Topology and Elasticity of Three Dimensional Nematics. Application to Biomechanics

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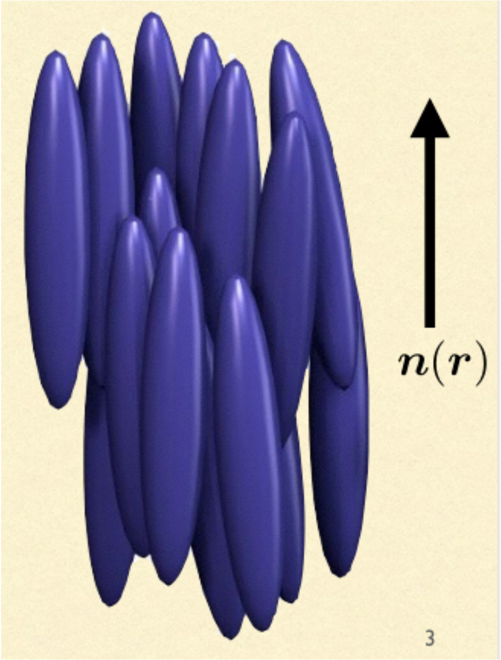
Nematic Order (Liquid Crystal)

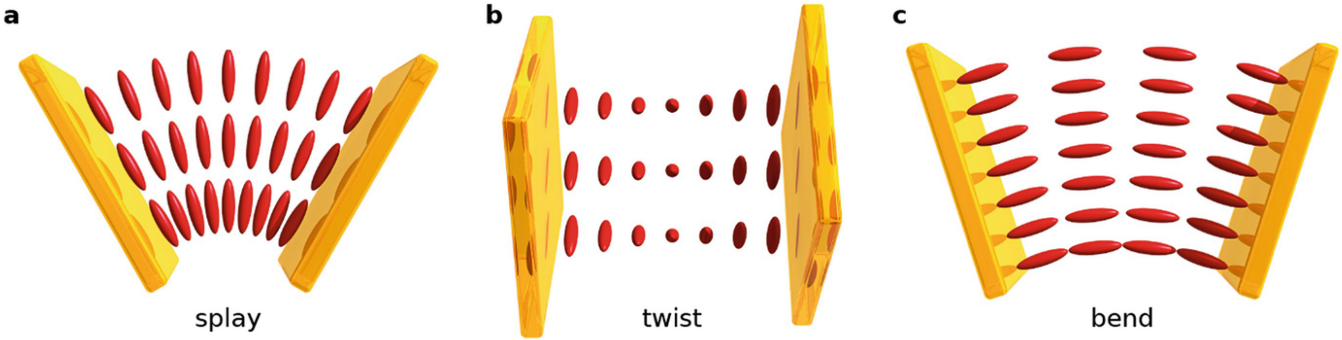


Nematic director

No positional order - it flows like a liquid

Orientational order - generalized elasticity

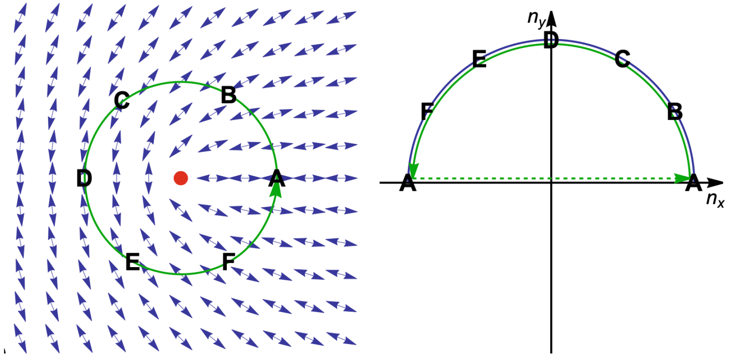
Elastic energy of deformation – three modes:



$$\mathcal{F}_d = \frac{1}{2}K_1(\nabla \cdot \hat{\mathbf{n}})^2 + \frac{1}{2}K_2(\hat{\mathbf{n}} \cdot \nabla \times \hat{\mathbf{n}})^2 + \frac{1}{2}K_3(\hat{\mathbf{n}} \times \nabla \times \hat{\mathbf{n}})^2.$$

Topological Invariants

Two dimensions



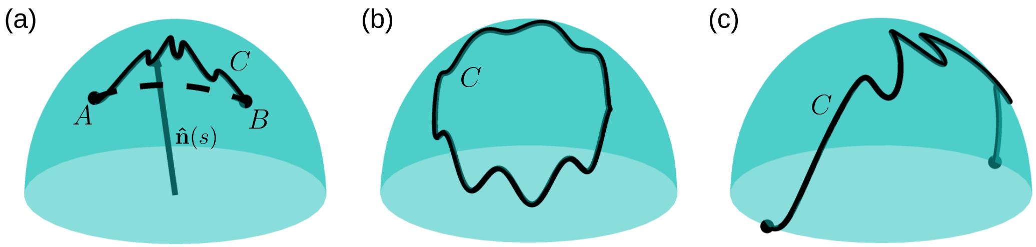
$$\oint d\theta = \oint \frac{d\theta}{ds} ds = 2\pi m$$

Classes defined by m

$\nabla \times \nabla\theta = 2\pi m \delta(\boldsymbol{x})$

Is a topological defect density

Three dimensions



$\int_C |\hat{\mathbf{n}} \times d\hat{\mathbf{n}}| = C$ arclength

$\int_C \hat{\Xi} \cdot (\hat{\mathbf{n}} \times d\hat{\mathbf{n}}) = AB$ distance

$\int_C \hat{\Xi} \cdot (\hat{\mathbf{n}} \times d\hat{\mathbf{n}}) = 0$

$\int_C \hat{\Xi} \cdot (\hat{\mathbf{n}} \times d\hat{\mathbf{n}}) = \pi$

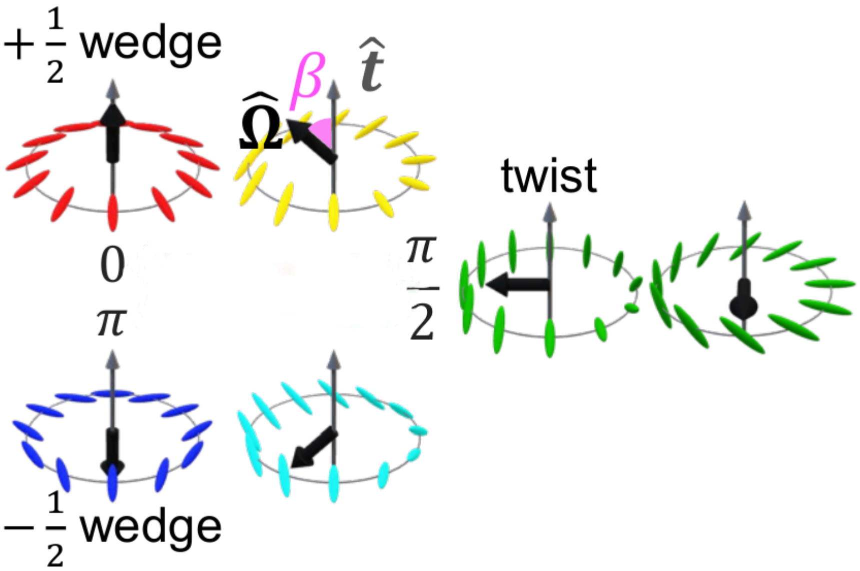
$$\oint \frac{\hat{\mathbf{n}}(0) \cdot d\hat{\mathbf{n}}}{|\hat{\mathbf{n}}(0) \times \hat{\mathbf{n}}|} = (0, \frac{1}{2}) \mod 2\pi$$

Only two classes: no defect and 1/2

Topological density may not exist

A density is useful for particle to field transformations, and introducing regularized approximations with the appropriate far field behavior

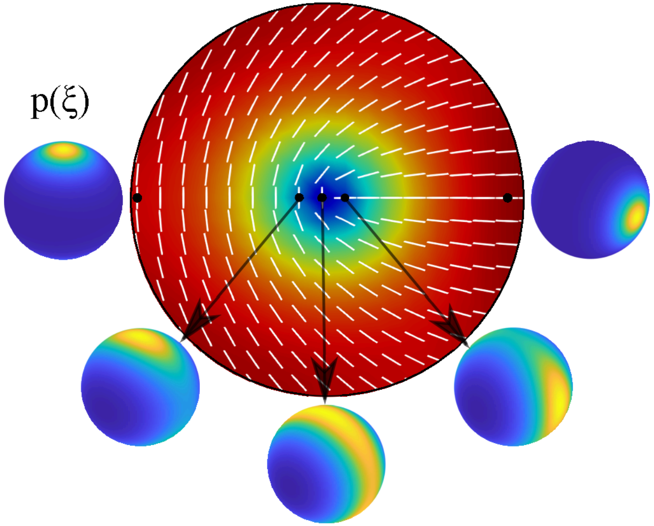
Disclination Geometry



Topology is simple: only one class: a 1/2 disclination

Geometry is complex: two unit vectors to characterize the line: the local tangent $\hat{\boldsymbol{t}}$ and the rotation vector $\hat{\boldsymbol{\Omega}}$.

Tensor Order Parameter



$$Q = \int_{\mathcal{S}^2} \left(\boldsymbol{\xi} \otimes \boldsymbol{\xi} - \frac{1}{3}\mathbf{I} \right) p(\boldsymbol{\xi}) d\Sigma(\boldsymbol{\xi})$$

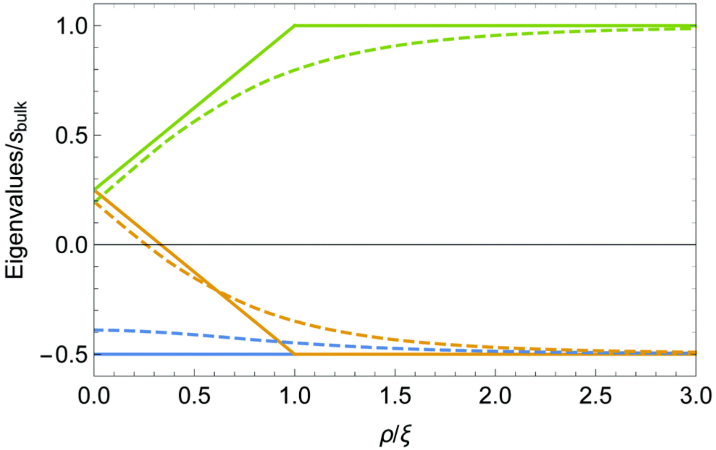
Macroscopically,

$$Q = S \left(\hat{\boldsymbol{n}} \otimes \hat{\boldsymbol{n}} - \frac{1}{3}\mathbf{I} \right) + P \left(\hat{\boldsymbol{m}} \otimes \hat{\boldsymbol{m}} - \hat{\boldsymbol{l}} \otimes \hat{\boldsymbol{l}} \right)$$

S is the uniaxial order parameter, $\hat{\boldsymbol{n}}$ the director, and P the biaxial order parameter.

The distribution is uniaxial far from the defect, becomes biaxial as the defect is approached, and then uniaxial at the core $S = P$.

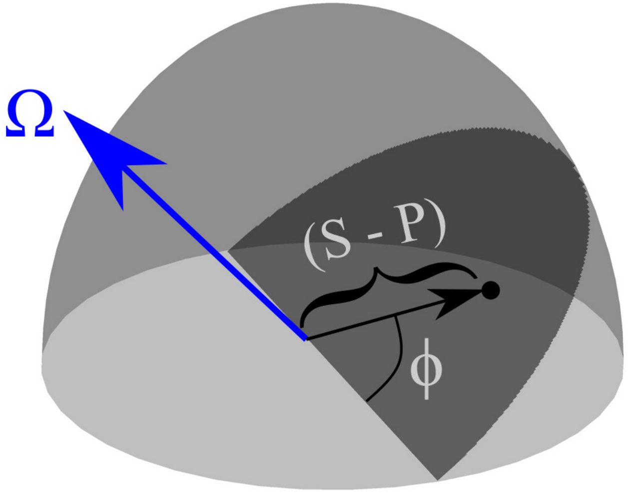
There is no singularity in this representation, just an eigenvalue crossing



C. Long, X. Tang, R. Selinger, J. Selinger, Soft Matter 17, 2265 (2021)]

Disclination Density Tensor

No topological density known, but $\boldsymbol{Q}$ is a properly regularized field.
A density can be defined: near the line $S = P$, a two dimensional description is $\boldsymbol{Q}_\perp = (\delta S = S - P, \phi)$



$$\boldsymbol{\rho}(\mathbf{r}) = \frac{1}{2}\int_C \frac{d\mathbf{R}}{ds}\delta(\mathbf{r} - \mathbf{R}(s))ds = \frac{1}{2}\hat{\mathbf{t}}\;\delta(\boldsymbol{\zeta}_\perp) = \nabla \times \left(\frac{1}{2}\delta S^2 \nabla \phi\right)\delta(\boldsymbol{Q}_\perp)$$

$$\boldsymbol{\rho}(\mathbf{r}) = \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{D}(\mathbf{r})\delta(\boldsymbol{Q}_\perp) \quad D_{\gamma i} = \epsilon_{\gamma\mu\nu}\epsilon_{ikl}\partial_k Q_{\mu\alpha}\partial_l Q_{\nu\alpha}$$

Define a disclination density tensor

$$\boldsymbol{D}(\mathbf{r}) = \omega(\mathbf{r})\left(\hat{\boldsymbol{\Omega}} \otimes \hat{\boldsymbol{t}}\right) \quad \omega(0) = S_N^2/\xi^2$$

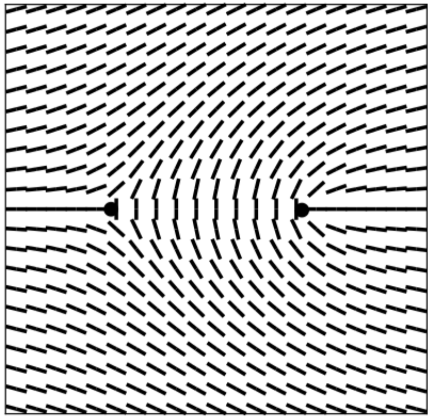
Kinematics:

$$\partial_t \rho_i = \partial_k\left(v_i\rho_k - v_k\rho_i\right), \quad \mathbf{v}(s) = \frac{d\mathbf{R}(s)}{dt}$$

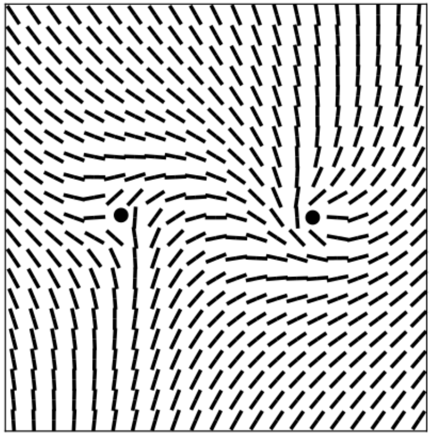
$$\mathbf{v}(s) = 2\left.\frac{\hat{\boldsymbol{t}} \times (\hat{\boldsymbol{\Omega}} \cdot \mathbf{g})}{\omega(\mathbf{r})}\right|_{\mathbf{r}=\mathbf{R}(s)} \qquad g_{\gamma k} = \epsilon_{\gamma\mu\nu}\partial_t Q_{\mu\alpha}\partial_k Q_{\nu\alpha}$$

Topology controlled motion

Optimal Orientation



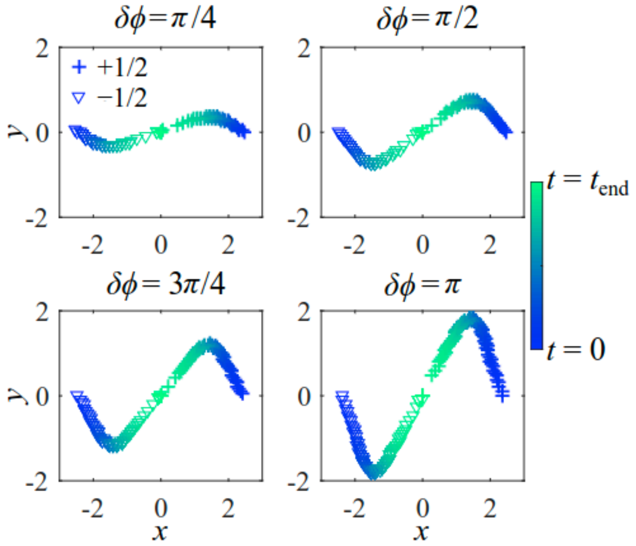
Twisted Orientation



Interaction energy [Tang and Selinger (2017)]

$$E = \frac{\pi K}{2} \ln \frac{R}{a} + \frac{K \delta\phi^2}{2} \frac{\ln(R/2a)}{\ln(R/a)^2}$$

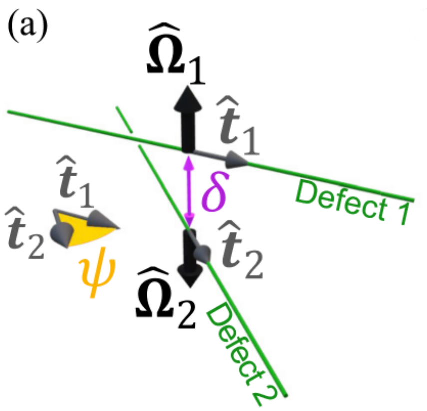
Force and torque acting on the defects. Force is directed along the line joining the centers



Topology requires transverse motion

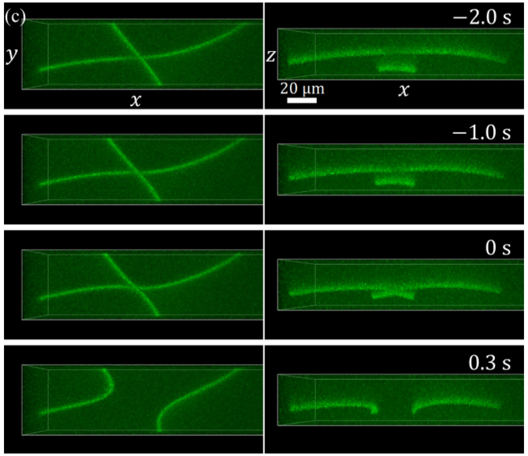
$$\mathbf{v}_+ = -2 \left[\frac{\hat{\mathbf{R}}_{12}}{R} - \frac{\delta\phi}{R \ln(R/a)} \left(\hat{\mathbf{z}} \times \hat{\mathbf{R}}_{12} \right) \right]$$

Disclination recombination



$$\mathbf{v}_1 = 2\left(\hat{\boldsymbol{\Omega}}_1 \cdot \hat{\boldsymbol{\Omega}}_2\right)\left(\hat{\boldsymbol{t}}_1 \cdot \hat{\boldsymbol{t}}_2\right)\frac{\hat{\boldsymbol{R}}_{12}}{R}$$

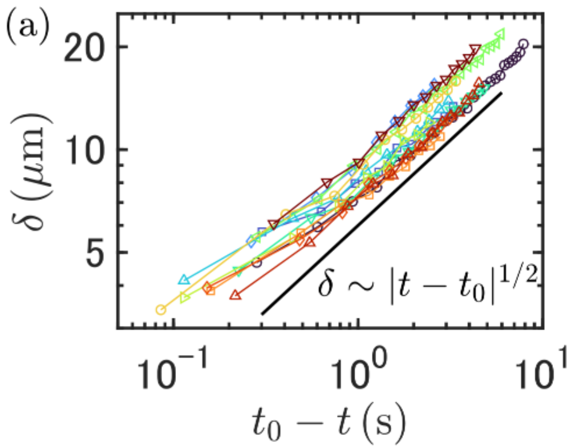
assuming the director found the core in one rotates according to the to the rotation vector of the other. At the closest point

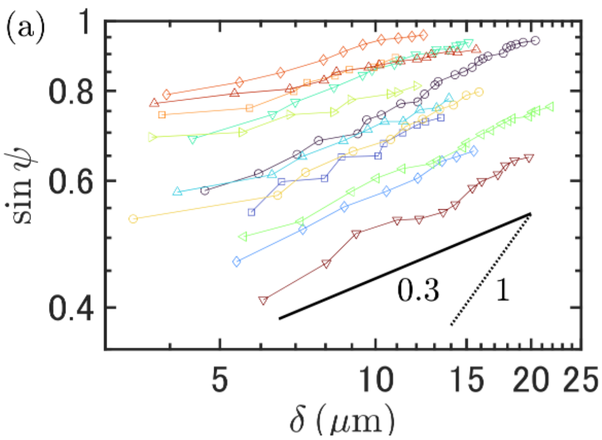


[Zushi, Schimming, Takeuchi, PRR 6, 023284 (2024)]

$$\frac{d\delta}{dt} = \frac{4\left(\hat{\boldsymbol{\Omega}}_1 \cdot \hat{\boldsymbol{\Omega}}_2\right)\cos\psi}{\delta} \approx -\mu_1\frac{\cos\psi}{\delta} \qquad \frac{d\psi}{dt} = \frac{4\left(\hat{\boldsymbol{\Omega}}_1 \cdot \hat{\boldsymbol{\Omega}}_2\right)\sin\psi}{\delta^2} \approx -\mu_2\frac{\sin\psi}{\delta^2}$$

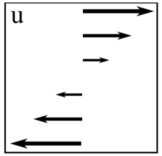
Over 12 observed recombination events ($\sin\psi \sim \delta^{\mu_2/\mu_1}$)

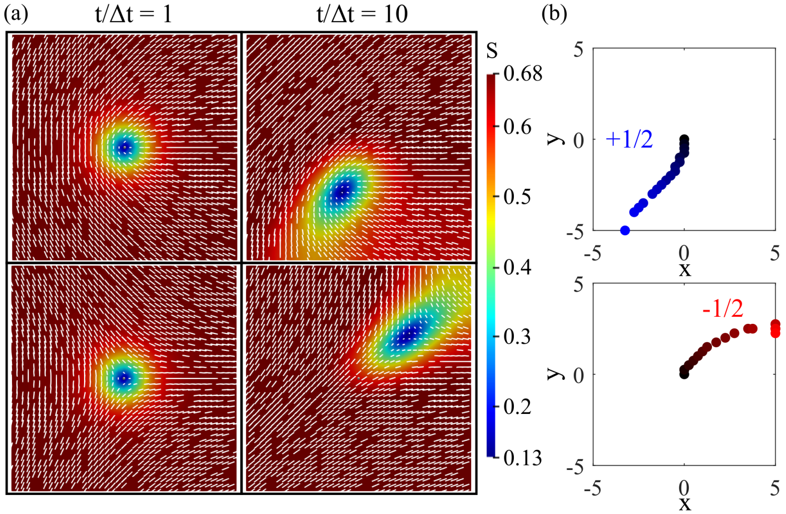




Disclination sorting by flow

Consider an imposed shear flow $\boldsymbol{u}(x,y) = \gamma y \hat{\boldsymbol{x}}$





The velocity of the line is

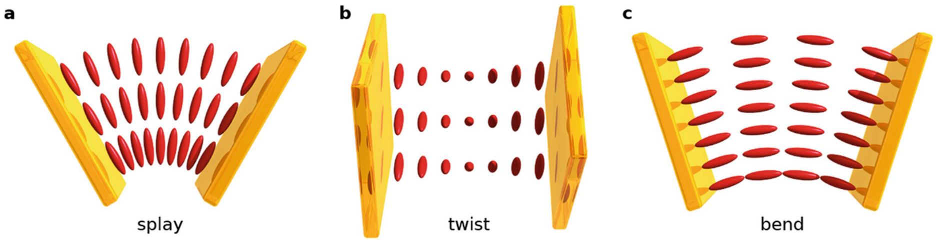
$$\mathbf{v} = 2\left.\frac{\hat{\mathbf{t}} \times (\hat{\boldsymbol{\Omega}} \cdot \mathbf{g})}{\omega}\right|_{\mathbf{r}=\mathbf{R}}, \qquad g_{\gamma k} = \epsilon_{\gamma\mu\nu}\partial_t Q_{\mu\alpha}\partial_k Q_{\nu\alpha}$$

- Choose $\hat{\boldsymbol{\Omega}} = \pm\hat{z}$.
- In the Beris-Edwards model for $\partial_t \boldsymbol{Q}$, the only nonzero term in $\hat{\boldsymbol{\Omega}} \cdot \boldsymbol{g} = (2/3)\lambda \boldsymbol{E}$, where λ is the flow aligning parameter, and $\boldsymbol{E} = (\gamma/2)\left(\hat{\boldsymbol{y}} \otimes \hat{\boldsymbol{x}} + \hat{\boldsymbol{x}} \otimes \hat{\boldsymbol{y}}\right)$ the velocity strain rate.

$$\mathbf{v} = 2\gamma y \hat{\mathbf{x}} - 2m\frac{4\lambda\gamma a}{3S_N}\hat{\mathbf{y}}, \qquad m = \pm\frac{1}{2}$$

This is a kinematic effect:
- As the director rotates to the local value of the Leslie angle ($\approx 45^o$ in the figure), maintaining topological continuity leads to transverse defect motion.
- Direction of rotation set by the sign of the shear and charge of defect. Defect sorting.

Anisotropic Elasticity



$$\mathcal{F}_d = \frac{1}{2}K_1(\nabla\cdot\hat{\mathbf{n}})^2 + \frac{1}{2}K_2(\hat{\mathbf{n}}\cdot\nabla\times\hat{\mathbf{n}})^2 + \frac{1}{2}K_3(\hat{\mathbf{n}}\times\nabla\times\hat{\mathbf{n}})^2.$$

Thermotropics: $K_1 \approx K_2 \approx K_3 = K$, isotropic

Lyotropics $K_1 \neq K_3,\ K_2 \ll K_1, K_3$

In d = 2 $\hat{\boldsymbol{n}} = (\cos\theta, \sin\theta)$ $\mathscr{F}_d = \frac{K}{2}(\nabla\theta)^2$

Linear in the one constant approximation

Defect field superposition

In d = 3 with the constraint $|\hat{\boldsymbol{n}}| = 1$ the equations are nonlinear, even in one constant approximation

Tensor order parameter

Isotropic (one constant) $\mathscr{F}_d = \frac{L}{2}(\nabla \boldsymbol{Q})^2$ $K = (9/2)LS^2$

Anisotropy (to lowest order) $\mathscr{F}_d = L_1(\partial_k Q_{ij})^2 + L_2(\partial_j Q_{ij})^2 + L_3 Q_{lk}(\partial_l Q_{ij})(\partial_k Q_{ij})$

$$K_1 = 4L_1S^2 + 2L_2S^2 - \frac{4}{3}L_3S^3$$

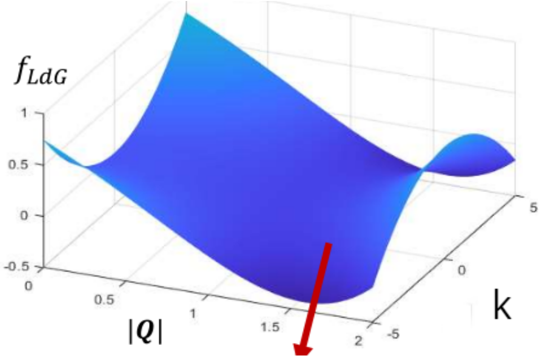
$$K_2 = 4L_1S^2 - \frac{4}{3}L_3S^3$$

$$L_3 = \frac{K_3 - K_1}{4S^3}$$

$$K_3 = 4L_1S^2 + 2L_2S^2 + \frac{8}{3}L_3S^3$$

Landau - de Gennes energy with cubic elastic nonlinearity $L_3 \neq 0$ is not bounded below

[Ball and Majumdar, Mol. Liq. Cryst. 525, 1 (2010)
Bauman and Philips, Calc. Var. 55, 81 (2016)]



Physically, since $Q = \int_{\mathcal{S}^2} \left(\xi \otimes \xi - \frac{1}{3}\mathbf{I} \right) p(\xi) d\Sigma(\xi)$

Its eigenvalues need to satisfy $-1/3 \leq \lambda_i \leq 2/3$

The Landau - de Gennes energy does not constrain the eigenvalues to this physically admissible range

Explicitly constrain Q (and use excluded volume energy of the Maier-Saupe form)

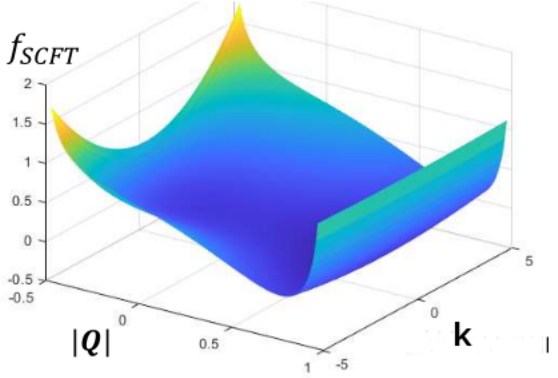
$$\mathcal{F}[Q, \Lambda] = -\kappa Q^2 + nk_B T \int_{\mathcal{S}^2} p(\xi) \ln(4\pi p) d\Sigma + \Lambda : \int_{\mathcal{S}^2} \left[Q - \left(\xi \otimes \xi - \frac{1}{3}\mathbf{I} \right) \right] p(\xi)) d\Sigma + \mathcal{F}_d(Q, \nabla Q)$$

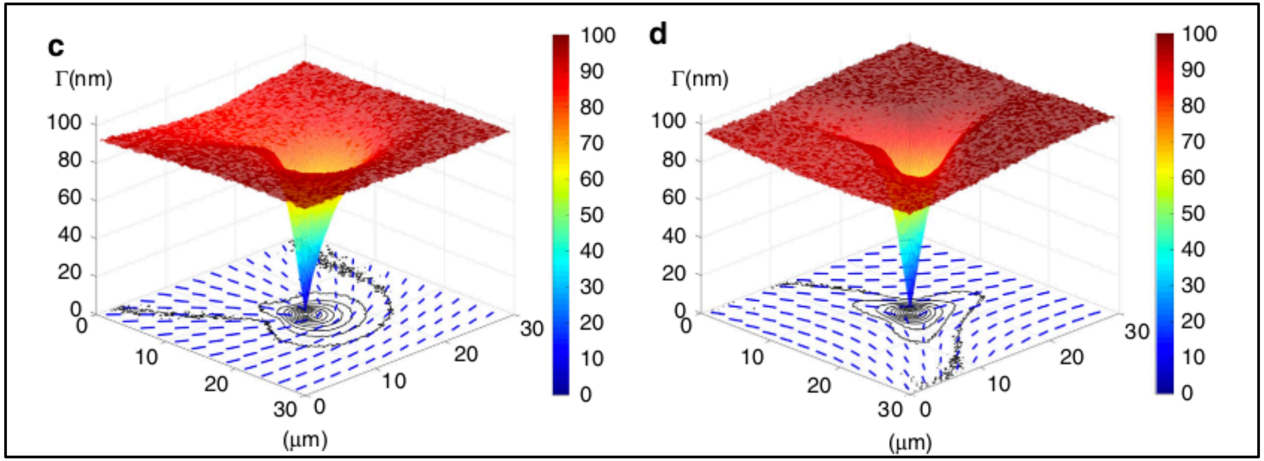
$$p(\xi) = \frac{1}{Z(\Lambda)} e^{\xi \Lambda \xi}, \quad Z = \int_{\mathcal{S}^2} e^{\xi \Lambda \xi} d\Sigma$$

Numerically

$$Q = \frac{\partial \ln Z}{\partial \Lambda} - \frac{1}{3}\mathbf{I}$$

Mean field, self consistency.
Unique solution. Numerically

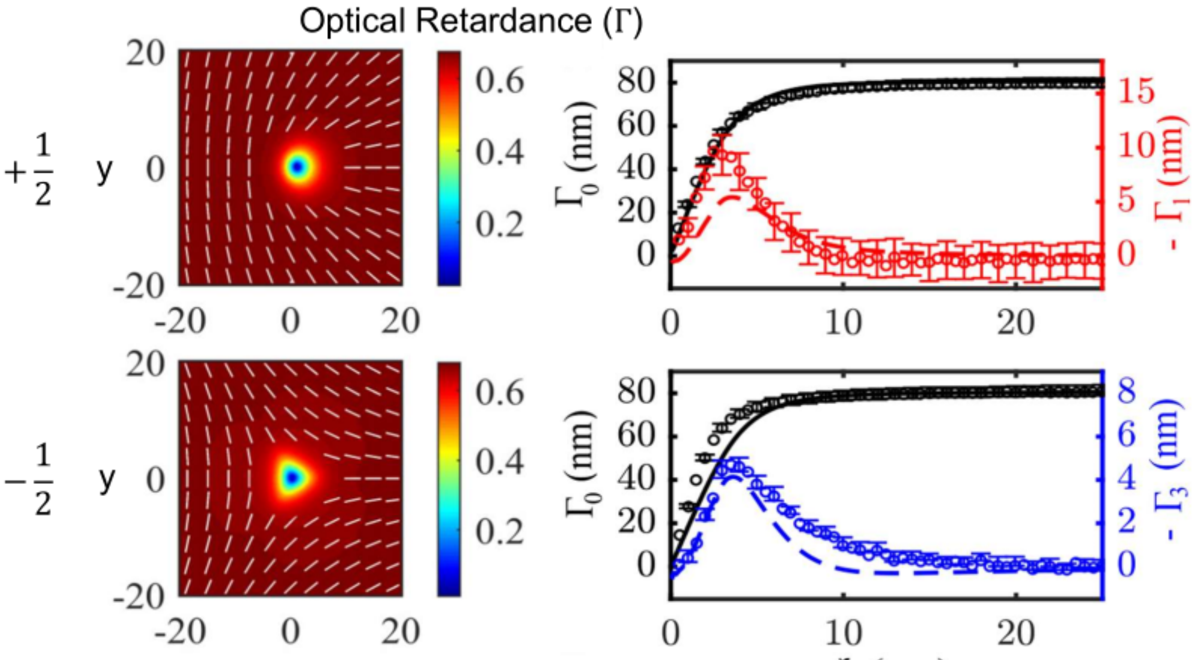




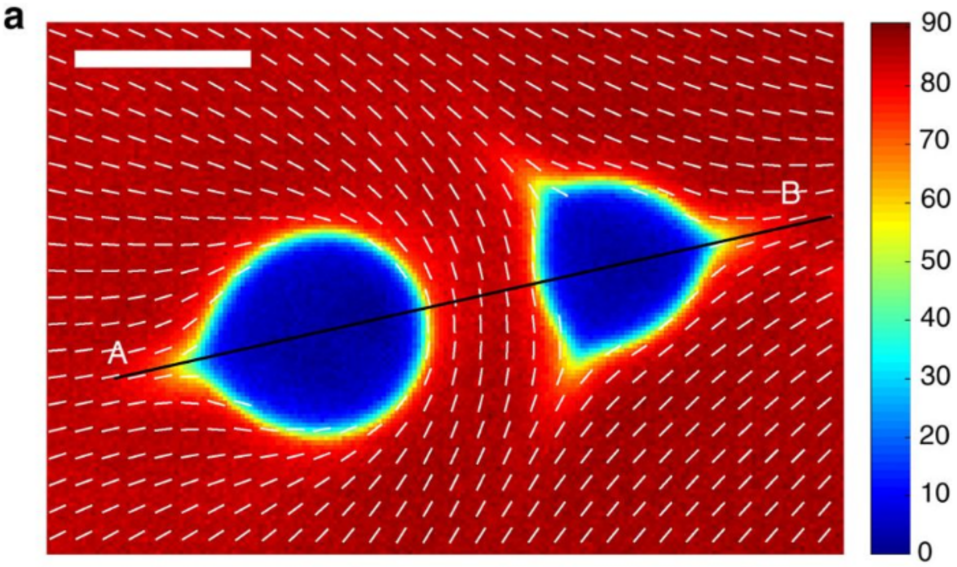
Optical retardance $\Gamma \propto S - P$ in a lyotropic chromonic liquid crystal

[Zhou, Shiyanovskii, Park, and Lavrentovich. Nat. Comm. 8, 14974 (2017)]

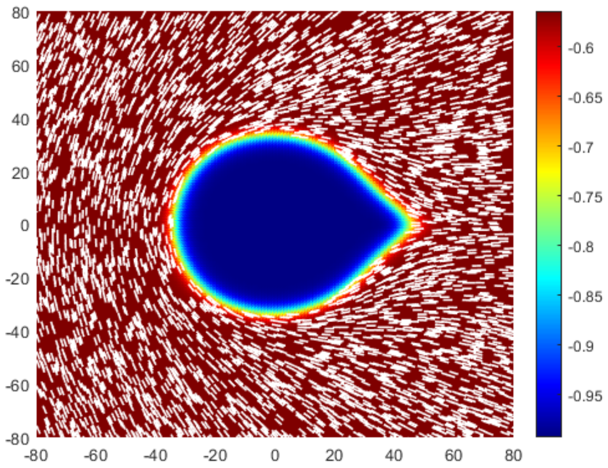
Pronounced anisotropy of the core profile

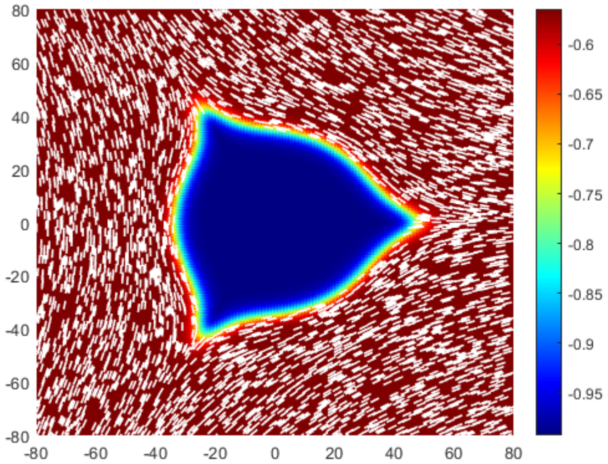


Equilibrium isotropic/nematic domains: "tactoids"



[Zhou, Shiyanovskii, Park, and Lavrentovich. Nat. Comm. 8, 14974 (2017)]



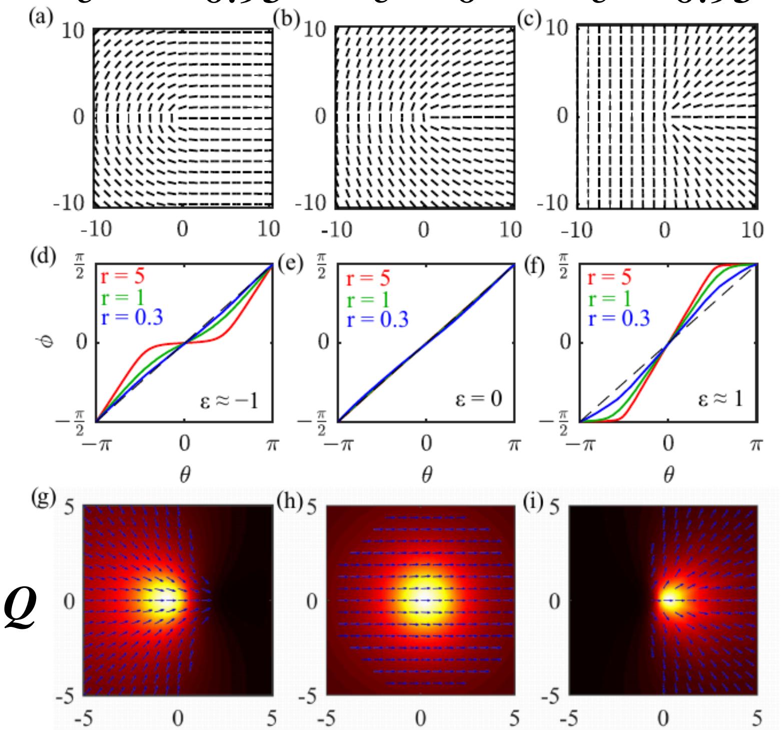


Single disclination (Dzyaloshinskii)

Far field solution, uniaxial and d = 2
(implicit integral equation)

$$\epsilon = (K_3 - K_1)/(K_3 + K_1)$$

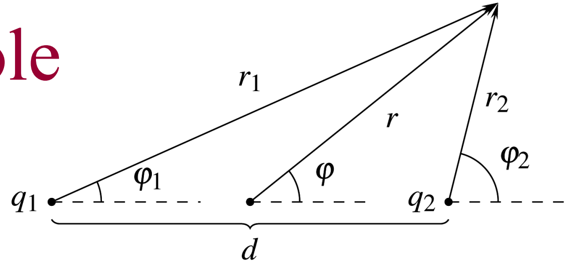
$\epsilon = -0.95$ $\epsilon = 0$ $\epsilon = 0.95$



$\nabla \cdot \boldsymbol{Q}$

Disclination dipole

(perturbatively in ϵ)

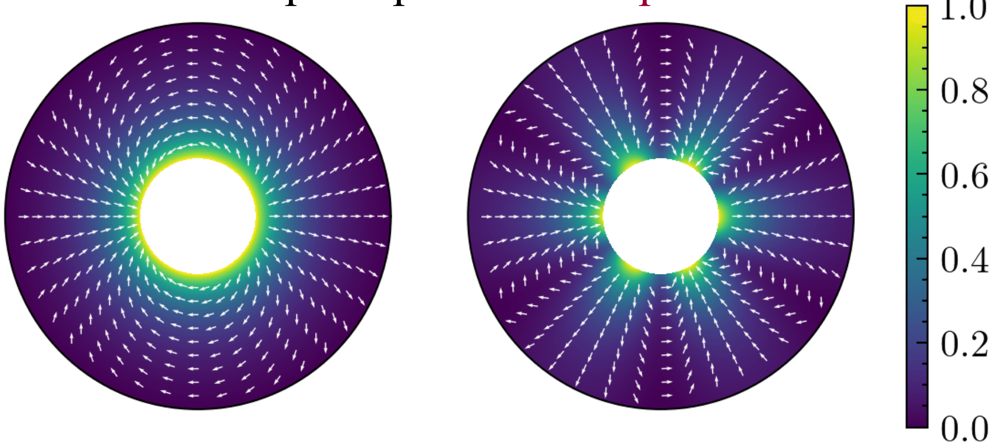


From the Frank-Oseen energy

$$\nabla^2\theta = \epsilon\left[\sin(2\theta)(\theta_x^2 - \theta_y^2 - 2\theta_{xy}) + \cos(2\theta)(\theta_{yy} - \theta_{xx} - 2\theta_x\theta_y)\right]$$

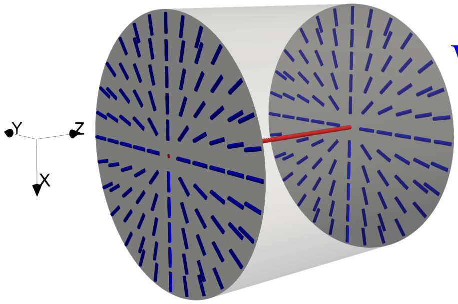
$$\theta = (q_1 + q_2)\varphi - \frac{d(q_1 - q_2)}{2r}\sin\varphi + \epsilon\frac{d}{4r}\sin(3\varphi) + \mathcal{O}\left(\frac{d}{r}\right)^2$$

isotropic dipole new dipolar term



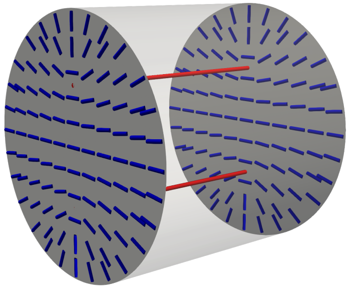
Velocity of a test -1/2 disclination
in the far field of the dipole

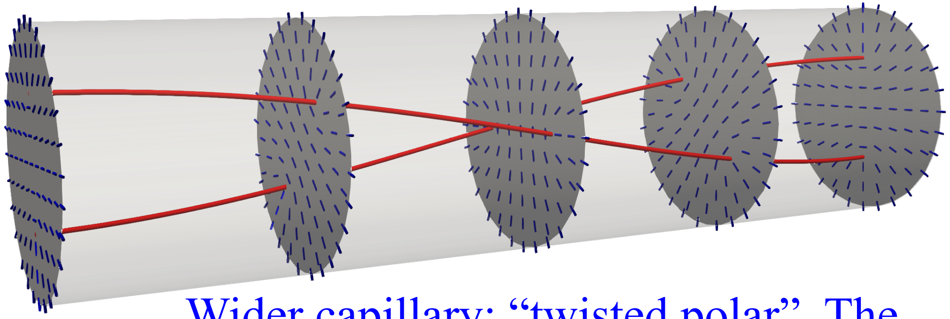
Chiral symmetry breaking

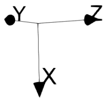


Wider capillary: “polar planar”

Thin capillary “polar radial”

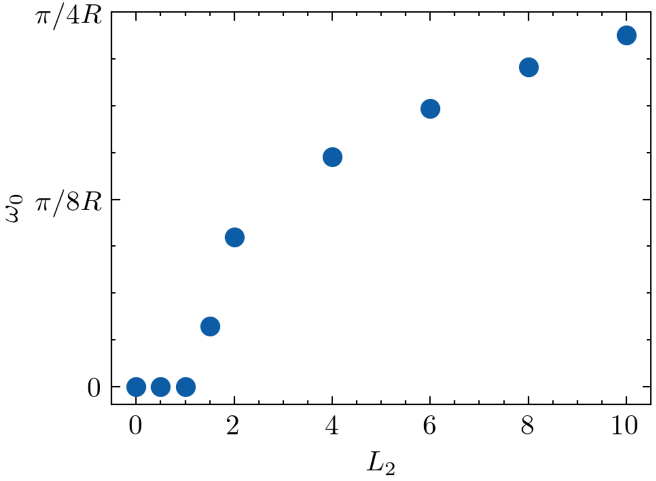




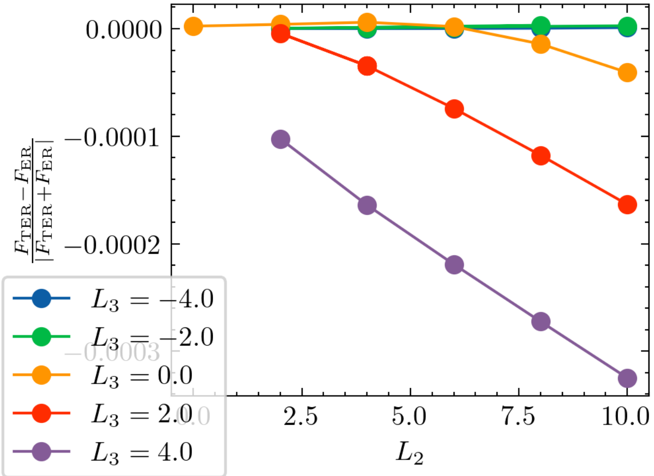


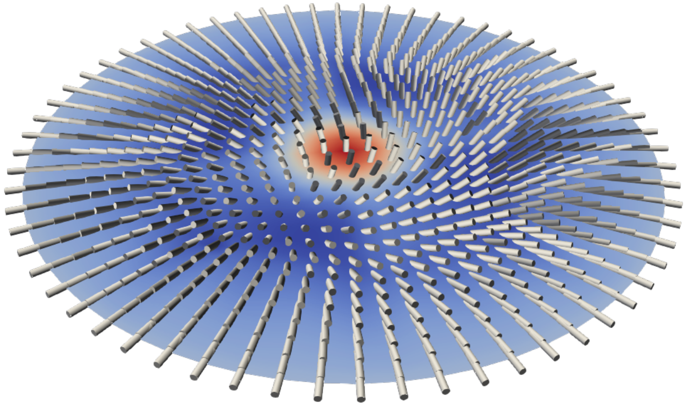
Wider capillary: “twisted polar”. The two disinclination lines wind around each other breaking chiral symmetry

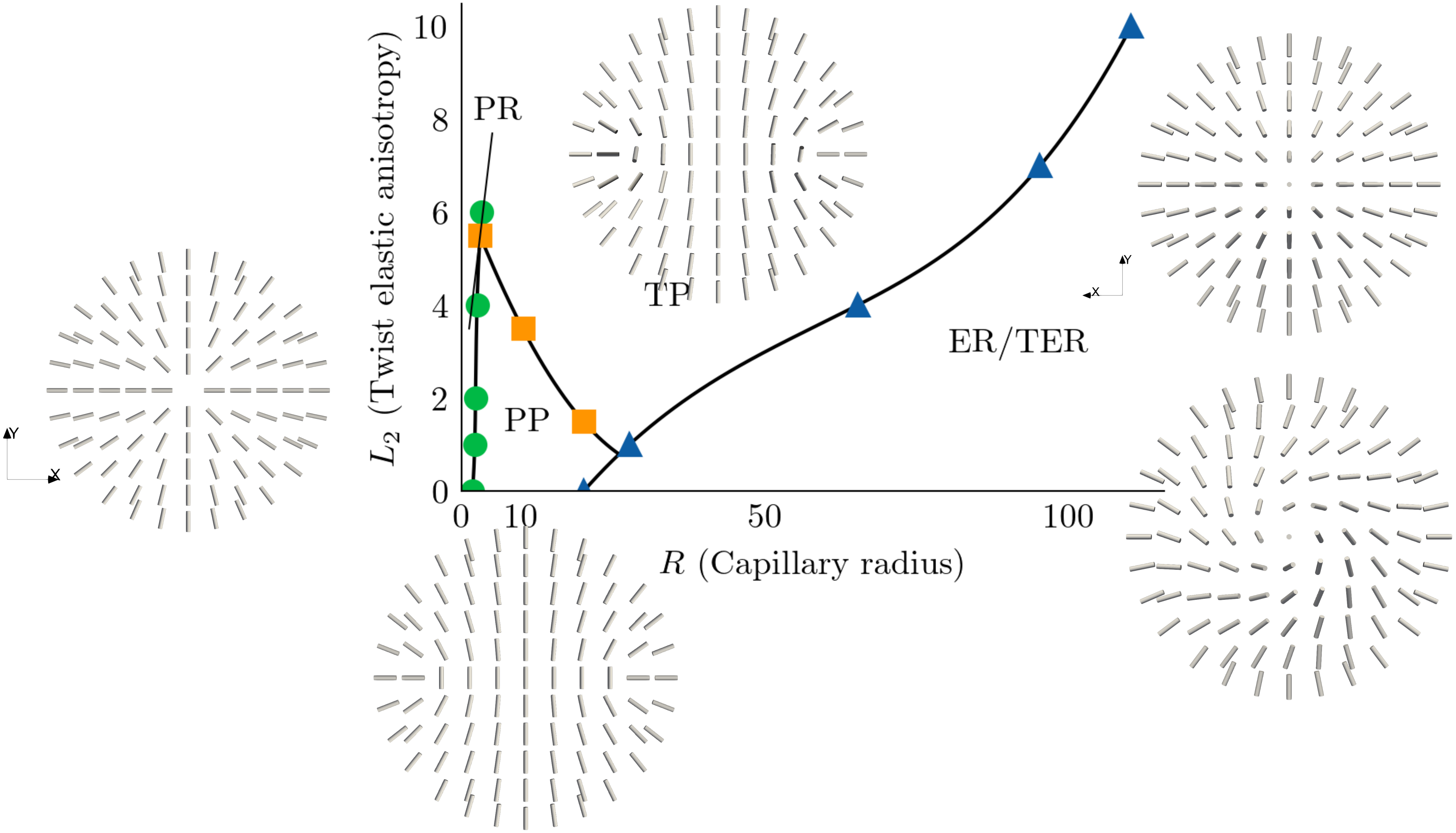
Onset of pitch as twist constant decreases



Bend/splay anisotropy matter



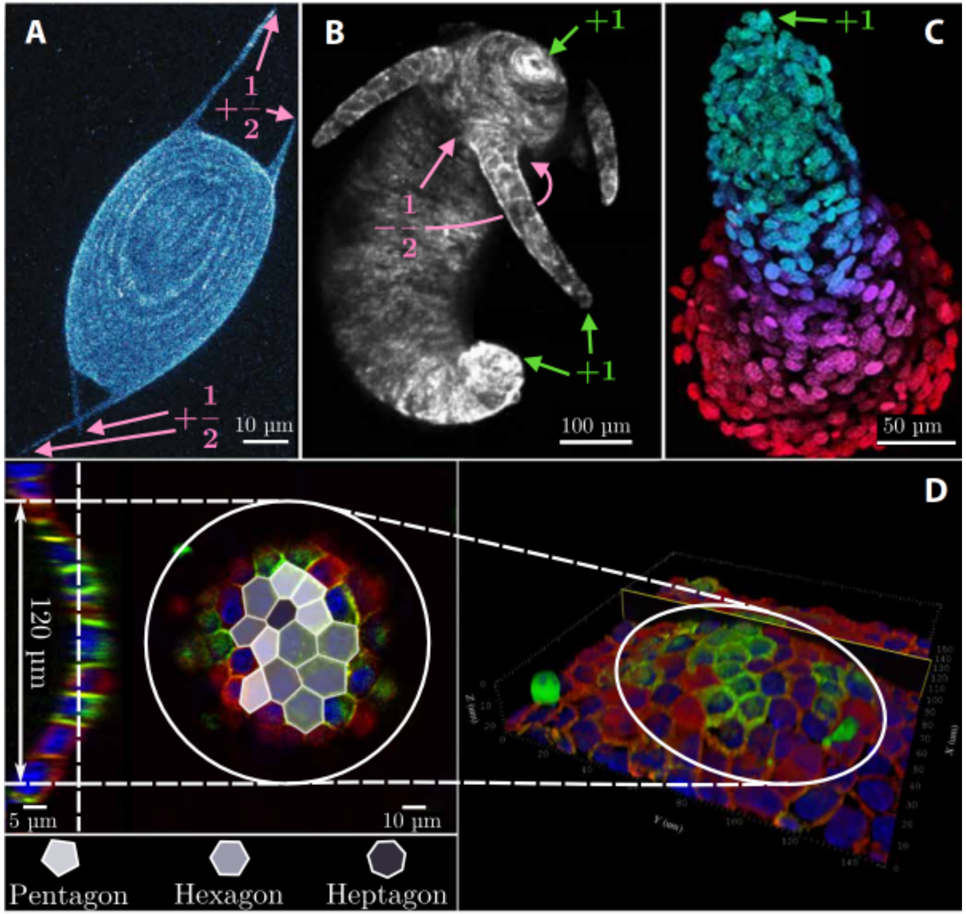




10
8
6
4
2
0
PR
TP
PP
ER/TER
0
10
50
100
L_2 (Twist elastic anisotropy)
R (Capillary radius)
Y
X
Y
X

Mechanics of orientationally ordered biological media

Morphogenesis



[L. Hoffman, …, L. Giomi, Science Adv. 8, eabk2712 (2022)]

Experimental evidence indicates that topological defects could serve as organizing centers in the morphogenesis of tissue.

(A) Monolayer of microtubules and kinesin enclosed in a lipid vesicle

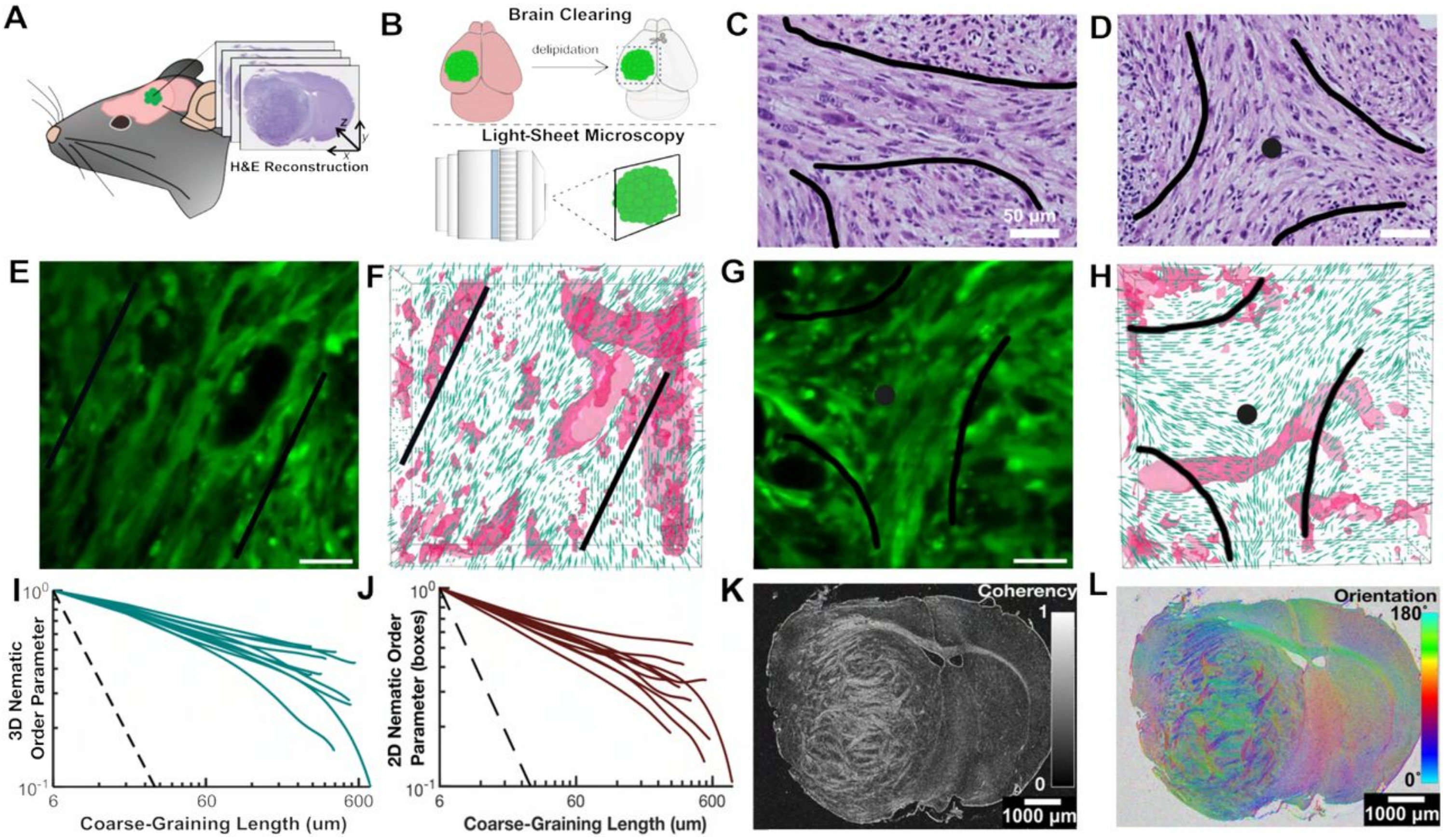
(B) Example of *Hydra* featuring +1 disclinations in proximity of the mouth, the foot, and the tip of each tentacle and two –1/2 defects at the base of each tentacle

(C) Multicellular protrusion in collectively migrating myoblasts under confinement, with a +1 defect at the tip

(D) Dome formed by a layer of MDCK epithelial cells. Penta/Hepta defects are disclinations of the hexagonal cell structure

Is Topology associated robustness key to the development and maintenance of living structures ?

Nematic order in gliomas



Oncostreams: gliomas (in vivo, mouse and human) exhibit self-organized, aligned, multicellular structures - active nematic.

Disclinations clearly visible in stained tissue and laser images

Nematic correlations are long ranged 300-3000 microns

Degree of nematic order correlates with tumor aggression. Order contributes to malignancy

[A. Argento, …, Pedro Lowenstein, bioRxiv May 2025]

A Few Questions

Is there nematic order (both passive and active) in Biological systems ?

- Many recent different systems seem to suggest that this is the case
- Caveat: difficulty and accuracy of experiments in living systems

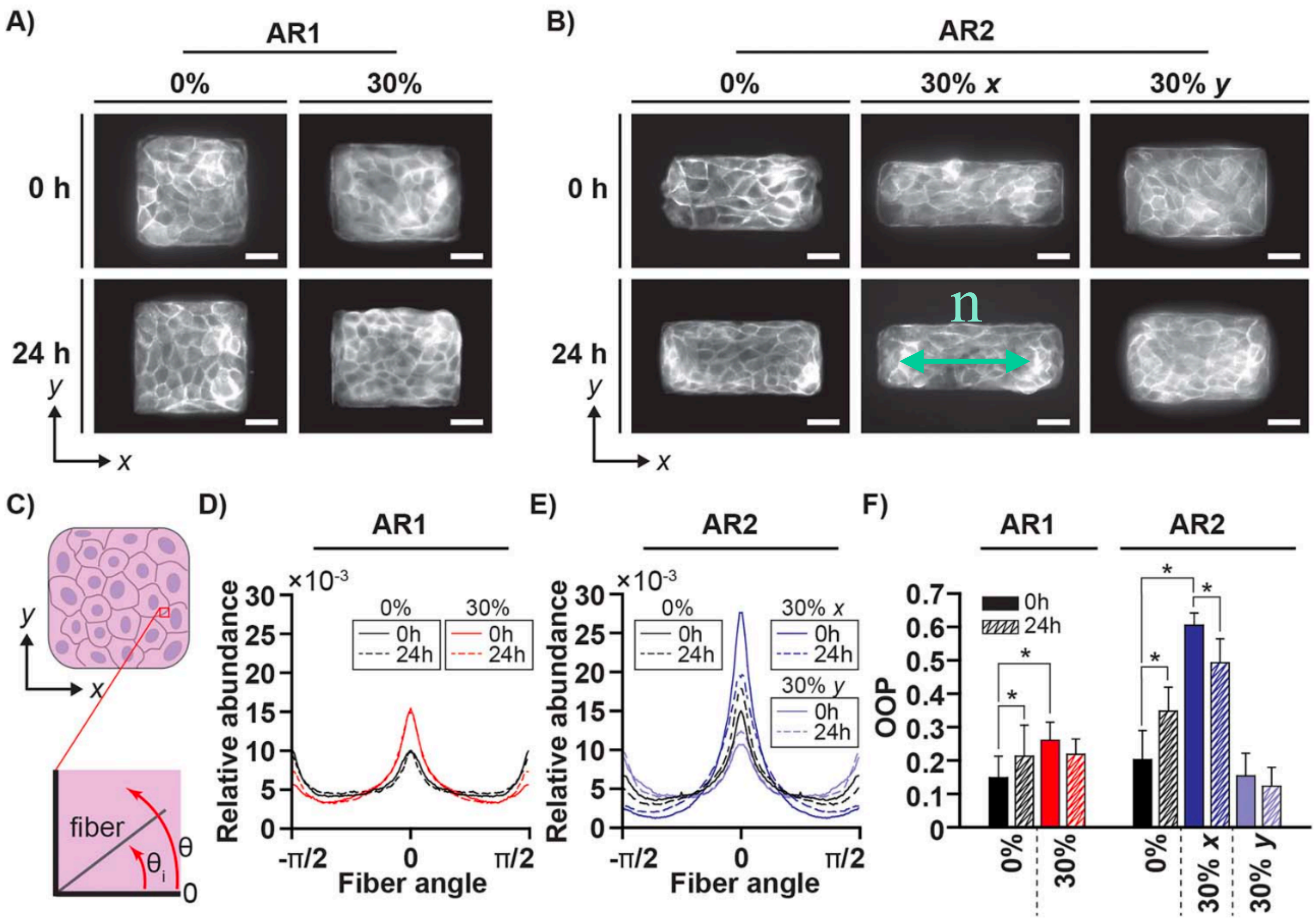
Genetics and biochemistry control/feedback with mechanics (the physical world)

- How Biology controls Mechanics - tissue development and repair
- What is the feedback between mechanics and Biology - remodeling, cell division
- Tissue and organ development modified by mechanical interventions
- Design and build artificial tissue

How does one model the mechanics of living tissue; is it an oriented soft solid ?

- Why would evolution lead to orientational order. Softer elasticity ?
  Topologically induced robustness ?

Tissue has long range nematic order



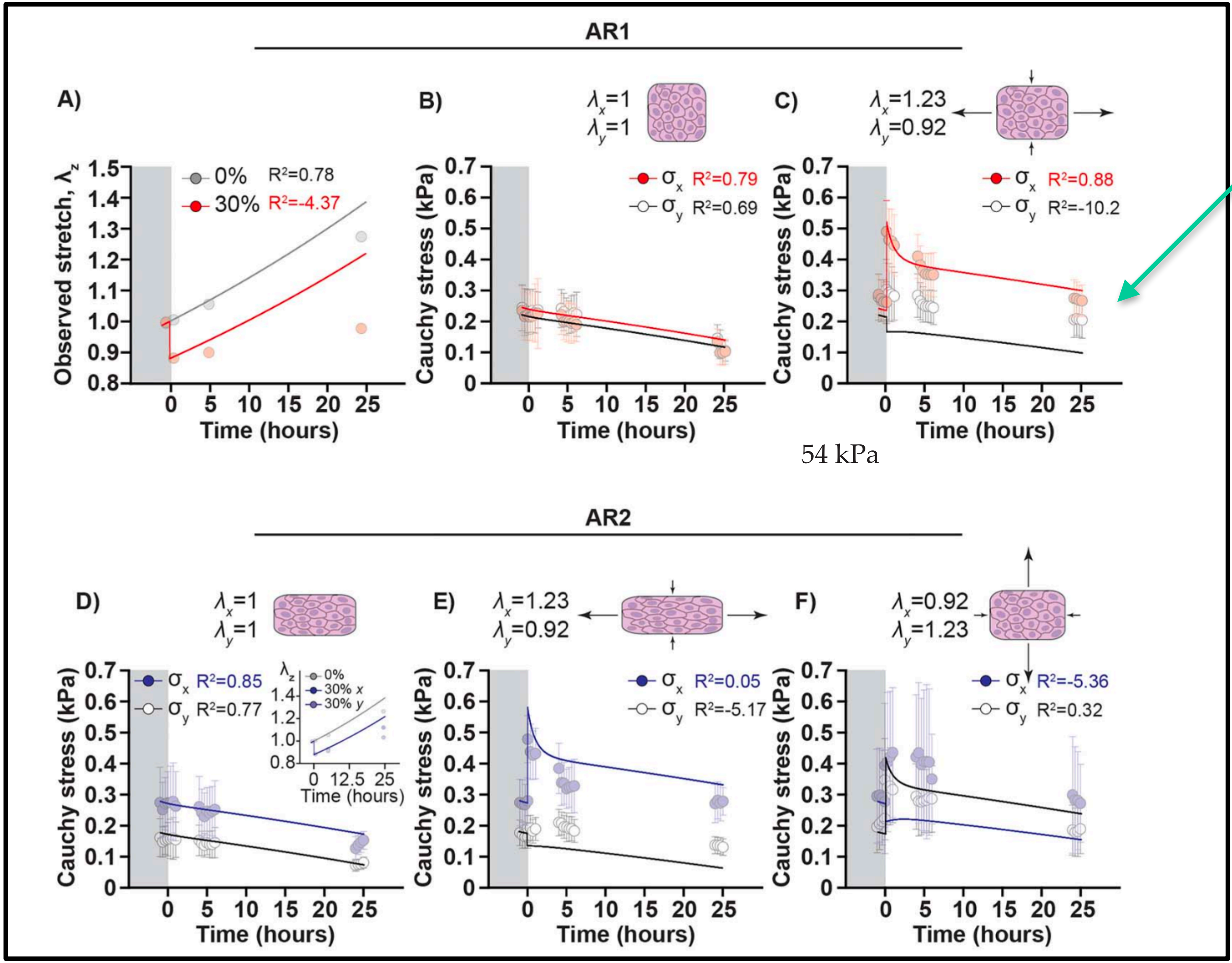
Lithographically micro patterned MDCK tissue. Square (AR1), and rectangular (ARn) shapes

Tissue stained for actin fibers
n is the "director"

Biomechanics:

- Degree or order changes under stretching
- Change depends on relative orientation of director and stretch
- Order changes over time - mechano adaptation

[B. Cook and P. Alford, Integrative Biology 15, 1 (2023)]



Isotropic solid response, $\mu \approx 0.54$ kPa

Cell proliferation relieves stress over a scale of hours

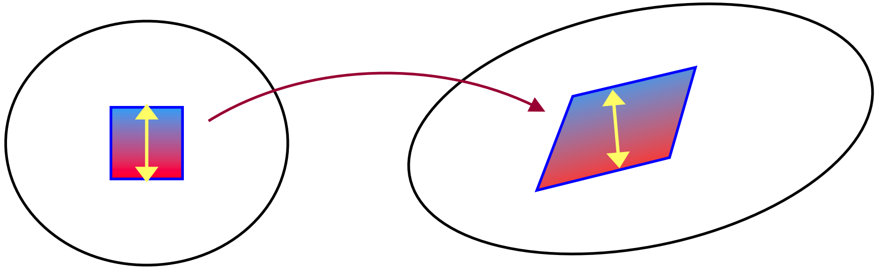
Under longitudinal strain $\delta S \approx 0.25$

Reduction in effective shear modulus relative to isotropic

Reduction in alignment under transverse stretch

Elastic distortion $\qquad W_{ij} = \delta_{ij} - \partial_j u_i \quad (\boldsymbol{W} = \boldsymbol{I} - \boldsymbol{U}^{el})$

Kinematics $\qquad \dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{W}\dot{\boldsymbol{G}}, \quad$ with. $\; L_{ij} = \partial_j v_i$



$\dot{\boldsymbol{G}}$ the anelastic growth rate tensor. Anelastic growth occurs because

Changes in nematic order $\boldsymbol{Q} = S\left(\hat{\boldsymbol{n}} \otimes \hat{\boldsymbol{n}} - \frac{1}{3}\boldsymbol{I}\right)$

Cell proliferation. Cells are largely incompressible, but mass is not conserved.

Free energy (not a functional of $\boldsymbol{G}$)

$$\mathscr{F}\left[\boldsymbol{W}(\boldsymbol{x},t), \boldsymbol{Q}(\boldsymbol{x},t), \nabla\boldsymbol{Q}(\boldsymbol{x},t)\right] = \int_{\Omega(t)} dV\,\rho\left[f_{el}(\boldsymbol{W}(\boldsymbol{x},t), \boldsymbol{Q}(\boldsymbol{x},t)) + f_n(\boldsymbol{Q}(\boldsymbol{x},t), \nabla\boldsymbol{Q}(\boldsymbol{x},t))\right]$$

Use dissipation inequality to obtain evolution equations for distortion and nematic order

$$\int_{\Omega(t)} \boldsymbol{T} : \boldsymbol{L}\; dV \geq \frac{d}{dt}\int_{\Omega(t)} \rho f\; dV$$

Evolution Equations

1. Mechanical stress includes two contribution from nematic order (if isotropic, otherwise uniaxial elasticity)

$$\boldsymbol{T} = 2\mu(\boldsymbol{\varepsilon} - \alpha\boldsymbol{Q}) + K\,\nabla\boldsymbol{Q} \odot \nabla\boldsymbol{Q}$$

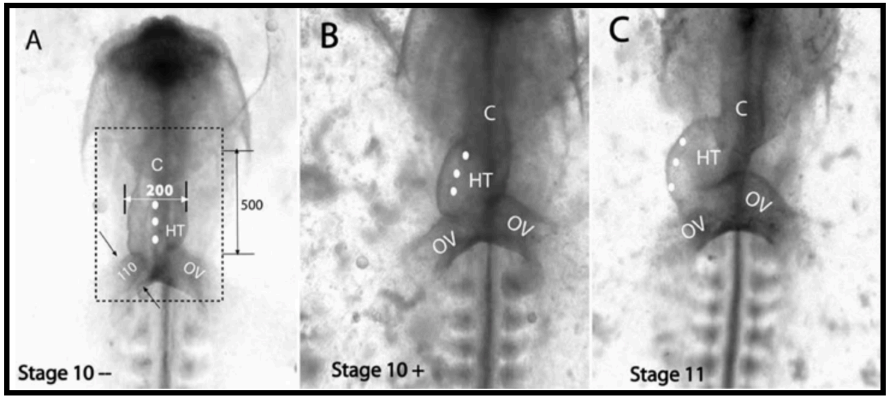
2. Evolution of nematic order (also for isotropic elasticity)

$$\dot{\boldsymbol{Q}} = 2\mu\alpha(\boldsymbol{\varepsilon} - \alpha\boldsymbol{Q}) - \Gamma\left[\frac{\delta\mathscr{F}_n}{\delta\boldsymbol{Q}}\right]_{tr} - \gamma'[\boldsymbol{\sigma}]_{tr}$$

3. Tissue growth. Affected by local stress (homeostasis) and nematic order

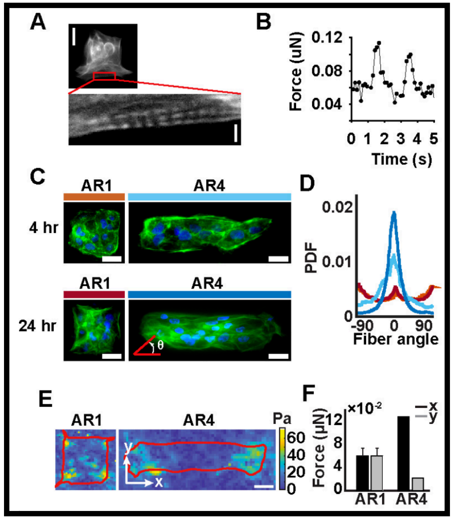
$$\dot{\boldsymbol{G}} = \gamma\boldsymbol{\sigma} - \gamma'\left[\frac{\delta\mathscr{F}_n}{\delta\boldsymbol{Q}}\right]_{tr}$$

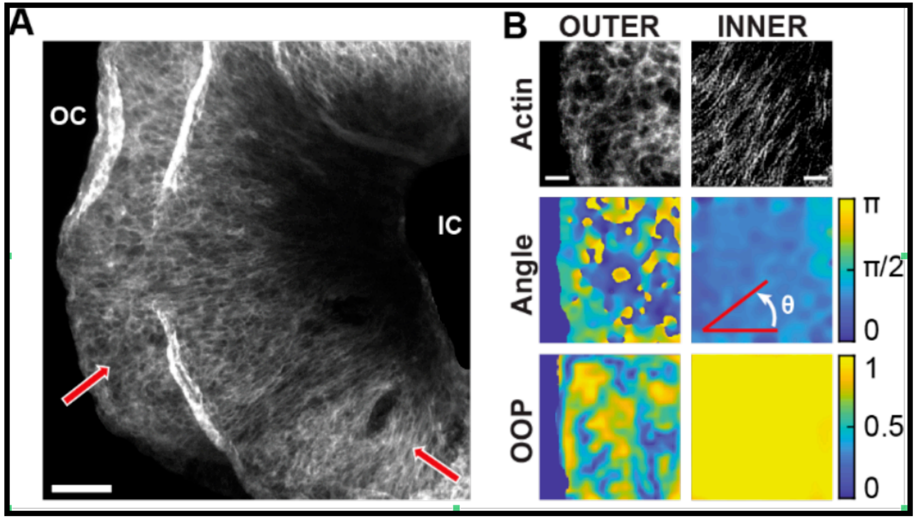
Cardiac Looping in Embryos



[A. Subramanian, …., L. Taber, Ann. Biomed. Eng. 34, 1355 (2006)]

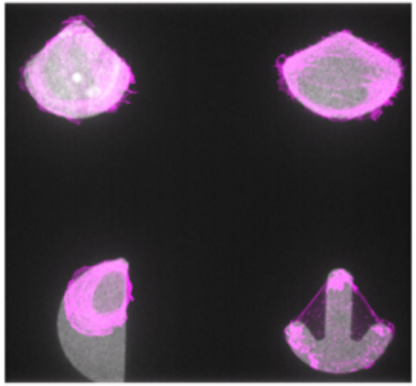
Changes in cell shape driven by actin polymerization in heart tube are responsible for the bending component of c-looping, while unbalanced forces in the OVs (omphalomesenteric vein), due to a combination of cell migration and cytoskeletal contraction, initiate dextral rotation (torsion).



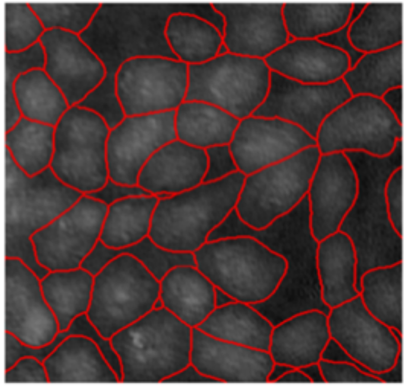


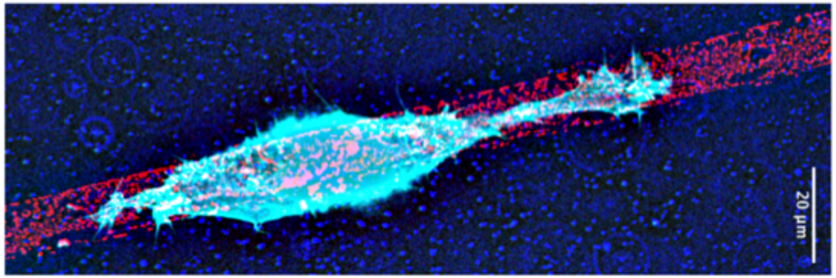
Epithelial Tissue

Play with cells in the lab: Fibronectin pattern (grey) and adherent cells (cyan)

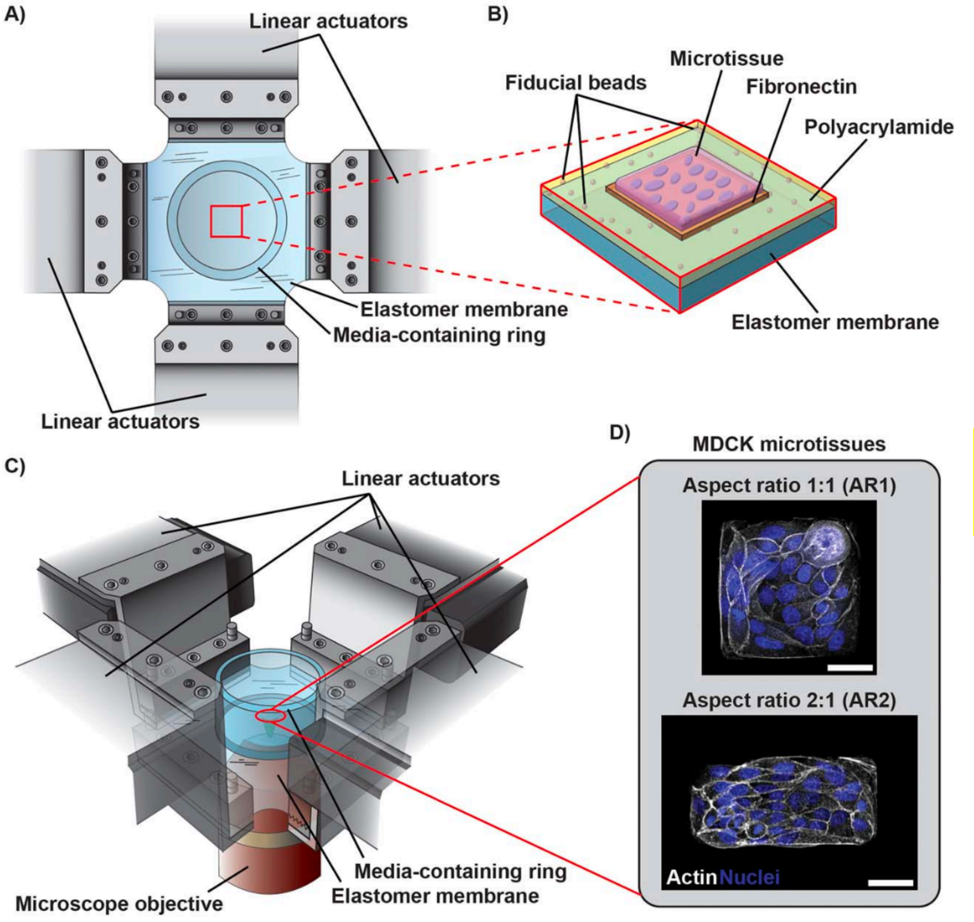


Actual tissue with many cells





Single cell migrating on a predefined track



Order and defects happen in a deformable manifold

Tissue will change shape during growth or in experiments. Potentially cell differentiation (“creation of space”)

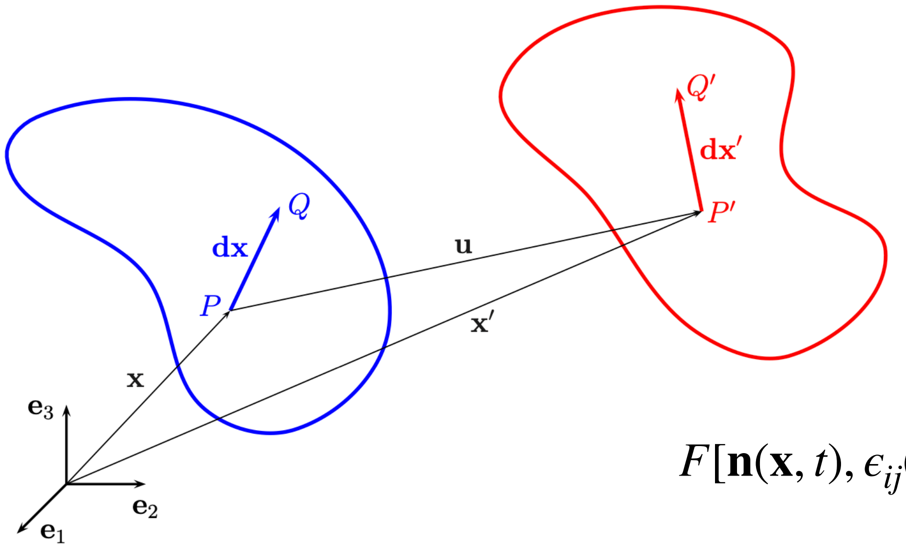


Figure 2.1: Kinematics of deformable bodies

$$(ds')^2 - (ds)^2 = 2\epsilon_{jk} dx_j dx_k$$

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_m}{\partial x_i}\frac{\partial u_m}{\partial x_j}\right)$$

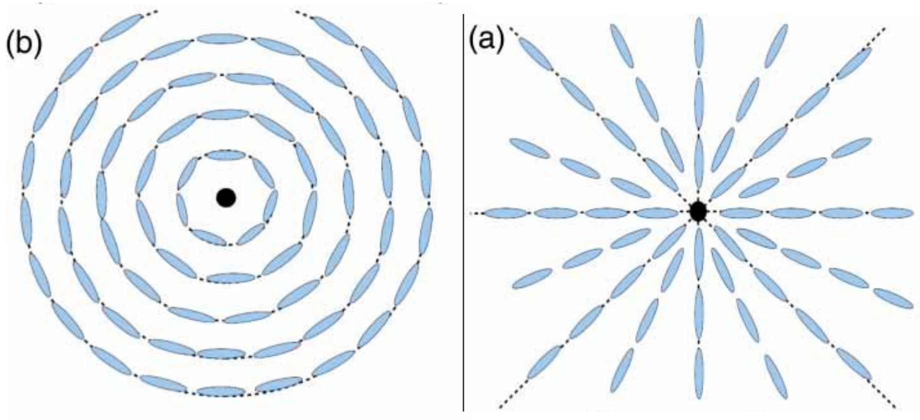
$$F[\mathbf{n}(\mathbf{x},t), \epsilon_{ij}(\mathbf{x},t)] = F_{el}[\epsilon_{ij}(\mathbf{x},t)] + F_d[\mathbf{n}(\mathbf{x},t)] + F_c[\mathbf{n}(\mathbf{x},t), \epsilon_{ij}(\mathbf{x},t)]$$

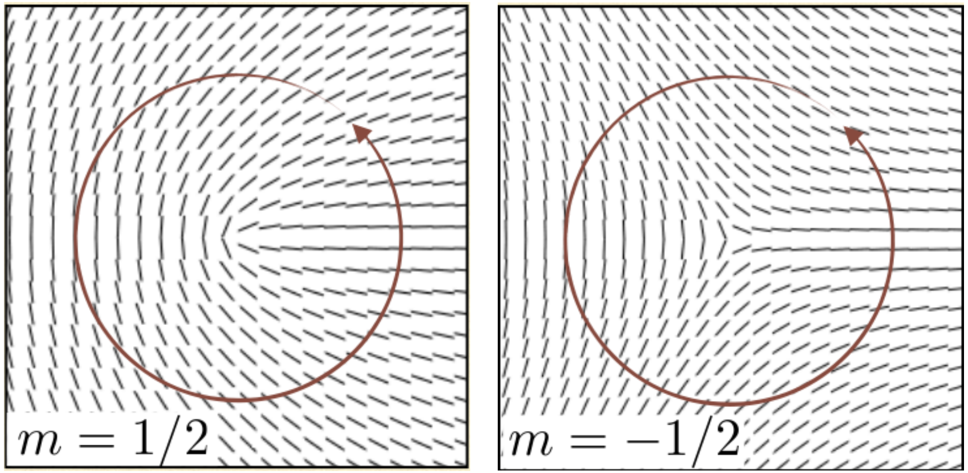
Defect Classes in Nematics

$$\hat{\boldsymbol{n}} = (\cos\theta, \sin\theta) \qquad \oint d\theta = \oint \frac{d\theta}{ds} ds = 2\pi m, \qquad m = \pm 1/2, \pm 1, \ldots$$

Integer charge (m = +1)

Half Integer charge (m = +/- 1/2)

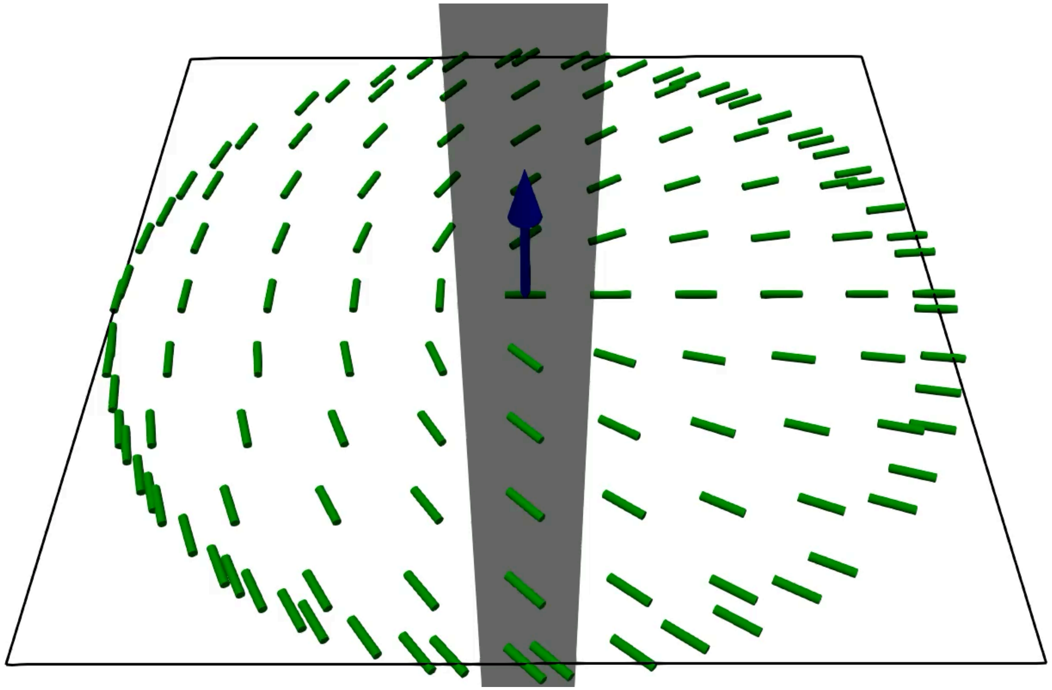




Not stable in three dimensions.
“Escape to the third dimension”

They are two different classes in two dimensions

They belong to the same (and only) class in three dimensions (m = 1/2)



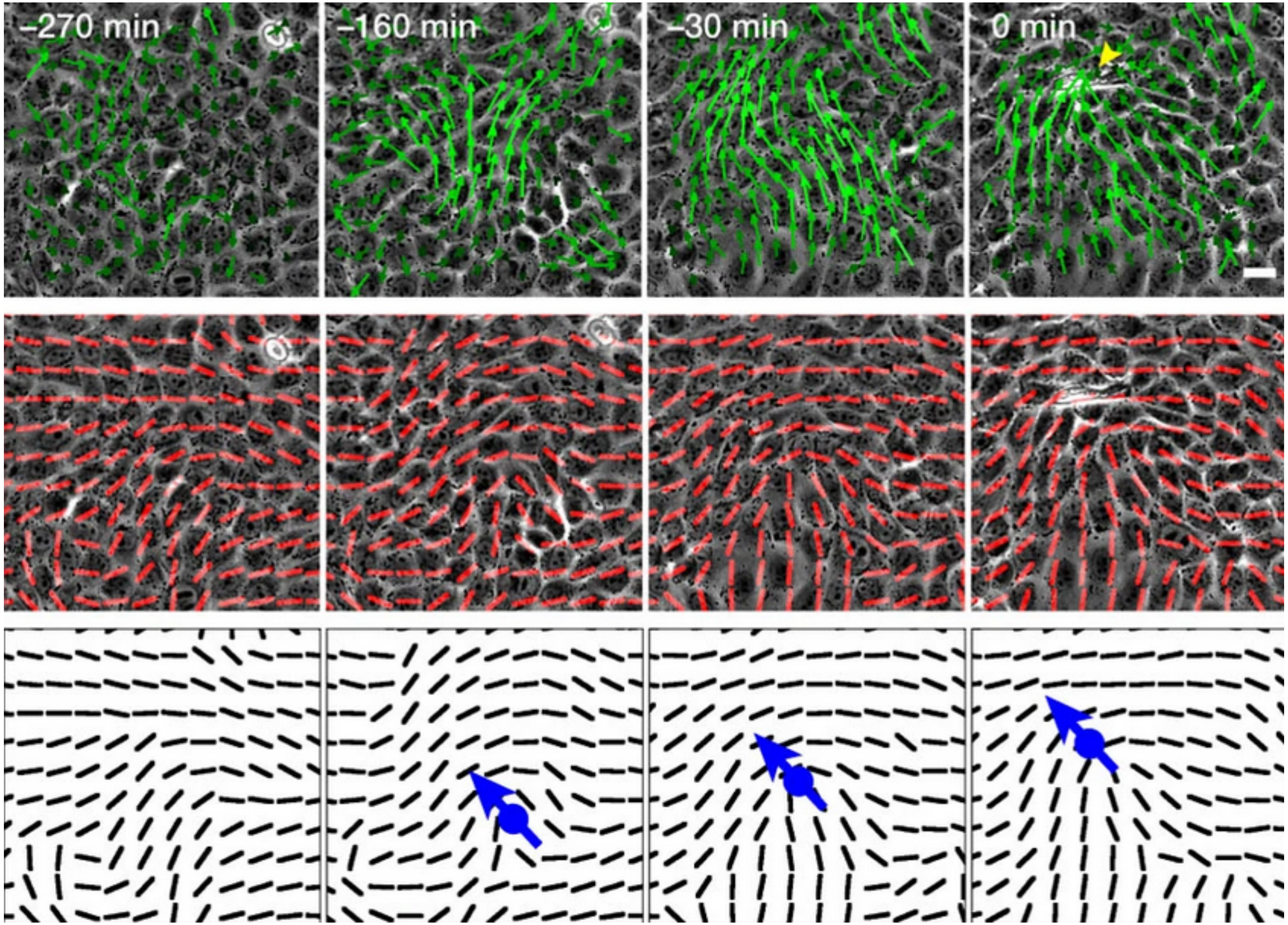
Cell death and extrusion

Epithelial tissues (MDCK) remove excess cells through extrusion, preventing the accumulation of unnecessary or pathological cells.

Death and extrusion occur at +1/2 disclinations. Defect induced stresses promote apoptosis and extrusion. Mechano-transduction

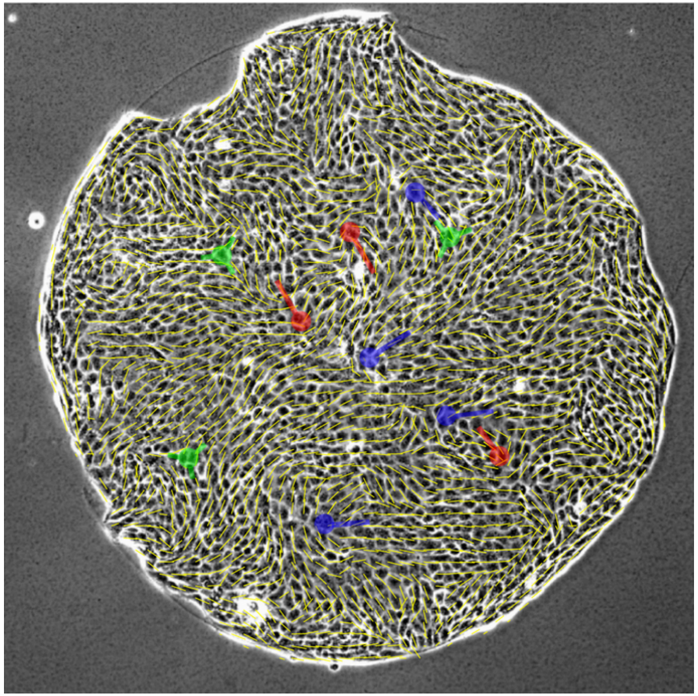
Modeled as extensile active nematic

Control extrusion hotspots by inducing defects through micros contact printing



[TB Saw et al. Nature 544, 212 (2017)]

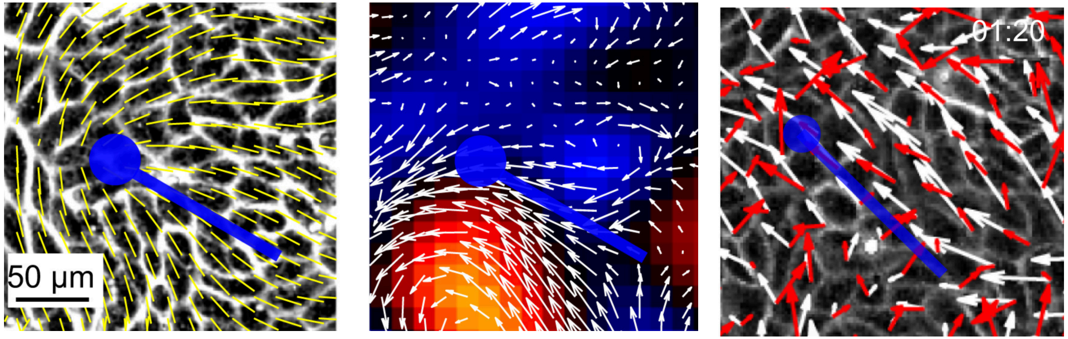
Biomechanics of MDCK tissue



[P. Bera, …, J. Notbohm, Newton 1, 100231 (2025)]

Madin-Darby canine kidney (MDCK) epithelial tissue

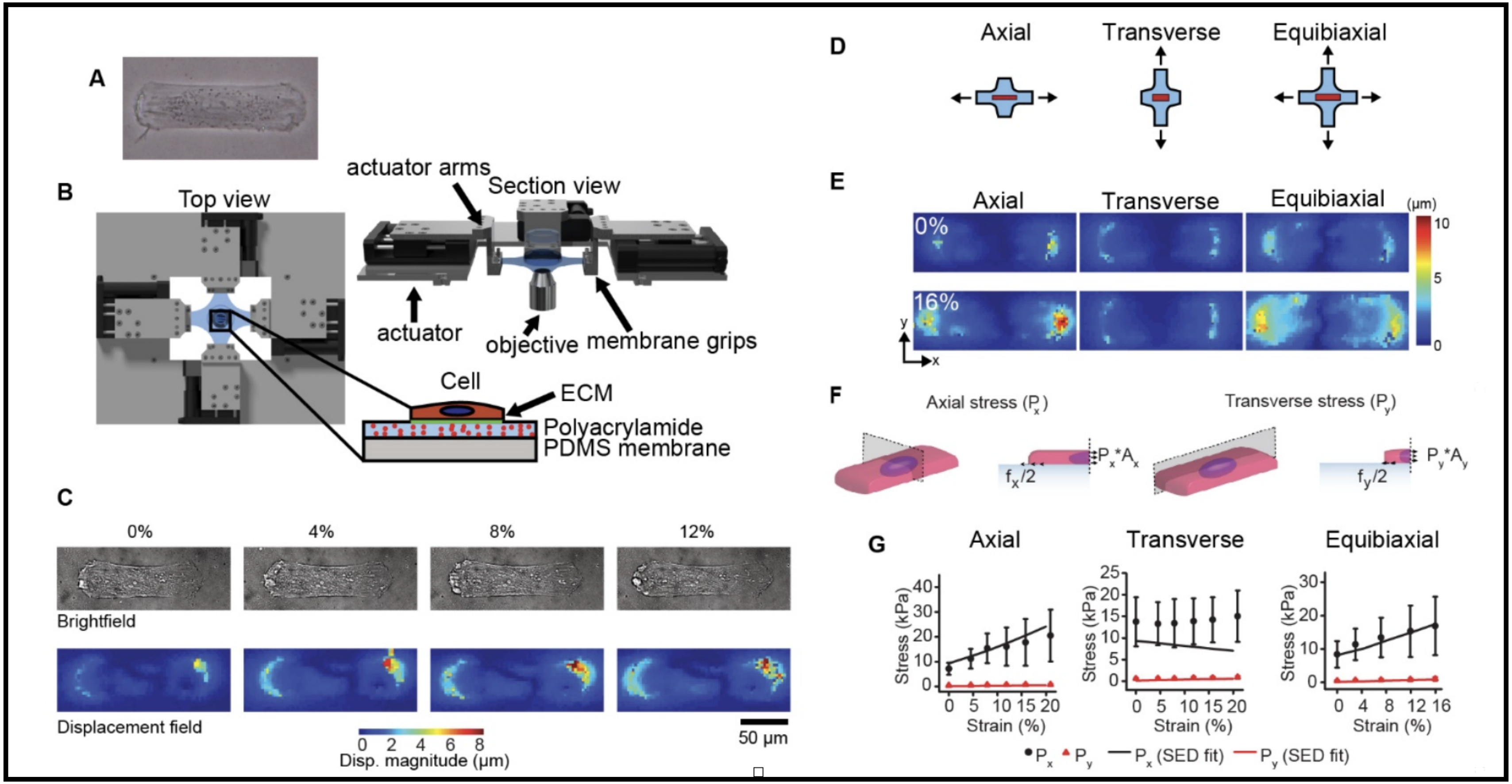
Easy to keep alive, manipulate, and pattern



Cell shapes consistent with nematic order and active nematic flows (vorticity shown). Also measured tractions (red arrows), with Traction Force Microscopy

There has to be more to tissue mechanics than a flowing, active, nematic fluid. Tissues also respond elastically

CμBS (UofM)



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