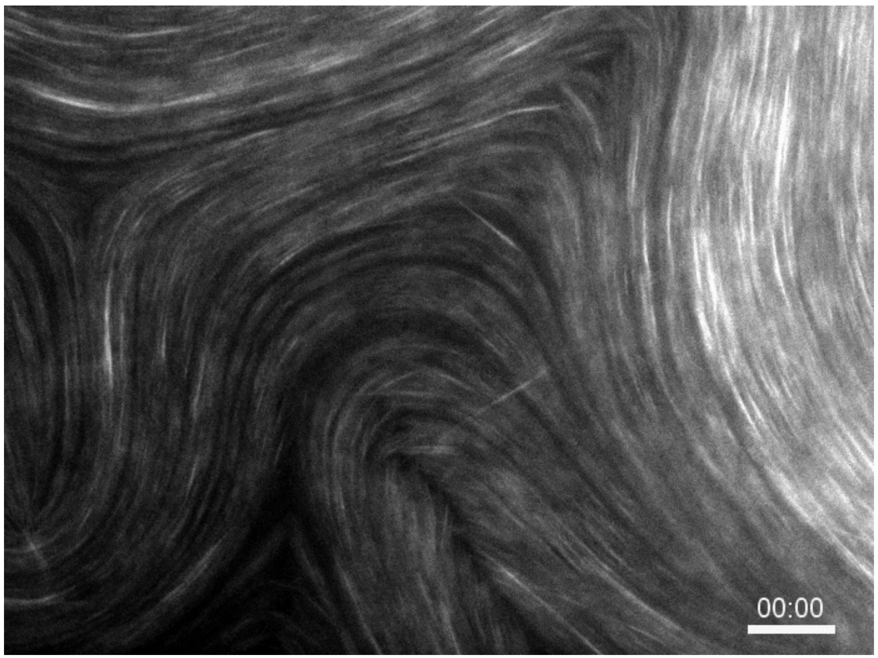
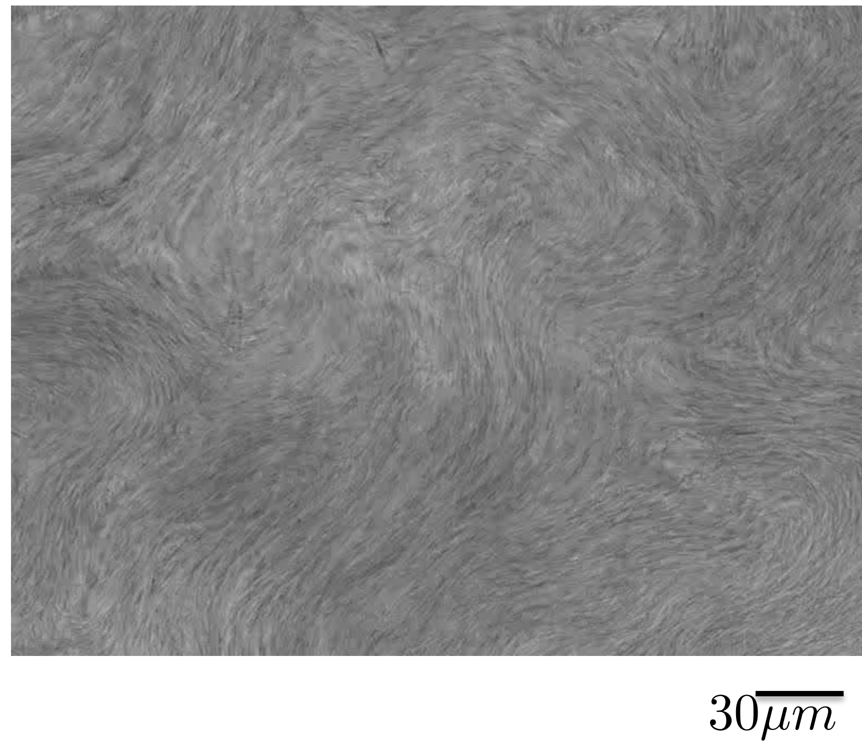
2D suspensions of microtubule-
kynesin bundles at oil/water interface

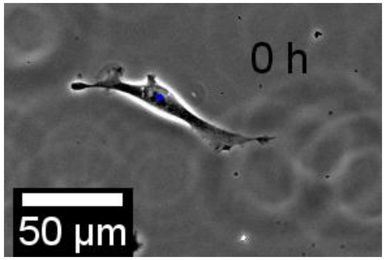
E. Coli swimming in nematic LC



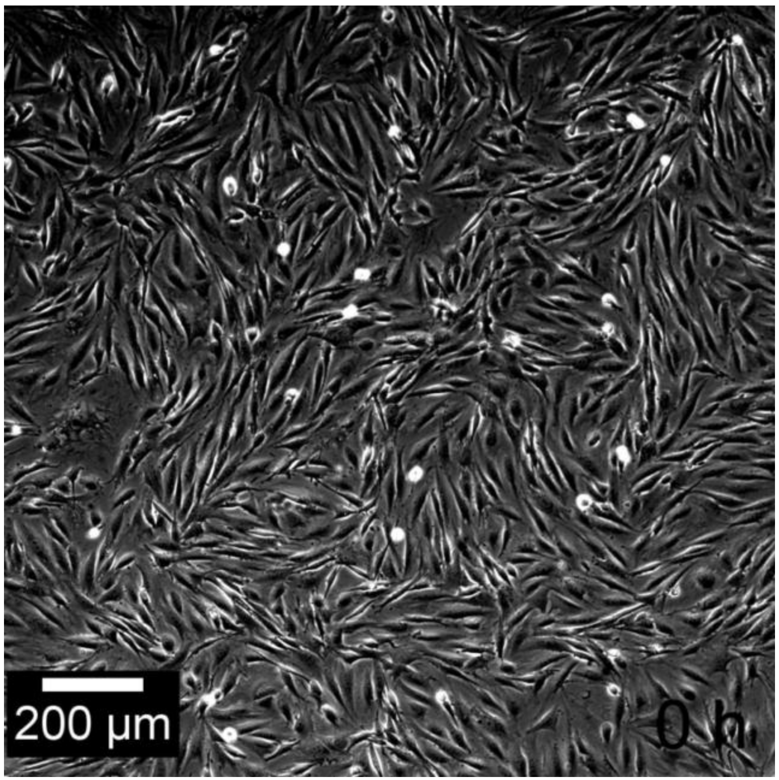


Sanchez et al, Nature 2012

Zhou et al PNAS 2014

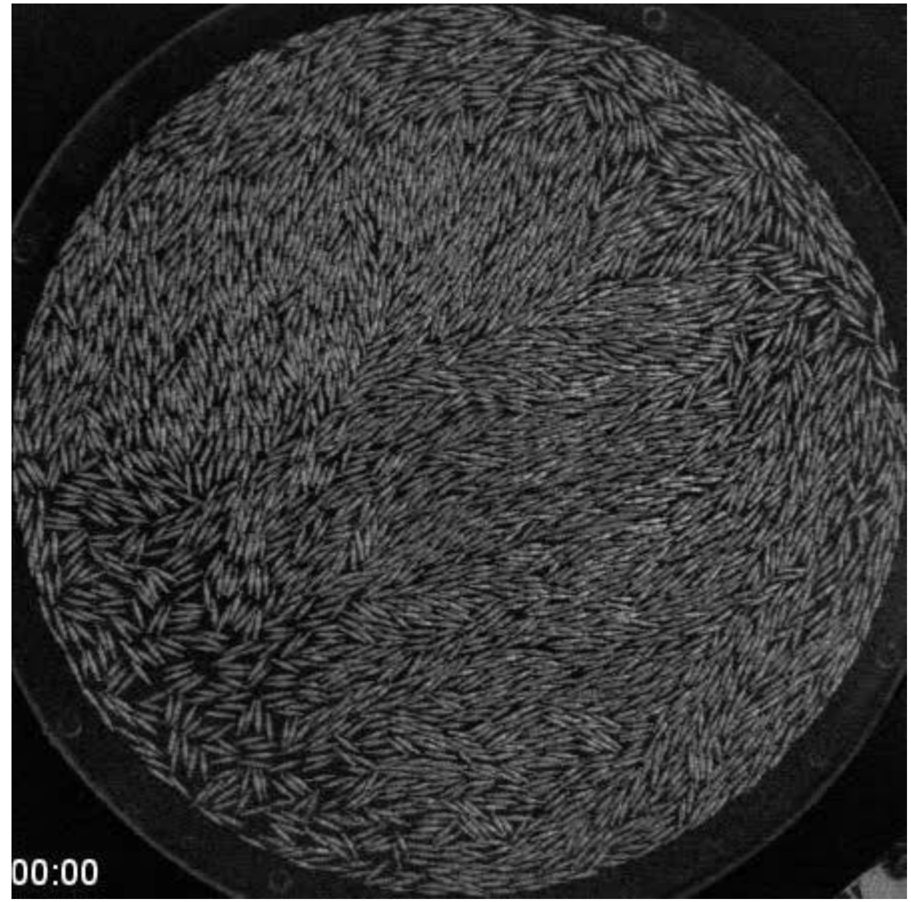


fibroblasts



Duclos et al, Soft Matter (2014)

Vertically vibrated granular rods



Narayan et al., Science (2007)

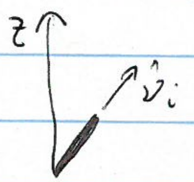
ACTIVE NEMATIC

I want to consider systems w/ momentum conservation. Strictly speaking a suspension: active particles in a fluid - should distinguish between total density of suspension and ~~flows~~ concentration of active units
→ for simplicity a one-component fluid

HYDRODYNAMICS : large λ, long times

- conserved fields $\begin{cases} \rho & \text{density} \\ \rho\vec{v} & \text{momentum density} \end{cases}$

We have a phase transition (isotropic → nematic) associated with a spontaneously broken <u>continuous</u> symmetry



O.P. $\quad Q_{\alpha\beta} = \left\langle \sum_i \left(\hat{\nu}_{\alpha i}\hat{\nu}_{\beta i} - \frac{1}{d}\delta_{\alpha\beta}\right)\delta(\vec{r}-\vec{r}_i)\right\rangle$

$d=2$

uniaxial $\quad Q_{\alpha\beta} = S\left(\hat{n}_\alpha \hat{n}_\beta - \frac{1}{d}\delta_{\alpha\beta}\right) \qquad Q_{\alpha\beta}Q_{\alpha\beta} = S^2/2$

- broken symmetry field $\hat{n}$ → Goldstone mode

Deep in ordered state → ~~only~~ S = constant

Consider only director deformations: they cost energy

$$F = \frac{1}{2}\int_{\vec{r}} \left[K_1 (\vec{\nabla}\cdot\hat{n})^2 + K_3 (n \times \nabla \times n)^2\right]$$

splay

bend

assume $K_1 = K_3$

$$-\frac{\delta F}{\delta \hat{n}} = \vec{h} = \nabla^2 \hat{n}$$

a driving force that tends to restore the uniform state

HYDRODYNAMICS

Navier - Stokes $\begin{Bmatrix} \rho \\ \vec{v} \end{Bmatrix}$ + dynamics of director $\hat{n}$

coupling of orientation and flow

- incompressible : $\rho = \text{const.}$ $\quad \partial_t \rho + \vec{\nabla} \cdot \rho \vec{v} = 0 \Rightarrow \vec{\nabla} \cdot \vec{v} = 0$

- Navier Stokes :

$$\cancel{\rho(\partial_t + \vec{v} \cdot \vec{\nabla}) v_\alpha} = \underbrace{\eta \nabla^2 v_\alpha}_{\text{viscous forces}} - \partial_\alpha p + \underbrace{\partial_\beta \sigma^N_{\alpha\beta}}_{\text{elastic deformations of the director couple to flow}}$$

0

But most active LC are in the low Re regime

$$Re \sim \frac{\text{inertial } \cancel{\text{forces}}}{\text{viscous forces}} \sim \frac{\rho v^2/L}{\eta v/L^2} \sim \frac{\rho v L}{\eta}$$

$Re \ll 1 \quad \rightarrow$ Stokes equation

$$\sigma^N_{\alpha\beta} = \frac{\lambda}{2}(n_\alpha h_\beta + n_\beta h_\alpha) \underbrace{- \frac{1}{2}(n_\alpha h_\beta - n_\beta h_\alpha)}_{\text{torque}}$$

- director dynamics

$$(\partial_t + \vec{v} \cdot \vec{\nabla}) n_\alpha + \underbrace{\omega_{\alpha\beta} n_\beta}_{\text{vorticity rotates LC molecules}} = \frac{1}{\gamma} h_\alpha + \lambda u_{\alpha\beta} n_\beta$$

δT

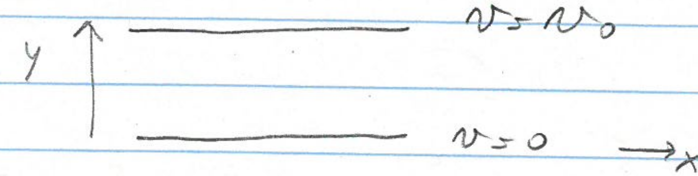
shear builds up alignment

$$u_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta + \partial_\beta v_\alpha)$$

$$\omega_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha)$$

Flow alignment parameter λ

LC in shear flow



$\hat{n} = (\cos\theta, \sin\theta)$

$$\partial_t \theta = -u(1 - \lambda \cos 2\theta) + \frac{K}{\gamma} \partial_y^2 \theta$$

$\dot{\gamma} = v_0 / L$ shear rate

$v_x = \dot{\gamma} y$

$u = u_{xy} = \dot{\gamma}/2$

homogeneous ss

- $\boxed{\cos 2\theta = 1/\lambda}$ if $|\lambda| \geq 1$ flow aligning

- $|\lambda| < 1$ no ss solution - flow tumbling

λ is a microscopic parameter that depends on molecular shape and degree of order

long, thin rods $|\lambda| > 1$

A nematic in shear flow picks an orientation that is determined by λ

flow exerts a torque on the director until it reaches this stable orientation

Activity

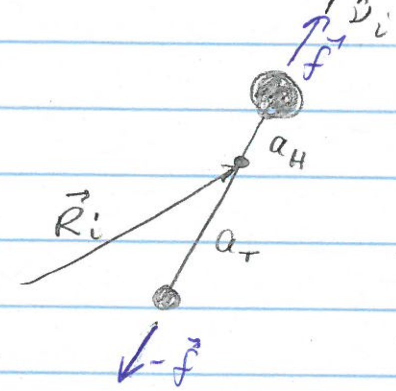
active stress

activity yields an additional energy input that provides additional driving forces on the fluid

$$\sigma_{ij}(\vec{\nabla}\vec{v}, \vec{h}) \longrightarrow \sigma_{ij}(\vec{\nabla}\vec{v}, \vec{h}, \Delta\mu)$$

e.g., $\mu_{ATP} - (\mu_{ADP} + \mu_P)$

$$[\partial_j \sigma_{ij}] = [\text{force density}]$$



$$\vec{F}^{act} = \sum_i \{ f\hat{\nu}_i \delta(\vec{r} - \vec{R}_i - a_H\hat{\nu}_i) - f\hat{\nu}_i \delta(\vec{r} - \vec{R}_i + a_T\hat{\nu}_i) \}$$

use $a_H = a_T$

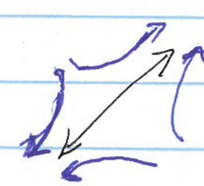
$$F^{act}_\alpha = \sum_i f\hat{\nu}_{i\alpha} \{ -(a_H + a_T)\hat{\nu}_{i\beta}\partial_\beta \delta(\vec{r} - \vec{R}_i) + \frac{1}{2}(a_H^2 - a_T^2)\hat{\nu}_{i\beta}\hat{\nu}_{i\gamma}\partial_\gamma \delta(\vec{r} - \vec{R}_i) + \dots \}$$

$r \gg a_T + a_H = L$

$$F^{act}_\alpha \simeq -fL \langle \sum_i \hat{\nu}_{i\alpha}\hat{\nu}_{i\beta} \delta(\vec{r} - \vec{R}_i) \rangle$$

$$F^{act}_\alpha = \alpha\partial_\beta (Q_{\alpha\beta} + \frac{1}{d} c\,\delta_{\alpha\beta})$$

$\alpha = -fL < 0$

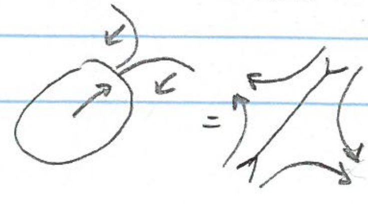


extensile : MT, E. coli

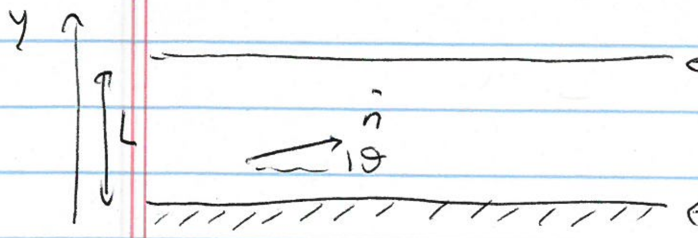
$$\boxed{\sigma^{act}_{\alpha\beta} = \alpha\, Q_{\alpha\beta} \boxed{+ \frac{\alpha}{d} c^2 \delta_{\alpha\beta}}}$$

$\alpha > 0$

contractile : actomyosin, Chlamydomonas



SPONTANEOUS FLOW



anchoring b.c. $\vartheta(0)=\vartheta(L)=0$

free boundary $\sigma_{xy}=0$

no slip $v_x(0)=0$

$\partial_y \sigma_{yy}=0 \rightarrow$ pressure

$\partial_y \sigma_{xy}=0 \rightarrow \sigma_{xy}=\text{const}=0$

$\sigma_{xy}=\eta\,\partial_y v_x + K\partial_y^2\theta$ quiescent uniform state

active

$$\sigma_{xy}=\eta\,\partial_y v_x + \alpha\,\hat{n}_x\hat{n}_y + K\partial_y^2\theta$$

can satisfy $\sigma_{xy}=0$ with $\partial_y v_x \neq 0$ and

director deformations $(n_y\neq 0)$

But director deformations cost elastic energy

$\sim K\partial_y^2\hat{n}$

elastic stress   active stress

$$K\nabla^2\hat{n} \sim \alpha\,\hat{n}\hat{n}$$

$$l_\alpha^2 \sim \frac{K}{|\alpha|}$$

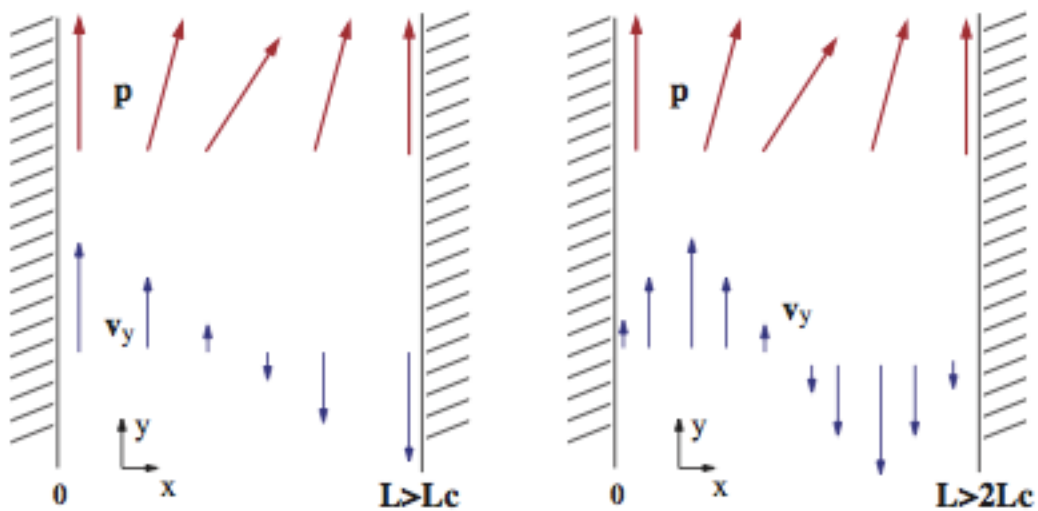
$L > l_\alpha$ activity wins $\rightarrow$ spontaneous flow

$L < l_\alpha$ anchoring wins $\rightarrow$ uniform state

Europhys. Lett., **70** (3), pp. 404–410 (2005)
DOI: 10.1209/epl/i2004-10501-2

Spontaneous flow transition in active ~~polar~~ nematic gels

R. Voituriez[1], J. F. Joanny[1] and J. Prost[1,2]



free slip walls

no slip walls

Contractile vs Extensile systems

ordered state $\hat{n}_0 = \hat{x}$

$$\sigma_{xy} = \frac{\eta}{2}(\partial_x v_y + \partial_y v_x) + \alpha n_x n_y$$

fluctuations:
$\delta\vec{n} = \hat{y}\,\delta n_y$
$|\hat{n}| = 1$

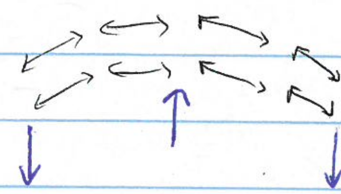
$$\sigma_{xy} \simeq \frac{\eta}{2}(\partial_x v_y + \partial_y v_x) + \alpha\,\delta n_y$$

SPLAY $\delta n_y(y)$

$\alpha > 0$
contractile

$$\partial_y v_x \sim -\frac{2\alpha}{\eta}\delta n_y$$

BEND $\delta n_y(x)$

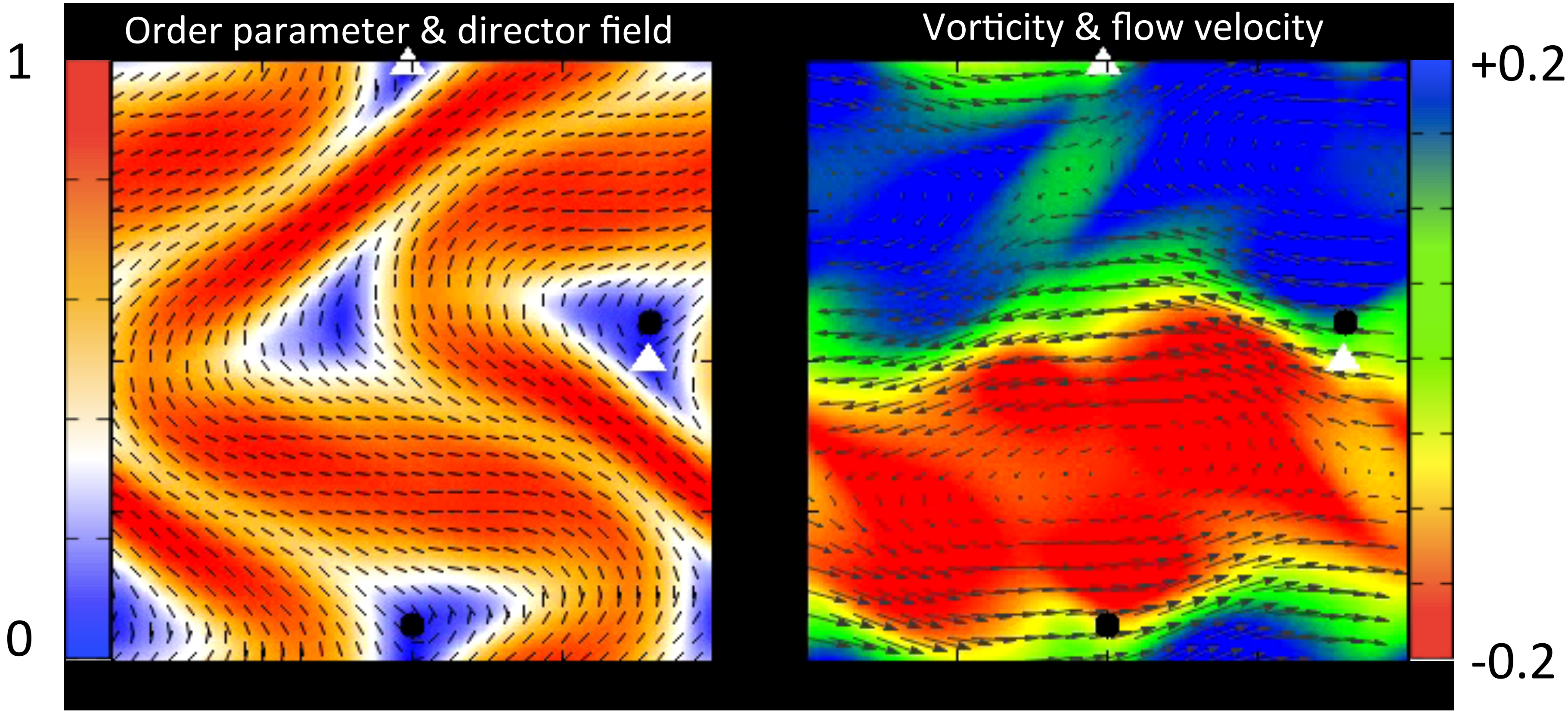


$\alpha < 0$ extensile

$$\partial_x v(y) \sim \frac{2|\alpha|}{\eta}\delta n_y$$

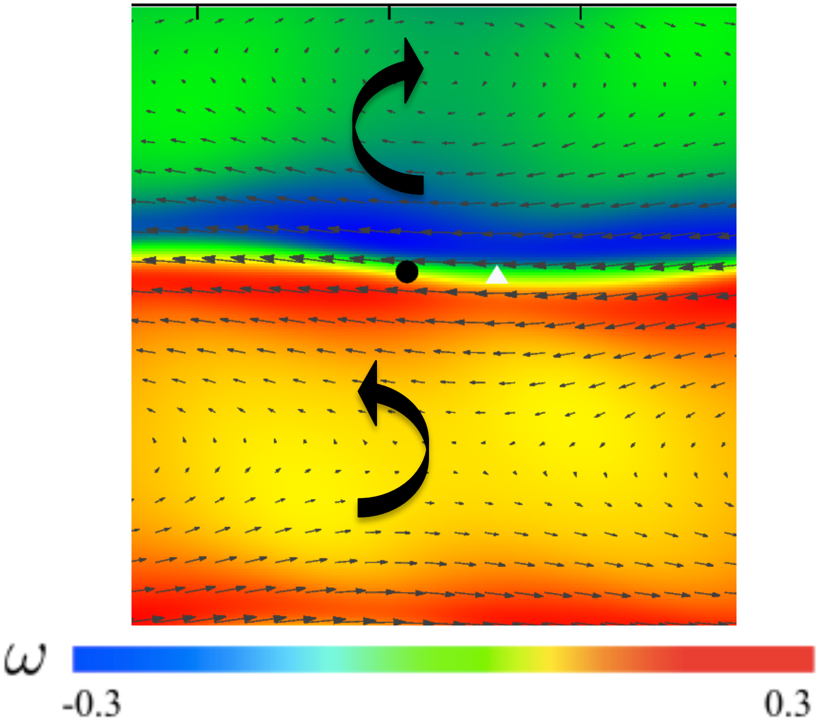
splay/bend fluctuations generate shear flows that enhances deformation, as shown $\rightarrow$ instability

Active nematic hydrodynamics yields self-sustained flow & defect proliferation

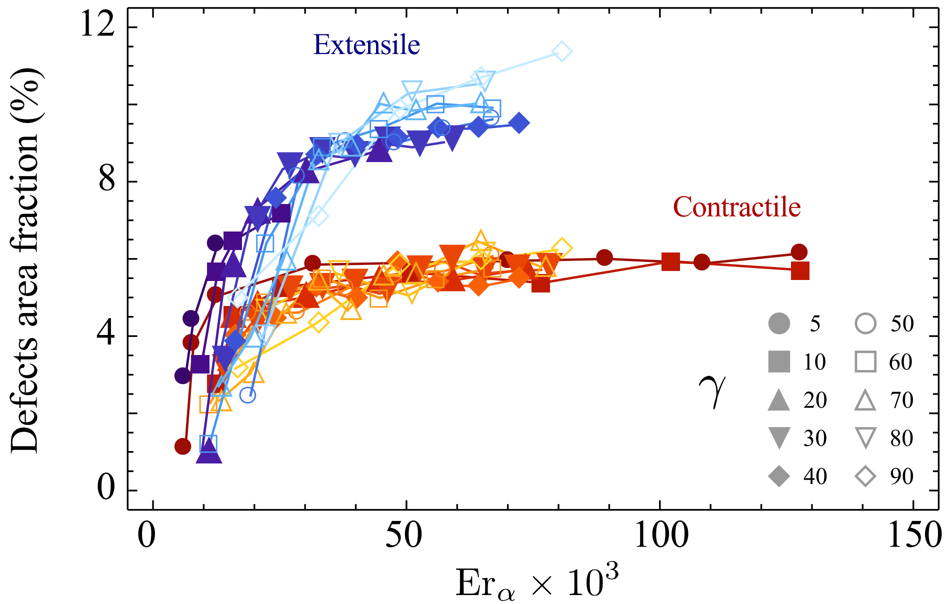


- Giomi, Bowick, Ma & MCM, PRL 110, 228101 (2013); Giomi *et al*, Phil Trans A 2014
- Thampi, Golestanian & Yeomans, PRL 2013; EPL 2014; Phil Trans A 2014
- Gao et al, PRL 2015

Spontaneous Vorticity & Defect Proliferation



defect-antidefect pairs in the order parameter are created at the interface between opposite-sign flow vortices



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* 2015

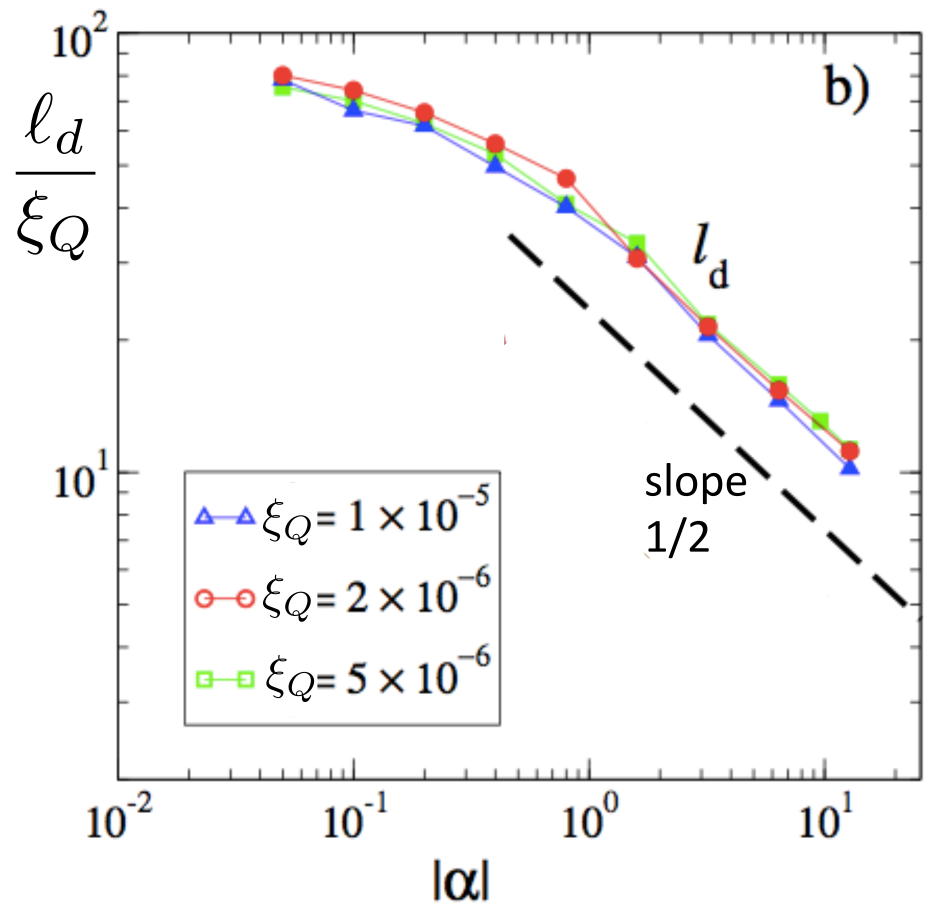
Scaling controlled by length ξ_α of linear instability

E. Hemingway, Mishra, Fielding, MCM

$\xi_a \sim \sqrt{K/|\alpha|}$

$\xi_Q \sim \sqrt{K/C}$ nematic correlation length

ℓ_d defect separation



To look at defect proliferation consider Q-tensor hydrodynamics:

$\boxed{2d}$

incompressible

$$\rho D_t \vec{v} = \eta \nabla^2 \vec{v} - \vec{\nabla} p + \vec{\nabla} \cdot \Sigma$$

$$D_t Q_{ij} = Q_{ik}\omega_{kj} - \omega_{ik} Q_{kj} + \lambda u_{ij} - \lambda Q_{ij} \, Tr[Q \cdot u] + \frac{1}{\gamma} H_{ij}$$

$$\Sigma_{ij} = -\lambda H_{ij} + Q_{ik} H_{kj} - H_{ik} Q_{kj} - \partial_i Q_{ke} \frac{\delta F}{\delta(\partial_j Q_{ke})}$$

$$H_{ij} = -\left(\frac{\delta F}{\delta Q_{ij}} - \frac{1}{d} \delta_{ij} \, Tr\left(\frac{\delta F}{\delta Q_{ij}}\right)\right)$$

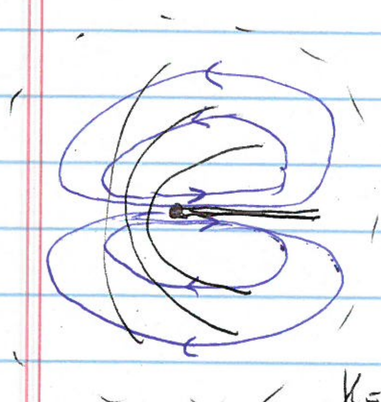
$$F = \int_{\vec{r}} \left\{ \frac{A}{2} (Q_{ij})^2 + \frac{C}{4} (Q_{ij})^4 + \frac{K}{2} (\partial_i Q_{jk})^2 \right\}$$

DEFECTS AS SPP

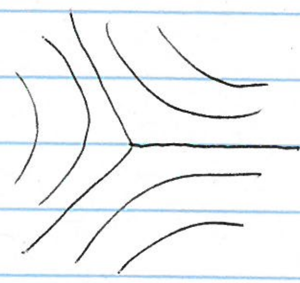
Flow field of defects obtained by solving

$$\begin{cases} \eta \nabla^2 \vec{v} - \vec{\nabla} p + \vec{f} = 0 \\ \vec{\nabla} \cdot \vec{v} = 0 \end{cases} \qquad \vec{f} = \vec{\nabla} \cdot \vec{\sigma}_a$$

$$\vec{f} = \frac{\alpha}{2r} \begin{cases} \hat{x} & k = +1/2 \\ -\cos 2\phi\, \hat{x} + \sin 2\phi\, \hat{y} & k = -1/2 \end{cases}$$



$k = +1/2$

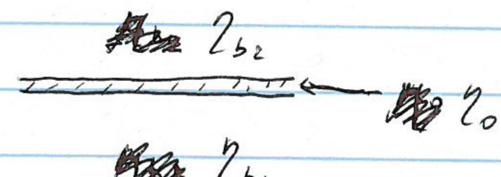


$k = -1/2$

$[\alpha] = [\text{2d pressure}]$

$v_{core} \sim \frac{\alpha}{\eta} R$ $\qquad$ $v_{core} = 0$

But → Suraj's poster



$$v_{core} \sim \frac{\alpha}{2(\eta_{b1} + \eta_{b2})} \ln\left(\xi / \underset{\substack{\uparrow \\ \text{core}}}{a}\right)$$

η_{bi} 3d viscosities

$$\xi \sim \sqrt{\frac{d\, \eta_0}{\eta_b}}$$

2d $[\eta] = m\, t^{-1}$

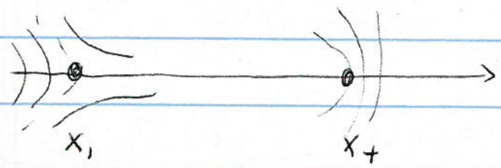
3d $[\eta] = m\, t^{-1}/\ell$

DEFECT DYNAMICS

$\boxed{\text{passive}}$: defects as point particles with frictional dynamics and attractive/repulsive interactions

$$E_{pair} = -2\pi K\, s_1 s_2 \log \frac{|\vec r_1 - \vec r_2|}{a} \qquad a \sim \text{core size}$$

$s_1 = +1/2 \;,\; s_2 = -1/2 \qquad E = \frac{\pi K}{2} \log \frac{|x_+ - x_-|}{a}$



$$\gamma \frac{dx_+}{dt} = -\frac{\partial E}{\partial x_+} = -\frac{\pi K}{2} \frac{1}{x_+ - x_-}$$

$$\gamma \frac{dx_-}{dt} = +\frac{\pi K}{2} \frac{1}{x_+ - x_-}$$

$\Delta = x_+ - x_-$

$$\frac{d\Delta}{dt} = -\frac{2\varkappa}{\Delta} \qquad \varkappa = \frac{\pi K}{2\gamma}$$

Note that $\gamma_{eff} = \gamma_0 \log(\Delta/a)$

$t_a = \Delta^2(0)/2\varkappa$

$\boxed{\text{active}}$

$$\gamma\left(\frac{dx_\pm}{dt} - v(x_\pm)\right) = F$$

$v(x) = v_+(x - x_+) + v_-(x - x_-)$ flow generated by defects

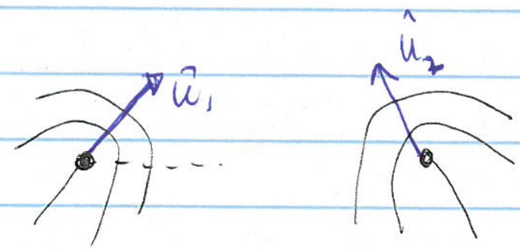
$$\gamma\left(\frac{dx_+}{dt} - v_0\right) = -\frac{\pi K}{2\Delta}$$

$$\gamma\left(\frac{dx_-}{dt}\right) = \frac{\pi K}{2\Delta}$$

$$\frac{d\Delta}{dt} = v_0 - 2\varkappa/\Delta \qquad t_a = -\frac{\Delta(0)}{v_0} - \frac{2\varkappa}{v_0^2} \log\left[1 - \frac{v_0}{2\varkappa}\Delta(0)\right]$$

Interactio + Torque of 2 $+1/2$ defects

$$E = -\frac{\pi K}{2}\left[\log\frac{|\vec{r}_1-\vec{r}_2|}{a} + \frac{1}{2}\ln(1-\hat{u}_1\cdot\hat{u}_2)\right]$$



$$\zeta_r \frac{d\psi_i}{dt} = \frac{\pi K}{2}\sum_j \cot\left(\frac{\psi_i-\psi_j}{2}\right)$$

$\psi_i-\psi_j=\pi$

torque $=0$

$\psi_i-\psi_j=0$

torque $\to\infty$

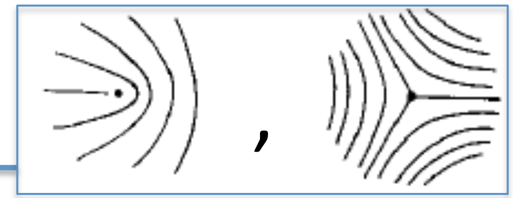
Active Backflow

Giomi, Bowick, Ma & MCM, PRL 2013

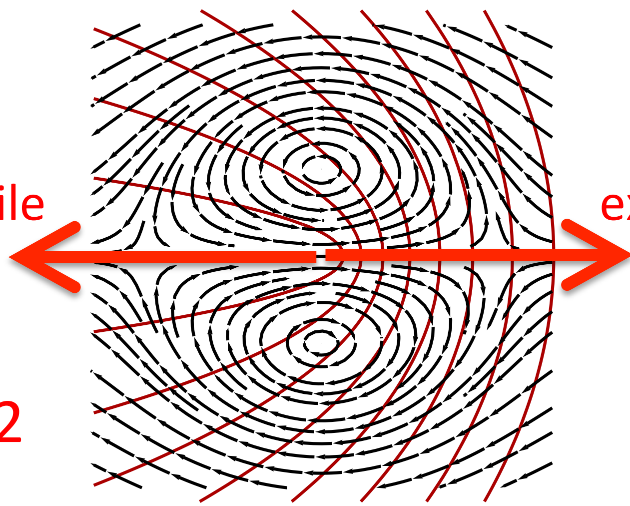
Director distortions from disclinations yield active stresses that act as a source for flows → solve for flow in Stokes limit

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

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

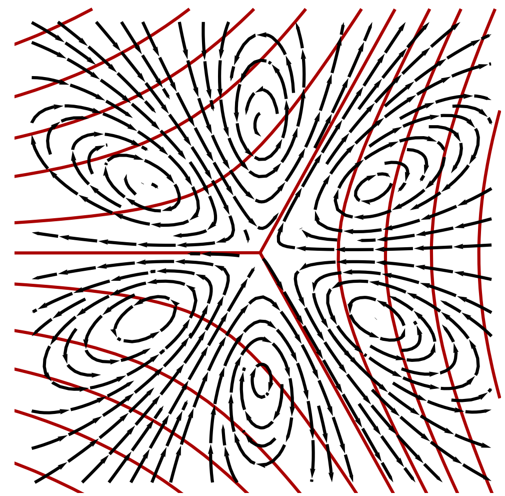


contractile



extensile

+1/2



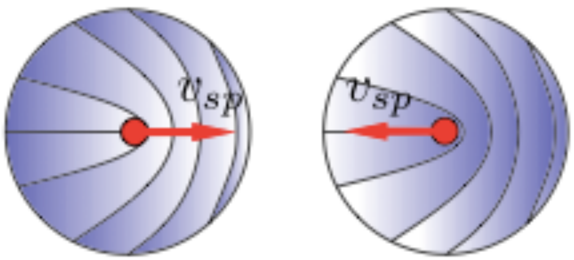
-1/2

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

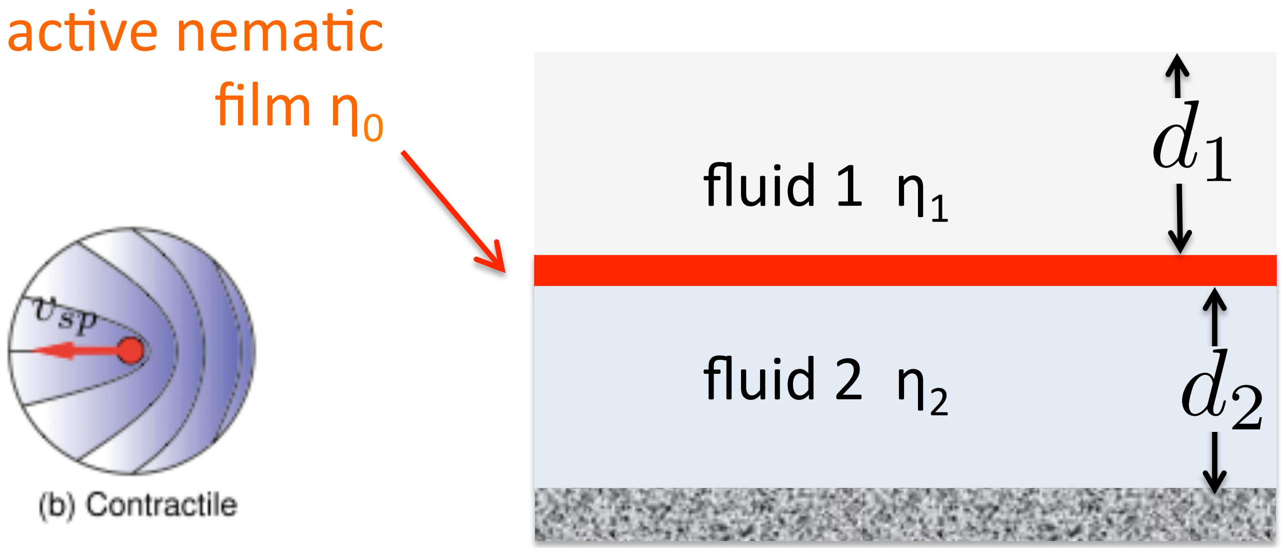
$v_{core} = 0$

Pismen, PRE 2014

Bounding fluids cut-off divergence



(a) Extensile (b) Contractile



$$v_{sp} \sim \frac{\alpha}{2(\eta_1 + \eta_2)} \ln\left(\frac{\xi}{\ell_c}\right)$$

$$\xi = \sqrt{d_2 \eta_R / \eta_2}$$

ℓ_c defect core

$$\eta_R = \eta_0 + \eta_1 d_1 + \eta_2 d_2$$

Active Defects as ``Self-Propelled'' Particles

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

$$x = x_+ - x_-$$

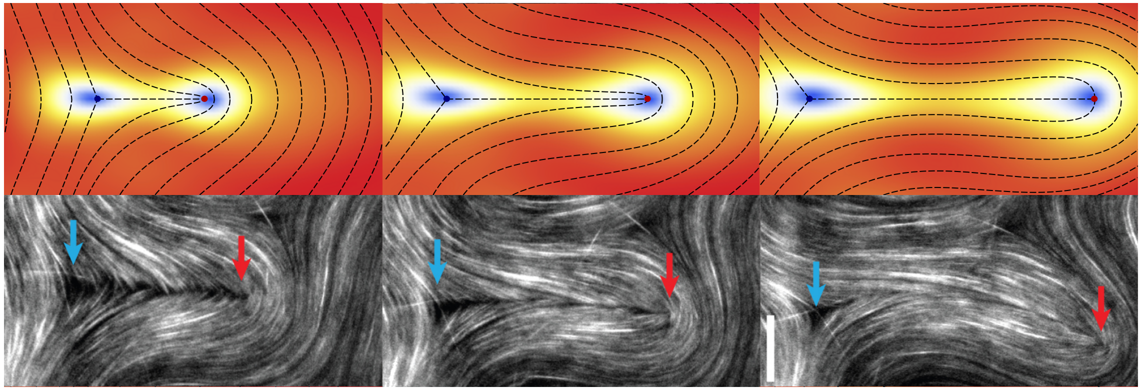
$$\zeta \dot{x} = -\nabla \left[K \ln(x/a) \right]$$

In the presence of active backflow defects ride with the flow

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

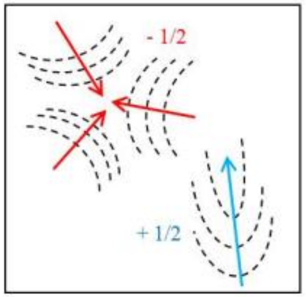
$$v_b(x) \simeq -(\alpha/\eta) R \delta(x - x_+)$$

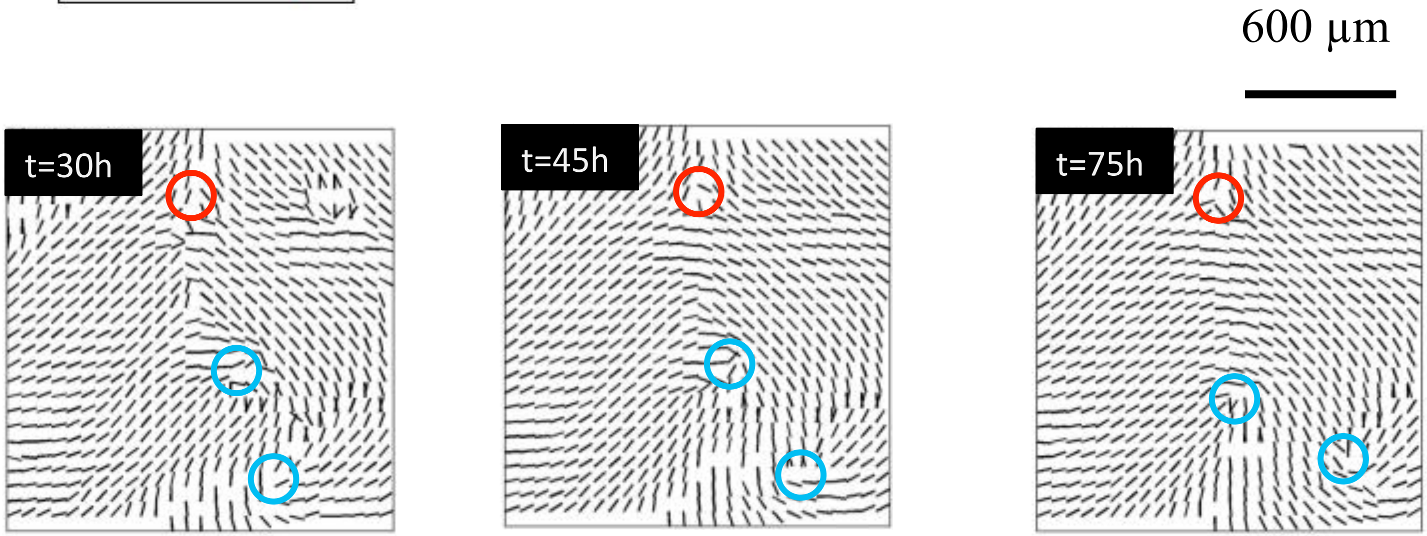
Extensile active nematic



Contractile system: fibroblasts monolayer

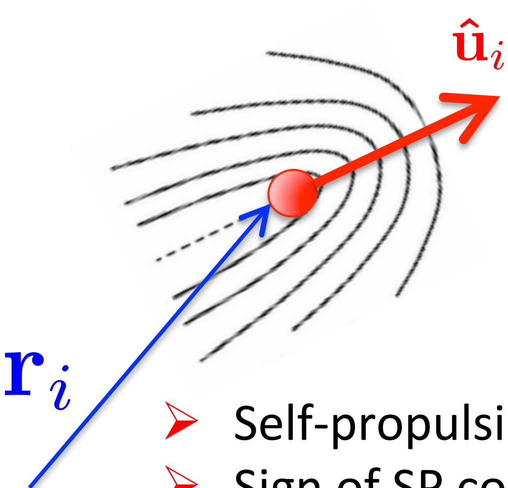
G. Duclos, … Silberzan, Soft Matter 2013





+1/2 defects as SP particles

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



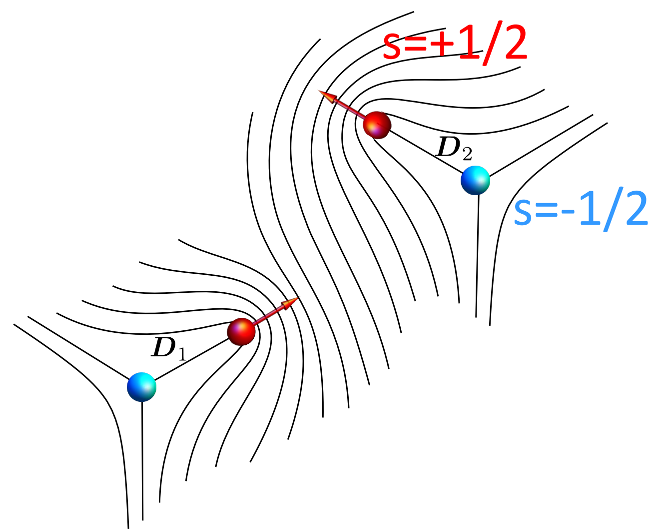
$$\frac{d\mathbf{r}_i}{dt} = v_0 \hat{\mathbf{u}}_i - \frac{1}{\zeta_t} \nabla_i E$$

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

- Self-propulsion proportional to activity
- Sign of SP controlled by extensile/contractile nature of active forces
- Forces and torques obtained from equilibrium interactions:

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

Torque obtained from interaction energy of two ±1/2 dipoles in the limit $D_1, D_2 \rightarrow \infty$

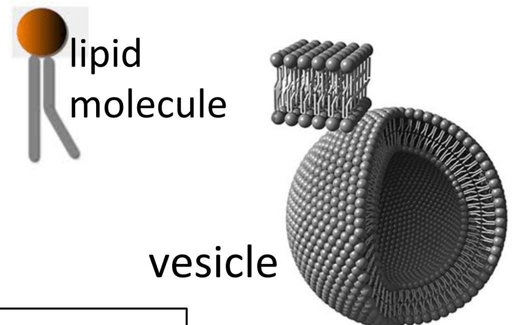


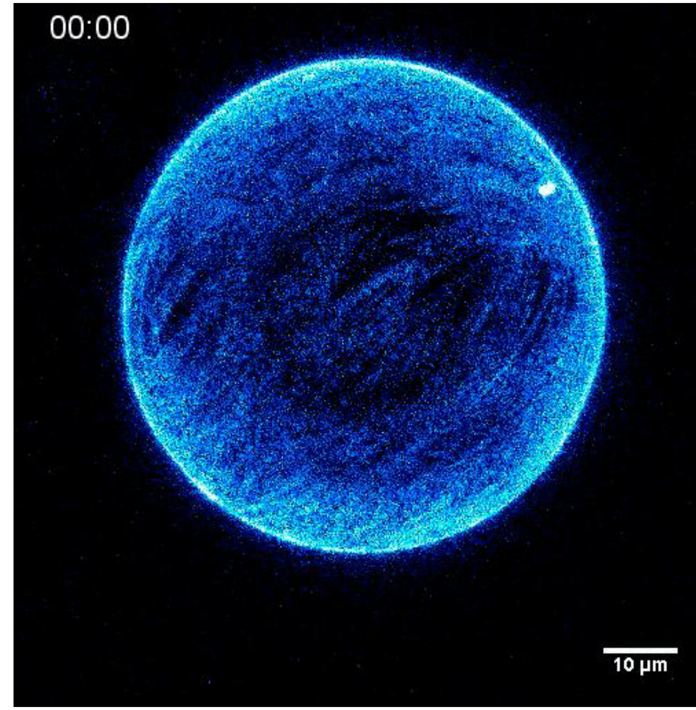
- Topological defects as fingerprints of symmetry (nematic vs polar)

- Direction of motion of +1/2 defect reveals extensile/ contractile nature of active stresses

Keber … MCM et al, Science 2014

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

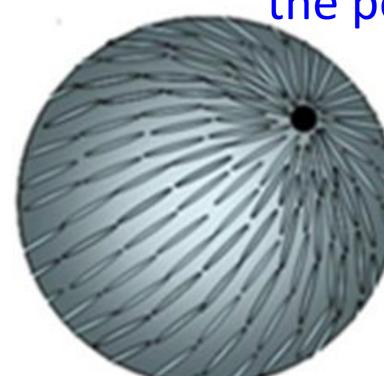




Nematic order on a sphere requires a +2 topological charge

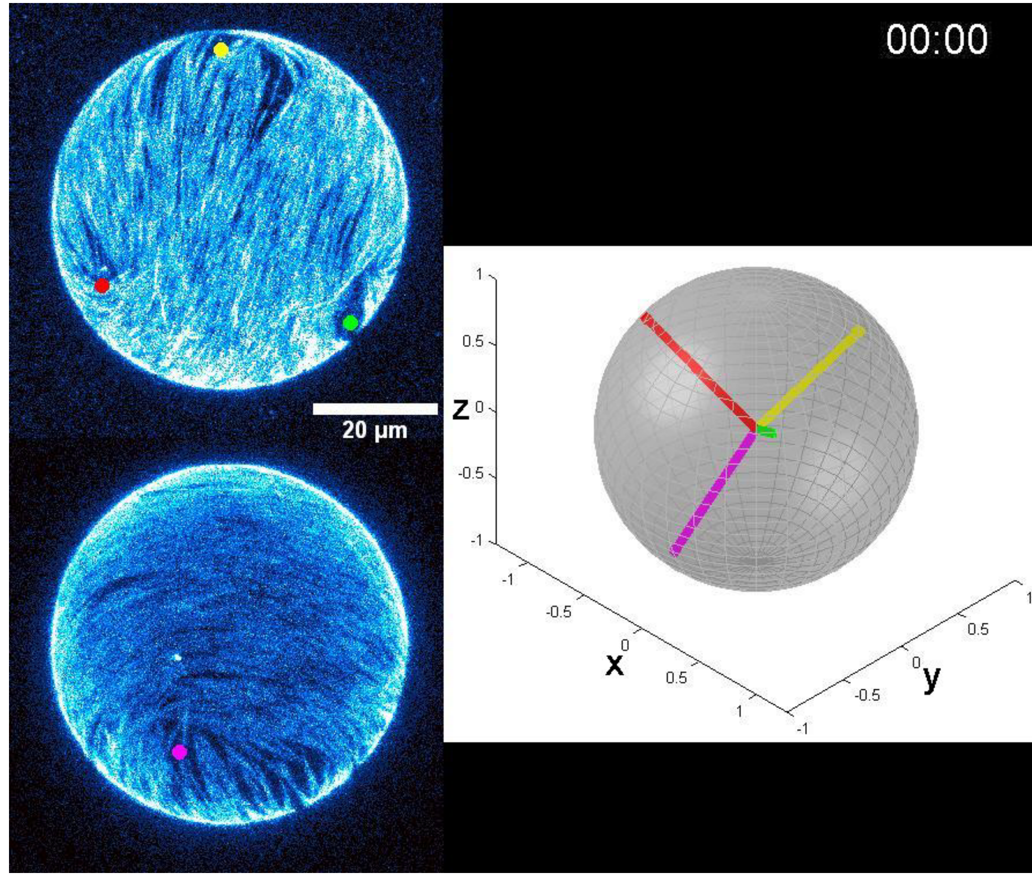
Four +1/2 defects at the corners of a tetrahedron

Two +1 defects at the poles

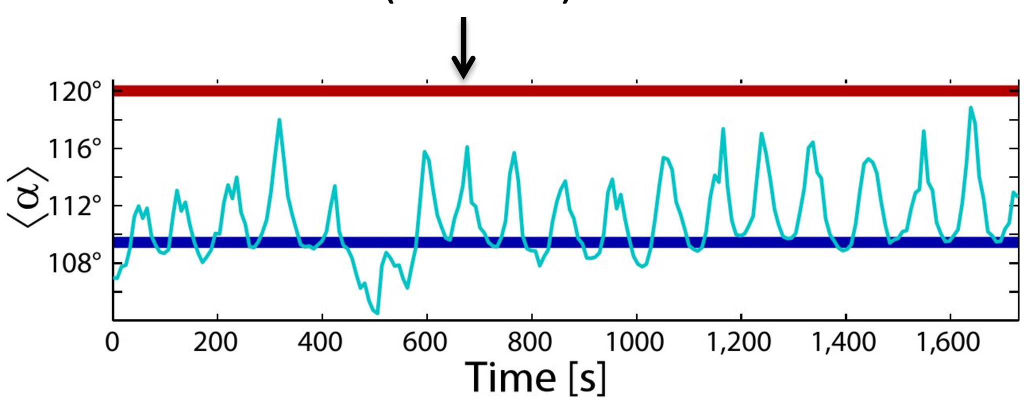


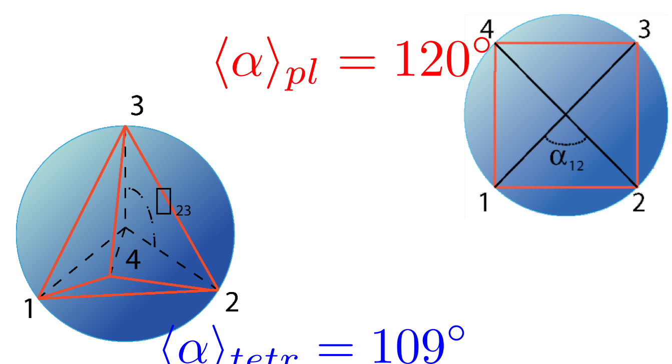
In active nematic defects oscillate between tetrahedral and planar configurations

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



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



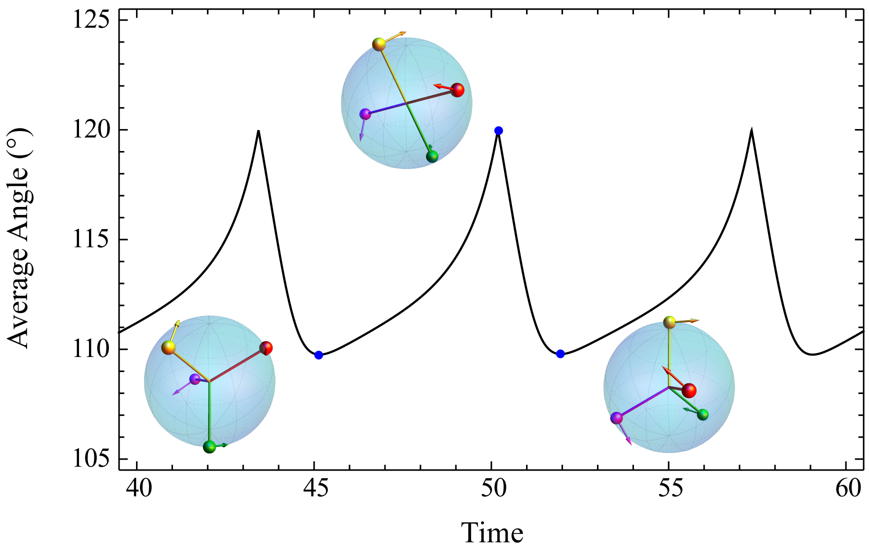


Oscillations for $\zeta_t R^2 > \zeta_r$

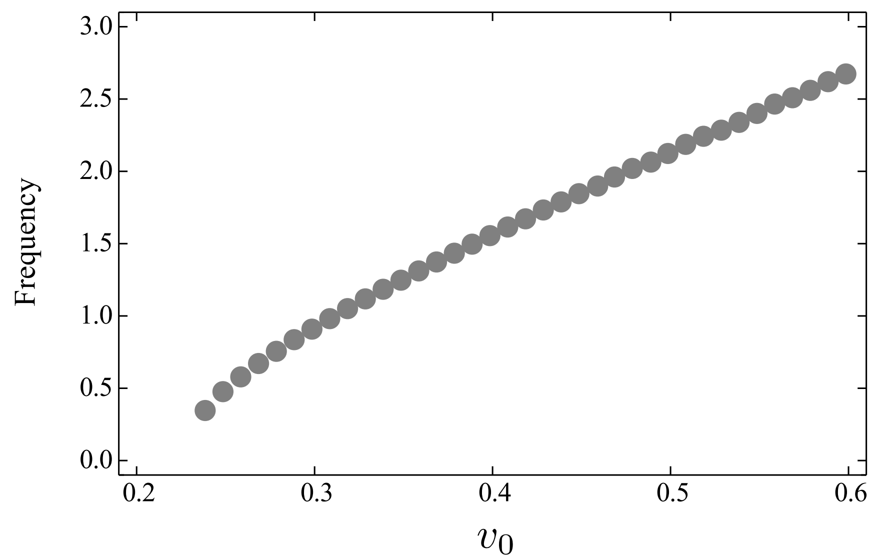
$$\langle \alpha \rangle = \frac{1}{6} \sum_{i<j} \arccos\left(\frac{\mathbf{r}_i \cdot \mathbf{r}_j}{R^2}\right)$$

Defect core translation lags reorientation

(*a*)

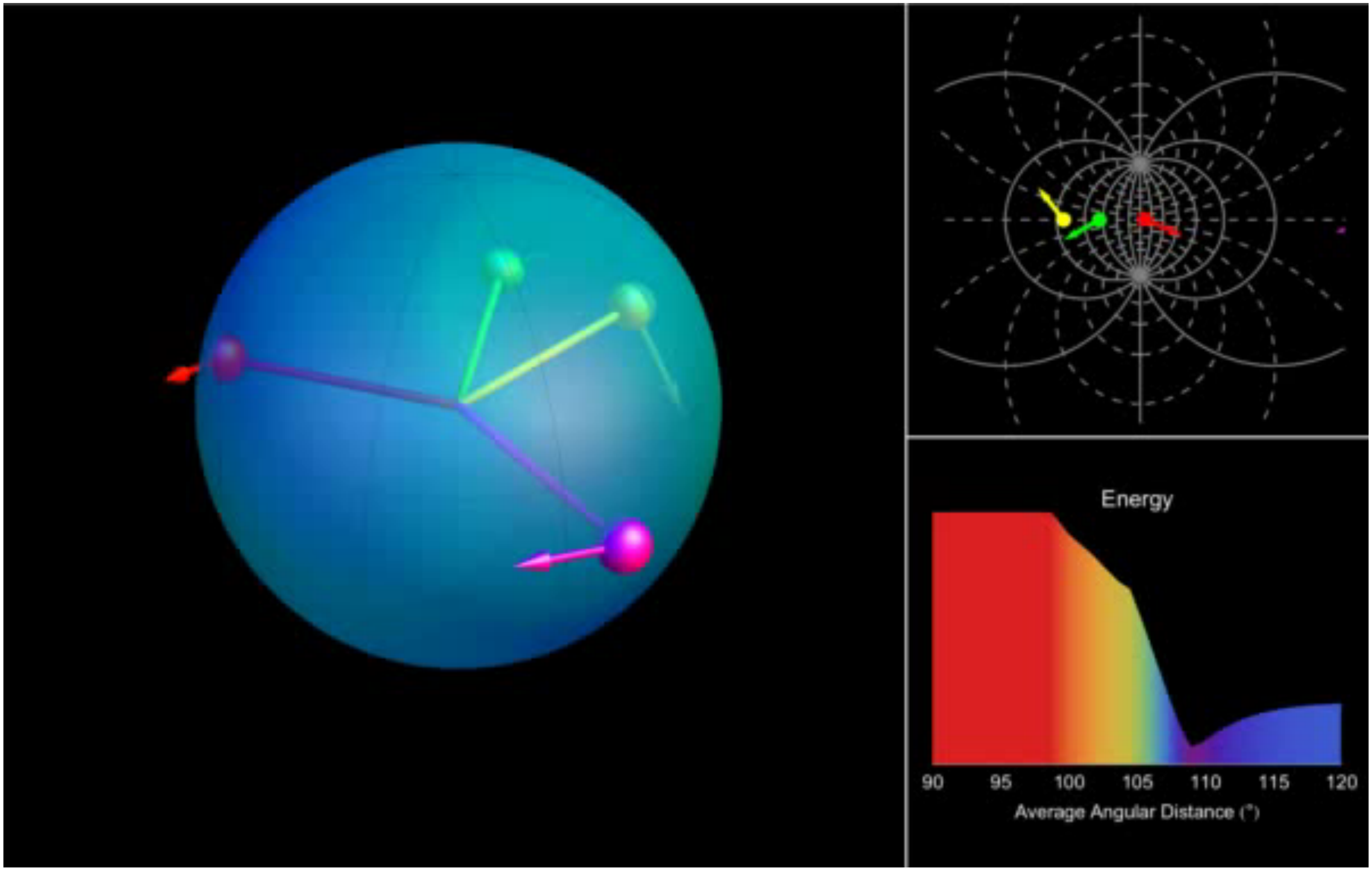


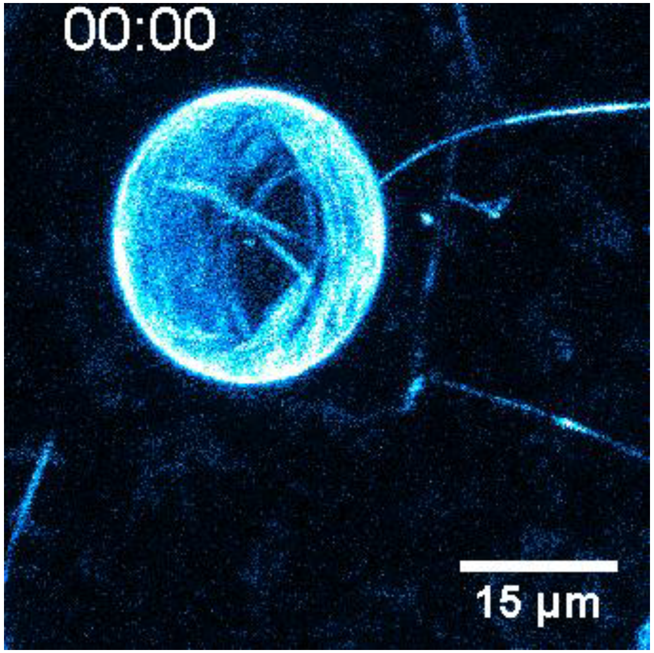
(*b*)



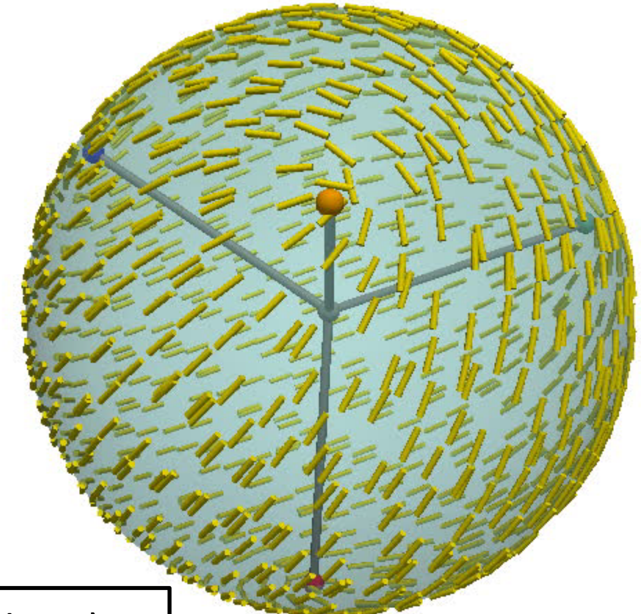
$$v_0 \sim \frac{\text{activity}}{\text{viscosity}} R$$

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


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



Smaller vesicles



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