$

$\langle \alpha \rangle_{pl} = 120°$



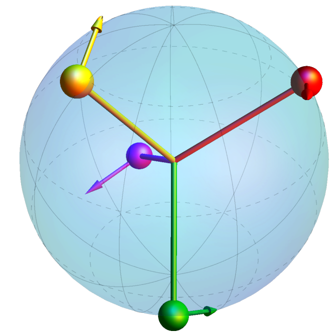
Defects as SP particles on a sphere

$$\hat{\mathbf{u}}_i = (\cos\psi_i, \sin\psi_i)$$



$$\frac{d\mathbf{r}_i}{dt} = v_0 \hat{\mathbf{u}}_i - \frac{1}{\zeta_t}\nabla_i E$$

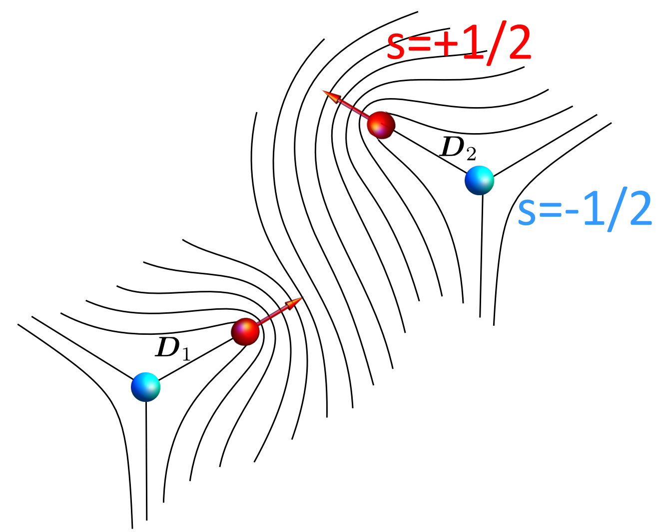
$$\frac{d\psi_i}{dt} = \frac{1}{\zeta_r} M_i$$



Equilibrium interactions and torques adapted to the surface of the sphere

$$E_{pair} \sim -s_1 s_2 K \ln|\mathbf{r}_1 - \mathbf{r}_2|$$

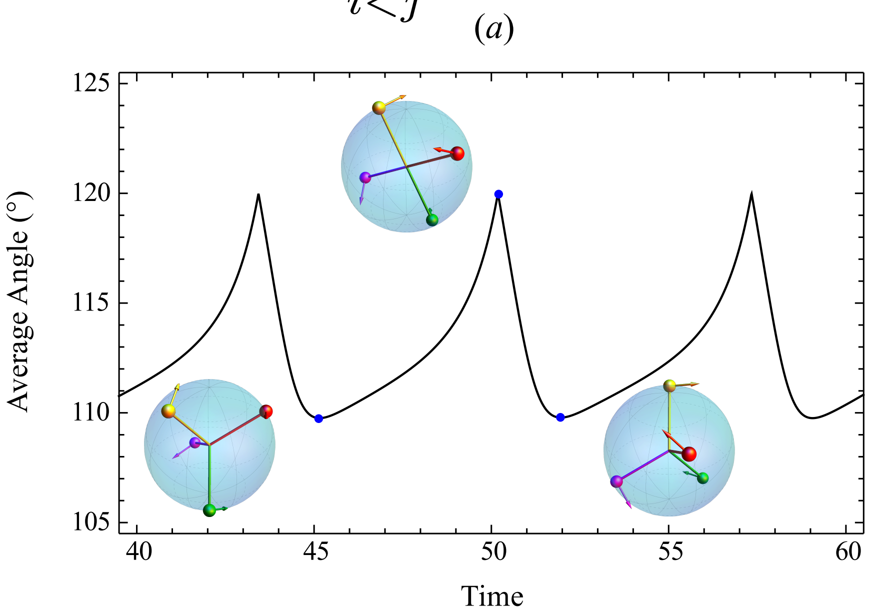
Torque obtained from interaction energy of two ±1/2 dipoles in the limit D_1,D_2→∞

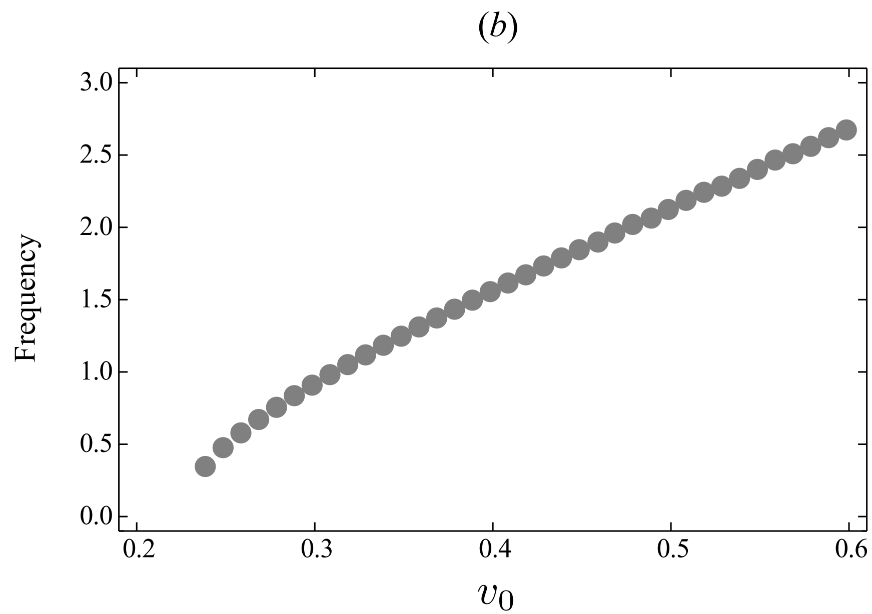


Oscillations for $\zeta_t R^2 > \zeta_r$

$$\langle \alpha \rangle = \frac{1}{6} \sum_{i<j} \arccos\left(\frac{\mathbf{r}_i \cdot \mathbf{r}_j}{R^2}\right)$$

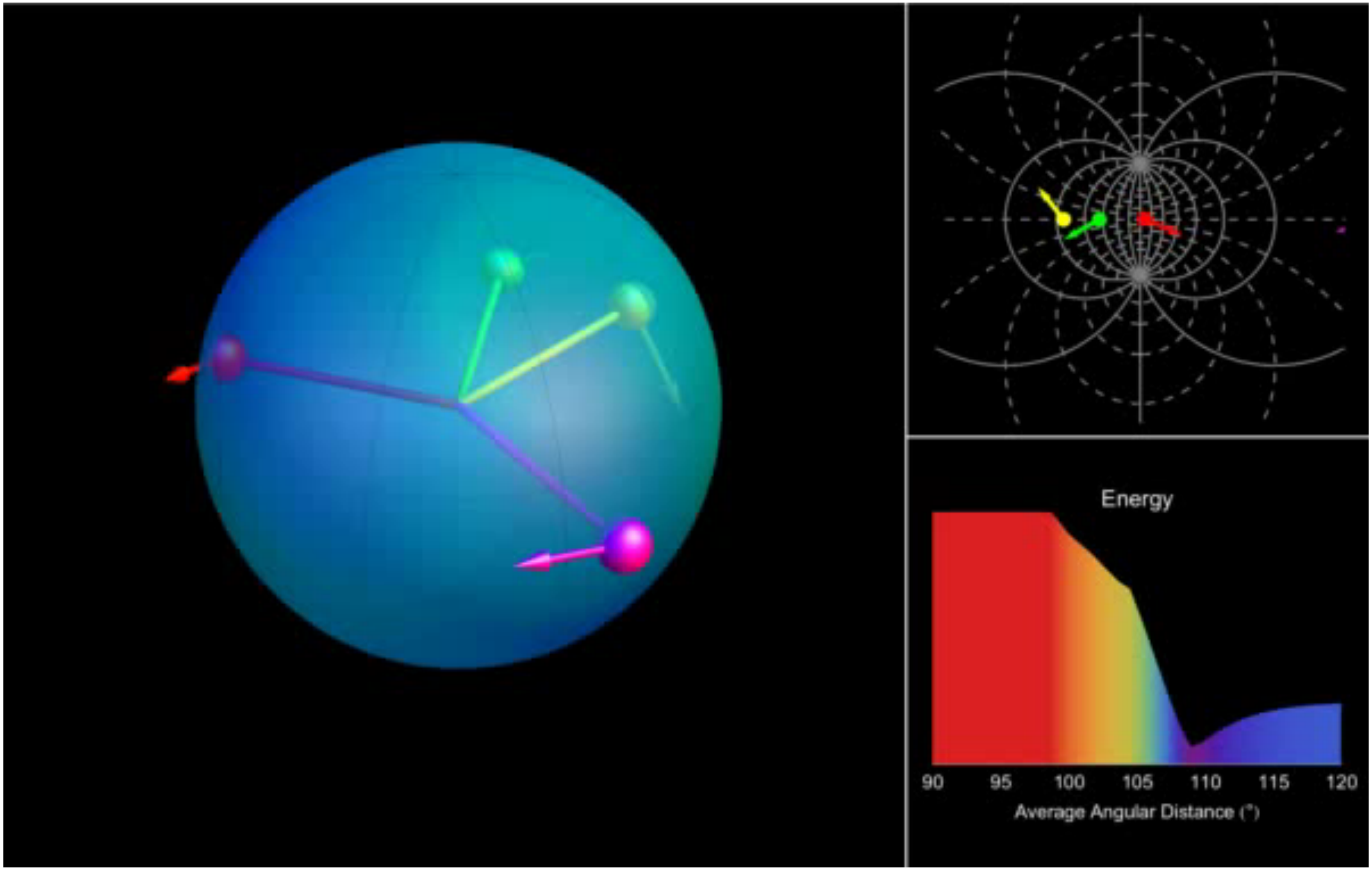
Defect core translation lags reorientation





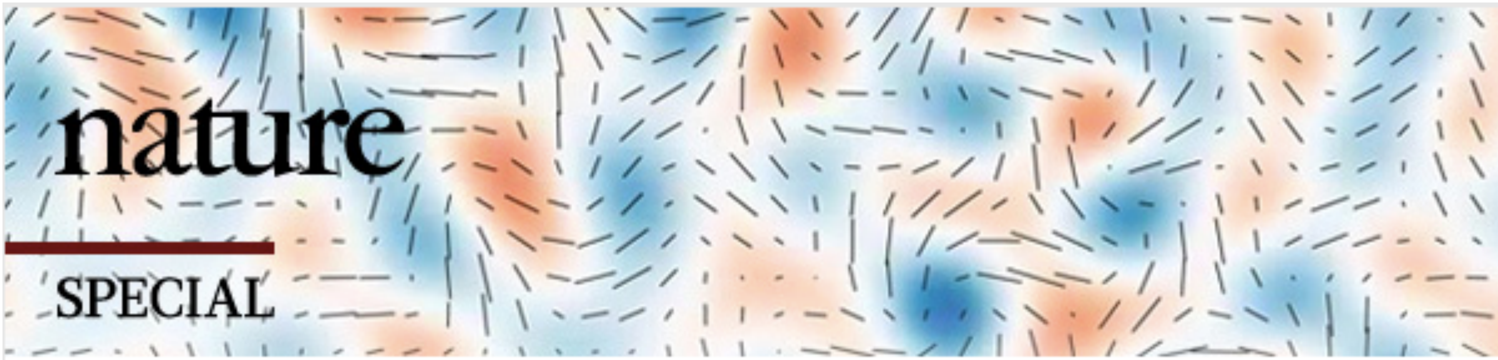
$$v_0 \sim \frac{\text{activity}}{\text{viscosity}} R$$

$$\text{frequency} \sim v_0 / R$$


Energy
90
95
100
105
110
115
120
Average Angular Distance (°)

Nematics everywhere: could it be *active*?

March 18, 2014



WAVES FROM THE BIG BANG

The detection of gravitational waves in the afterglow of the Big Bang — if confirmed — opens a new chapter in astronomy, cosmology and physics. The signature, seen by the BICEP2 radio telescope at the South Pole, packs at least three discoveries into one: It provides the most direct evidence for the existence of the waves predicted by Einstein; it is the proof of 'cosmic inflation' that physicists had been eagerly awaiting; and it opens a window into the unification of the fundamental forces of nature and into quantum gravity.