Active and Driven Soft Matter

Lecture 2: Hydrodynamics of Living Liquid Crystals

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Outline

- Tutorial: hydrodynamics of nematic liquid crystals
- Active hydrodynamic: active stresses, nematic vs polar order
- Spontaneous flow
- Asters, vortices and spirals

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Hydrodynamics of nematic liquid crystals

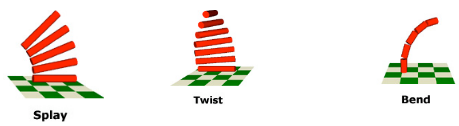
Hydrodynamic fields

- Conserved variables: density ρ, momentum $\vec{g}$, [energy]
- Broken symmetry fields: director n

Symmetry: n → -n

$$F = \int_{\vec{r}} \left(\frac{g^2}{2\rho} + f_0(\rho) \right) + F_K[\vec{n}] \longleftarrow$$ Frank free energy

$$F_K = \frac{1}{2} \int_{\vec{r}} \left[K_1 (\nabla \cdot n)^2 + K_2 [n \cdot (\nabla \times n)]^2 + K_3 [n \times (\nabla \times n)]^2 \right]$$



single - elastic constant approx:

$K_1 = K_2 = K_3 = K$

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Conservation Laws and Fluxes

$$\partial_t \rho = -\vec{\nabla} \cdot \vec{g} \qquad \partial_t g_i = -\partial_j \pi_{ij}$$

$$\partial_t \vec{n} = -\vec{J}$$

$$R \equiv T \frac{dS}{dt} = -\int_{\vec{r}} \left[(\vec{g} - \rho \vec{v}) \cdot \vec{\nabla} \frac{\mu}{m} + \left(\pi_{ij} - \rho v_i v_j - \delta_{ij} p \right) \partial_i v_j + \dot{n}_i h_i \right]$$

Hyd. field	Flux	Force
ρ	$\vec{g}$	$\vec{\nabla}\mu$
$\vec{g}$	π_{ij}	$\partial_i v_j$
$\vec{n}$	$\dot{\vec{n}}$	$\vec{h} = -\delta F / \delta \vec{n}$

single-elastic constant approx:

$K_1 = K_2 = K_3 = K$

$\vec{h} = K \nabla^2 \vec{n}$

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Nematic hydrodynamic

- incompressible $\rho = \text{constant} \Rightarrow \vec{\nabla}\cdot\vec{v}=0$
- low Reynolds number $\partial_j \sigma_{ij} = 0$
- $\sigma_{ij} = 2\eta u_{ij} - p\delta_{ij} + \frac{\lambda}{2}(h_i n_j + h_j n_i) + \frac{1}{2}(h_i n_j - h_j n_i)$
- $\partial_t n_i + \vec{v}\cdot\vec{\nabla} n_i + \omega_{ij} n_j = \delta^T_{ij}(\lambda u_{ij} n_j + \frac{1}{\gamma} h_i)$

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

$\omega_{ij} = \frac{1}{2}(\partial_i v_j - \partial_j v_i)$

$\delta^T_{ij} = \delta_{ij} - n_i n_j$

$\vec{h} = K\nabla^2 \vec{n}$

Coupling of orientation and flow
Flow alignment parameter λ depends on microscopic properties of nematogens: λ> 0 rod-like molecules, λ>0 discotic molecules

Asymmetric part of stress tensor
torque exerted by orientational degrees of freedom on the flow

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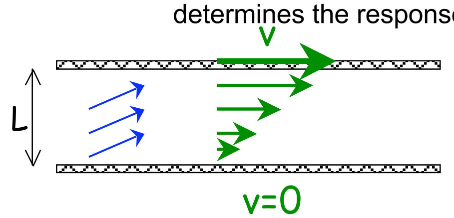
Flow alignment parameter λ

determines the response of the director to shear



Nematic film uniformly **sheared** between two plates
- no-slip boundary conditions

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

$u_{xy} = \frac{1}{2}\partial_y v_x = \mathrm{v}/2\mathrm{L}$

Homogeneous state (away from boundaries):

$\partial_t \theta = -u_{xy}(1 - \lambda\cos 2\theta)$

$\Rightarrow \cos 2\theta_0 = \frac{1}{|\lambda|} \quad \text{if} \quad |\lambda| > 1$

|λ|>1 flow alignment

| λ |<1 flow tumbling: inhomogeneous rolls

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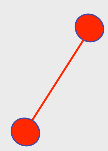
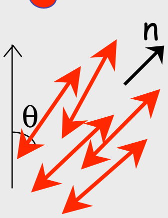
Active liquid crystals can exhibit two types of orientational order: polar and nematic

Apolar: melanocytes, rods



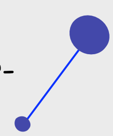
Apolar order: nematic



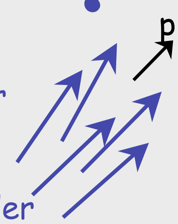
n=-n

Tensor order parameter: alignment $Q \sim \langle \Sigma_\alpha \cos^2\theta_\alpha \rangle$

Polar: fish, bacteria, motor-filaments



Polar order



p≠ -p

Vector order parameter: polarization $P \sim \langle \Sigma_\alpha \cos\theta_\alpha \rangle$

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Active Liquid Crystals

Three new ingredients:

1. Active LC can order in **nematic and polar states** $\rightarrow$ both order parameter fields Q and P must be included in the hydrodynamics
2. Activity yields an energy input on each particle that provides an **additional driving force**, not unlike a chemical potential

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

•motor-filament mixtures: $\Delta\mu$ ~ rate of ATP consumption

•swimming bacteria: $\Delta\mu$ ~ force exerted by swimmers on fluid

3. One should develop a two-fluid model that incorporates the exchange of momentum between active particles and solvent

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Active stress

Coupling between orientation and flow induced by activity. The simplest active terms allowed in the stress have the form

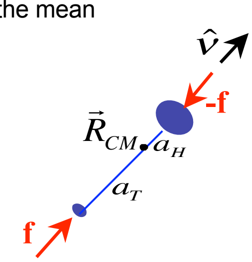
$$\sigma_{ij}^{\alpha} = \Delta\mu\alpha Q_{ij} + \Delta\mu\alpha' P_i P_j \quad \text{nematic \& polar}$$

$$+ \Delta\mu\beta\left(\partial_i P_j + \partial_j P_i\right) \quad \text{polar only}$$

Justification (Hatwalne et al, 2004): active particles (e.g., bacteria) extert a force dipole on the surrounding fluid. Calculate the mean force density on a fluid element:

$$F_i^{active} = \left\langle \sum_{\substack{active \\ particles}} \left[-f\hat{u}_i \delta(\vec{r} - \vec{R}_{CM} - a_H \hat{v}) + f\hat{u}_i \delta(\vec{r} - \vec{R}_{CM} + a_T \hat{v}) \right] \right\rangle$$

$$\simeq \partial_j \left[f(a_H + a_T)\left\langle \hat{v}_i \hat{v}_j \right\rangle + f(a_H^2 - a_T^2)\partial_i \left\langle \hat{v}_j \right\rangle + \ldots \right] \equiv \partial_j \sigma_{ij}^{active}$$



$\alpha > 0 \rightarrow$ contractile

$\alpha < 0 \rightarrow$ tensile

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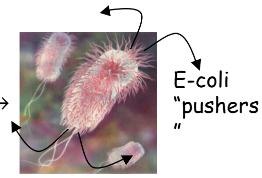
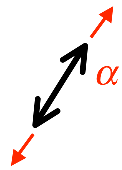
Contractile/tensile stresses

(more on this in Lecture 4)

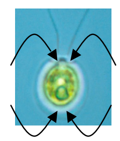
Most swimming bacteria push fluid out at the head and tail → **tensile** or pushers

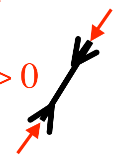




$\alpha < 0$

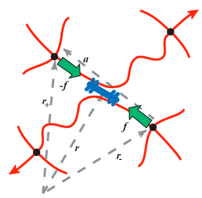
The algae chlamydomonas pull fluid in at the head and tail → **contractile** or puller





$\alpha > 0$

Actin filaments crosslinked by myosins are **contractile**



$\alpha > 0$

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Active Hydrodynamics: single incompressible fluid

$\rho = \text{constant}$

$\partial_j \sigma_{ij} = 0$

$$\partial_t n_i + (\vec{\mathrm{v}} - \beta\vec{n}) \cdot \vec{\nabla} n_i + \omega_{ij} n_j = \delta_{ij}^T (\lambda u_{ij} n_j + \frac{1}{\gamma} h_i)$$

$$\sigma_{ij} = -\pi\delta_{ij} + \eta\left(\partial_i \mathrm{v}_j + \partial_j \mathrm{v}_i\right) + \alpha n_i n_j + \beta\left(\partial_i n_j + \partial_j n_i\right) + O(\nabla^2)$$

mechanical stresses

active contractile/tensile (α>0 /α<0) stresses in polar & nematic

active stresses exclusive to polar systems

α, β ~ activity
~ ATP consumption rate
~ forces exerted by swimmers

α ~ mean active force
β ~ self-propulsion/treadmilling

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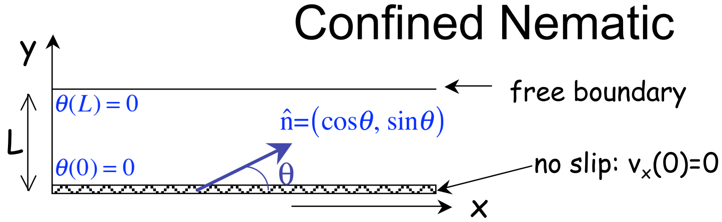
Confined Nematic



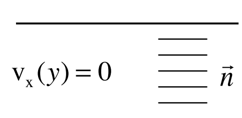
Passive Nematic

$$\partial_t\theta = K\partial_y^2\theta - (1-\lambda\cos 2\theta)\partial_y v_x$$
$$\sigma_{xy} = \eta\partial_y v_x + K(1-\lambda\cos 2\theta)\partial_y^2\theta$$

$$\rho = \text{constant}$$
$$\partial_y\sigma_{yy} = 0 \rightarrow \text{pressure}$$
$$\left.\begin{aligned}&\partial_y\sigma_{xy} = 0 \rightarrow \sigma_{xy} = \text{const}\\ &\sigma_{xy}(0) = \sigma_{xy}(L) = 0\end{aligned}\right\} \rightarrow \boxed{\sigma_{xy}(y) = 0}$$

Only solution is aligning and homogeneous

$$\theta(y) = 0 \quad \text{anchoring}$$
$$v_x(y) = 0 \quad \text{no flow}$$



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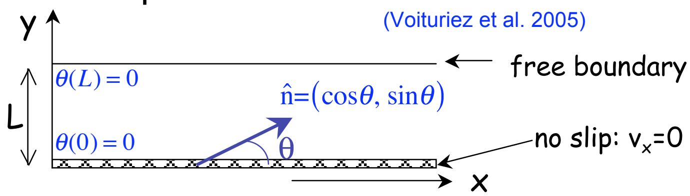
"Spontaneous flow" in confined active nematic

(Voituriez et al. 2005)



$$\boxed{\begin{array}{l}\rho = \text{constant}\\ \sigma_{xy}(y)=0\end{array}}$$

Active Nematic

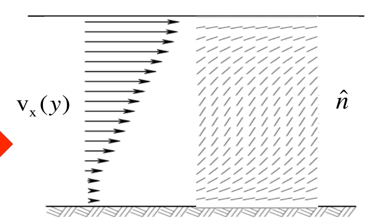
$$\left.\begin{array}{l}\partial_t\theta = K\partial_y^2\theta-(1-\lambda\cos 2\theta)\partial_y \mathrm{v}_x\\ \sigma_{xy}=\eta\partial_y\mathrm{v}_x+K(1-\lambda\cos 2\theta)\partial_y^2\theta+\alpha\sin 2\theta\end{array}\right\}\rightarrow\ \partial_y^2\theta\simeq-\frac{1}{l_\alpha^2}\sin 2\theta$$

steady state

$$l_\alpha^{-2}=\frac{\alpha(1-\lambda)}{K[2\eta+(1-\lambda)^2]}$$

spontaneous flow if $l_\alpha \geq L/\pi$

$$\alpha_c \sim \frac{\eta}{1-\lambda}\left(\frac{\pi}{L}\right)^2$$



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"Spontaneous flow" in polar active film

(Giomi, MCM & Liverpool, PRL)

Variations in filament concentration cannot be neglected $\rightarrow$ two-fluid description needed

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Hydrodynamics of active suspensions

$$\rho = \rho_{solvent} + Mc = \text{constant} \quad \vec{\nabla}\cdot\vec{\mathrm{v}}=0$$

$$\partial_t c = -\vec{\nabla}\cdot\vec{j} = -\vec{\nabla}\cdot c\left(\vec{\mathrm{v}}\text{-}\beta\vec{P}\right) + D\nabla^2 c$$

"self-propulsion": only in polar systems

$$\partial_j \sigma_{ij} = 0$$

$$\sigma_{ij} = \text{-}p\delta_{ij} + \eta\left(\partial_i \mathrm{v}_j + \partial_j \mathrm{v}_i\right) + \alpha n_i n_j + \beta\left(\partial_i n_j + \partial_j n_i\right)$$

mechanical stresses | active contractile\tensile stresses in polar & nematic | active polar stresses

$$\partial_t n_i + (\vec{\mathrm{v}}\text{-}\beta\vec{n})\cdot\vec{\nabla}n_i + \omega_{ij}n_j = \delta_{ij}^T(w\partial_j c + \lambda u_{ij}n_j + \frac{1}{\gamma}h_i)$$

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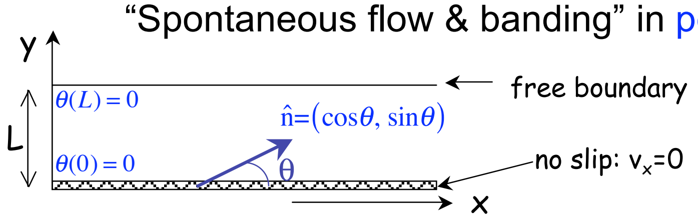
"Spontaneous flow & banding" in polar films



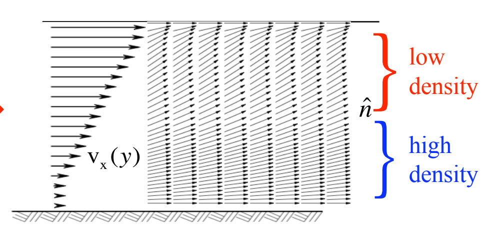
$$\rho = \text{constant}$$
$$\sigma_{xy}(y) = 0$$

$$\partial_y j_y = \partial_y(\beta n_y \text{ - } D\,\partial_y c)=0 \quad \rightarrow \quad \partial_y c = \beta\sin\theta / D$$
$$K\partial_y^2\theta = (1-\lambda\cos 2\theta)\partial_y \mathrm{v}_x$$
$$\sigma_{xy} = \eta\partial_y \mathrm{v}_x + \alpha\sin 2\theta = 0$$

Active currents balance diffusion across the channel yielding concentration gradients and spontaneously "banded" flow

spontaneous flow & concentration bands

$$\alpha > \alpha_c \sim \frac{\eta}{1-\lambda}\left(\frac{\pi}{L}\right)^2$$



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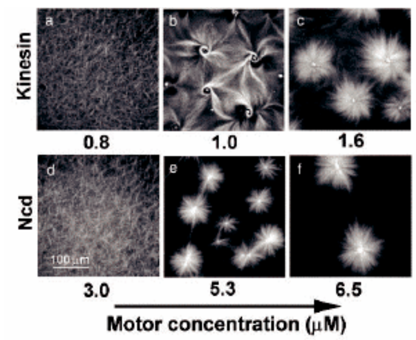
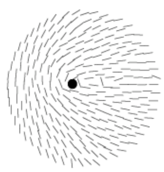
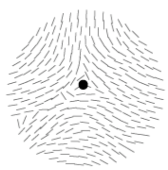
Topological defects

Activity-induced patterns in vitro bear striking resemblance to topological defect of polar state

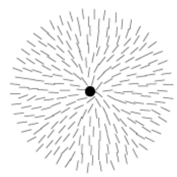
Because of n →-n symmetry, lowest energy defects in 2d nematic are s=±1/2 disclinations

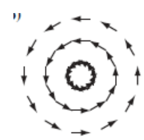






A polar state has the symmetry of a vector field with s=±1 defects





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Defects in polarized state

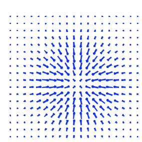
Kruse et al. 2005
Aranson & Tsimring 2005
MCM & TBL

neglect density modulations to study the topological defects of polarization field

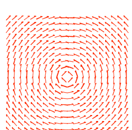
$$K_{1,3}^{\alpha} = K_{1,3} - \alpha(...)$$

$$\partial_t n_i = \delta_{ij}^T \left[K_3^{\alpha} \nabla^2 n_j + (K_1^{\alpha} - K_3^{\alpha}) \partial_j \vec{\nabla} \cdot \vec{n} \right] - \beta \vec{n} \cdot \vec{\nabla} n_i$$

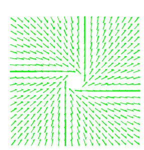
$$\boxed{\begin{aligned} \vec{n} &= (\cos\theta, \sin\theta) \\ \theta(r,\varphi) &= \varphi + \Psi(r) \end{aligned}}$$



$\Psi = 0, \pi$
aster



$\Psi = \pm\pi/2$
vortex



spirals:
$\Psi(\mathrm{r}) = \sin^{-1}\left(r/r_0 \right)$

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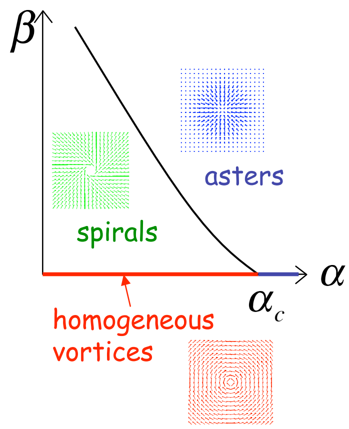
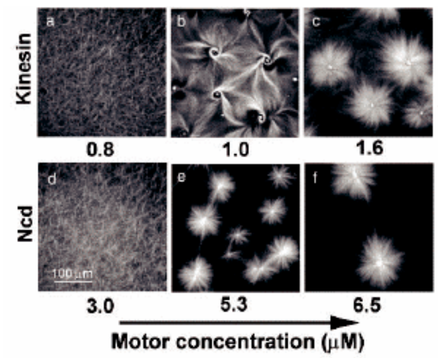


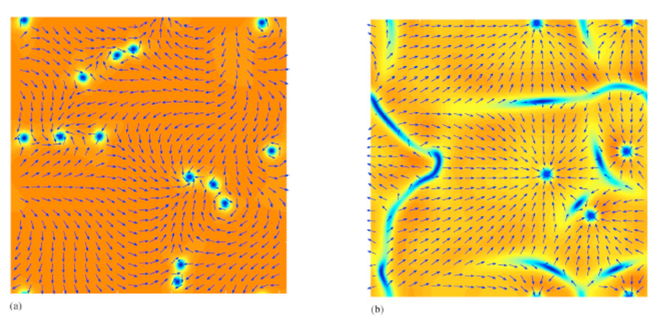


β~motor speed~ polarity

Consistent with simulation by F. Nedelec

α~ motor processivity (motor stalling at filaments' end)

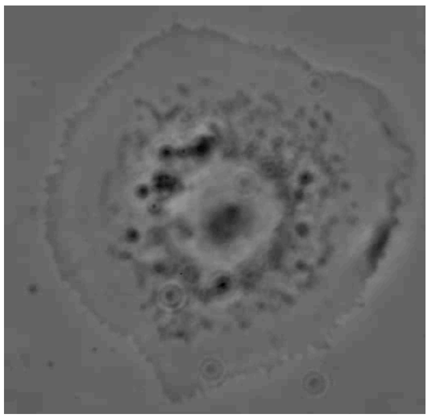
Numerical solution -- Aranson & Tsimring PRE **71**, 50901 (2005)



Polarization field **P** for vortices and asters structures. Color refers to magnitude |**P**|: red is max and blue is zero.

Actin waves in cultured Drosophila cells

Y. Asano et al. HFSPJ 2009



Pak3 depletion polarizes the actin lamellipodium → migration of non-motile cells & actin waves in immobile cells

Hydrodynamics of actin cytoskeleton as a polar LC in an annulus yields propagating actin waves above critical $\beta_{c,}$ as seen in experiments

β~ treadmilling rate

α~ myosin contractility

Summary

Active liquid crystals exhibit "spontaneously" many of the nonequilibrium phenomena that occur in passive LC under the action of external fields

Connection with biological phenomena only qualitative, yet tantalizing

→ activity-induced oscillations

→ rheology very rich and currently being explored