Active Matter

Lectures for the 2011 ICTP School on Mathematics and Physics of Soft and Biological Matter

Lecture 4: Hydrodynamics of “Living” Liquid Crystals

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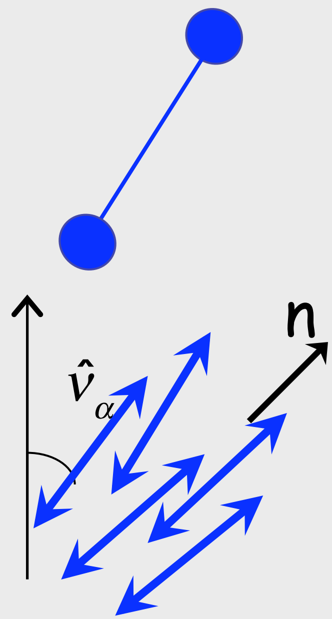
Outline

- Liquid crystals hydrodynamics
- Active hydrodynamic: active stresses, nematic vs polar order
- Generic instability of ordered states
- Confined active film: spontaneous flow

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

Apolar: melanocytes, rods



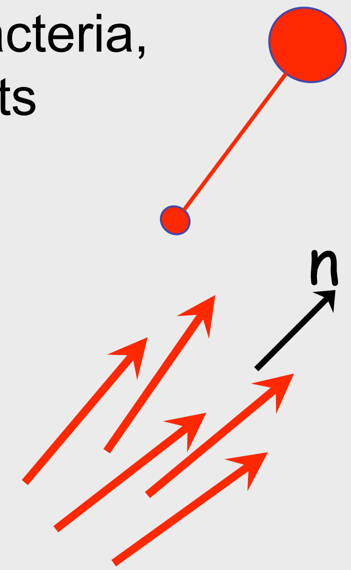
Apolar order: nematic

n=-n

Tensor order parameter: alignment

$$Q_{ij} = \left\langle \sum_\alpha \left(\hat{v}_{\alpha i} \hat{v}_{\alpha j} - \tfrac{1}{d} \delta_{ij} \right) \right\rangle = S(n_i n_j - \tfrac{1}{d} \delta_{ij})$$

Polar: fish, bacteria, motor-filaments



Polar order

n≠-n

Vector order parameter: polarization

$$\vec{P} = \left\langle \sum_\alpha \hat{v}_\alpha \right\rangle = P\ \vec{n}$$

Hydrodynamic eqs written in terms of director **n** in both cases, taking into account different symmetry

Liquid Crystals Hydrodynamics

Hydrodynamic fields

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

Nematic: symmetry n → -n

Polar: n ≠ -n

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

← Frank free energy

$$F_K = \frac{1}{2} \int_{\vec{r}} \left[K_1 (\nabla \cdot n)^2 + K_2 [n \cdot (\nabla \times n)]^2 + K_3 [n \times (\nabla \times n)]^2 + \underbrace{w(\nabla \cdot n)\delta\rho}_{\text{polar systems only}} \right]$$

Splay

Twist

Bend

single - elastic constant approx:

$$K_1 = K_2 = K_3 = K$$

Conservation Laws & Fluxes (nematic case)

$$\partial_t \rho = -\vec{\nabla} \cdot \vec{g}$$

$$\vec{g} = \rho \vec{\mathrm{v}}$$

$$\partial_t g_i = \partial_j \sigma_{ij}$$

$$\sigma_{ij} = \sigma_{ij}(\underbrace{\vec{\nabla}\vec{\mathrm{v}}, \vec{h}}_{\text{driving forces}})$$

(convective flux neglected)

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

$$\vec{h} = -\delta F / \delta \vec{n}$$

molecular field

single-elastic constant approx, 2d:

$$K_1 = K_2 = K, \quad K_3 = 0$$

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

- $\partial_t \rho = -\vec{\nabla} \cdot (\rho \vec{\mathrm{v}})$
- $\sigma_{ij} = 2\eta u_{ij} - p\delta_{ij} - \frac{\lambda}{2}(h_i n_j + h_j n_i) + \frac{1}{2}(h_i n_j - h_j n_i)$
- $\partial_t n_i + \vec{\mathrm{v}} \cdot \vec{\nabla} n_i + \omega_{ij} n_j = \delta^T_{ij}(\lambda u_{ij} n_j + \frac{1}{\gamma} h_i)$

$$u_{ij} = \tfrac{1}{2}(\partial_i \mathrm{v}_j + \partial_j \mathrm{v}_i)$$

$$\omega_{ij} = \tfrac{1}{2}(\partial_i \mathrm{v}_j - \partial_j \mathrm{v}_i)$$

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

Coupling of orientation and flow

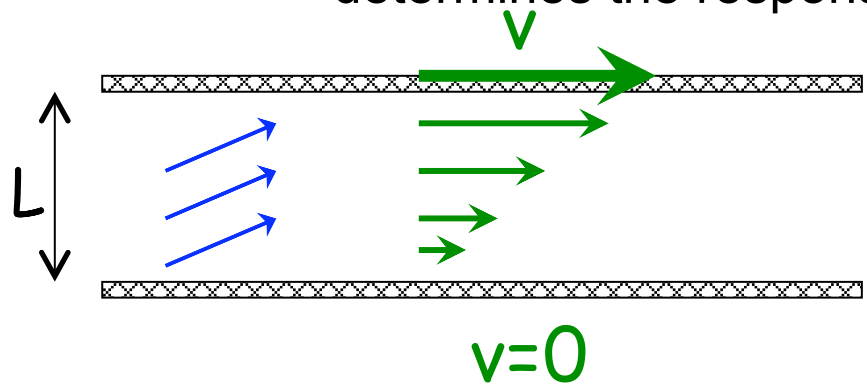
Flow alignment parameter λ depends on microscopic properties of nematogens: λ>0 rod-like molecules, λ<0 discotic molecules

Asymmetric part of stress tensor

torque exerted by orientational degrees of freedom on the flow

Flow alignment parameter λ

determines the response of the director to shear



Nematic film uniformly **sheared** between two plates

- no-slip boundary conditions

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

$$u_{xy} = \tfrac{1}{2}\partial_y \mathrm{v}_x = \mathrm{v}/2\mathrm{L}$$

Homogeneous state (away from boundaries):

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

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

$|\lambda|>1$ flow alignment

$|\lambda|<1$ flow tumbling: inhomogeneous rolls

Active Liquid Crystals

Three new ingredients:

1. Active LC can order in **nematic and polar states**
2. Activity yields an energy input on each particle that provides an **additional driving force**, not unlike a chemical potential

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

   •motor-filament mixtures: Δμ~ rate of ATP consumption

   •swimming bacteria: Δμ~ force exerted by swimmers on fluid

3. We need to develop a two-fluid model that incorporates the exchange of momentum between active particles and solvent

Active stress

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

$$\sigma_{ij}^{active} = \alpha\rho n_i n_j \qquad \text{nematic \& polar}$$

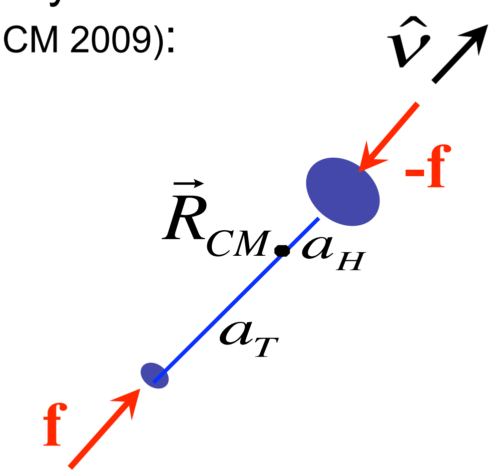
$$+\beta\rho\left(\partial_i n_j + \partial_j n_i\right) \qquad \text{polar only}$$

$$\alpha, \beta \sim \Delta\mu$$

Active particles (e.g., bacteria) extert a force dipole on the surrounding fluid. Active stress is the mean force density by active particles on a fluid element (Hatwalne et al, 2004; Baskaran & MCM 2009):

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

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

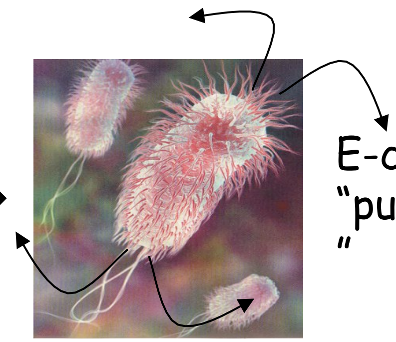


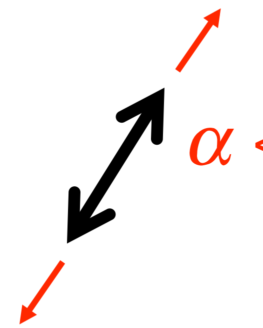
$\alpha > 0 \rightarrow$ *contractile / pullers*

$\alpha > 0 \rightarrow$ *tensile / pushers*

Contractile/tensile stresses

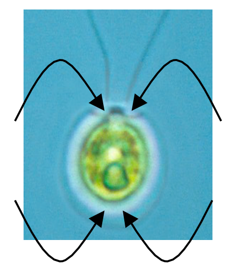
Most swimming bacteria push fluid out at the head and tail → **tensile** or pushers



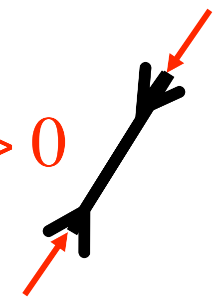


$\alpha < 0$

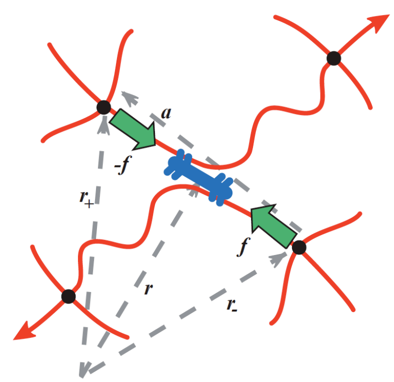
The algae chlamydomonas pull fluid in at the head and tail → **contractile** or puller
(but see Guasto et al, PRL 2010 indicating more complex flow field → Tom Powers' lecture)



$\alpha > 0$



Actin filaments crosslinked by myosins are **contractile**
(see F. MacKintosh's lectures)



$\alpha > 0$

Active Hydrodynamics: single incompressible fluid

incompressible $\rightarrow \rho = \text{constant}, \quad \vec{\nabla} \cdot \vec{\mathrm{v}}=0$

Re<<1 $\rightarrow$ Stokes aproximation $\partial_j \sigma_{ij} = 0$

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

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

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

“Generic” Instability of ordered states

Simha & Ramaswamy, PRL 2002

Small fluctuations about the quiescent ordered state (nematic, 2d)

$$\vec{v} = \vec{0} + \delta\vec{v}$$

$$\vec{n} = \vec{n}_0 + \delta\vec{n}_\perp \qquad \vec{n}_0 = \hat{x} \qquad \vec{n}_0 \cdot \delta\vec{n}_\perp \simeq 0 \rightarrow \delta\vec{n}_\perp = \delta n\ \hat{y}$$

$$v_i = \frac{i\alpha}{\nu q^2}\left[\delta_{ix} q_y + \delta_{iy} q_x\right]\delta n \sim \frac{1}{q} \qquad \nu = \eta / \rho$$

$$\partial_t \delta n = \lambda_- i q_y v_x + \lambda_+ i q_x v_y \qquad \lambda_\pm = \frac{\lambda \pm 1}{2}$$

For $|\lambda|<1$ unstable growth of bend fluctuations for pullers/tensile ($\alpha<0$) and of splay fluctuations for pushers/contractile ($\alpha>0$)

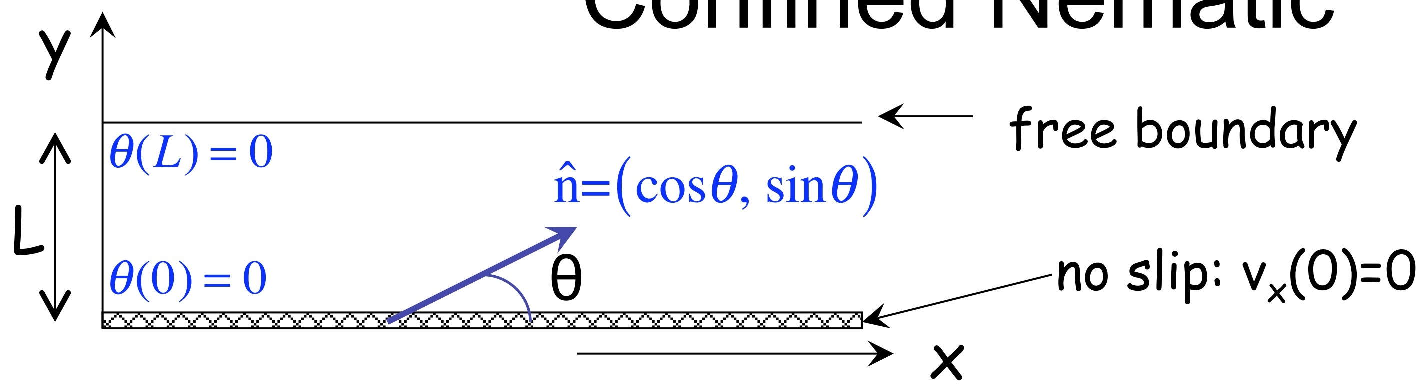
Suppressing the Generic Instability

The generic instability is intimately related to the ~$1/r^2$ behavior of the flow field generated by swimmers due to hydrodynamic interactions (Baskaran & MCM, PNAS 2009)

It can be suppressed by any mechanism capable of cutting off or screening this flow field, such as

- Boundaries
- Elastic or viscoelastic component of the medium response

Confined Nematic



Passive Nematic

$$\partial_t\theta = K\partial_y^2\theta - (1-\lambda\cos 2\theta)\partial_y \mathrm{v}_x$$

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

$\rho = \text{constant}$

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

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

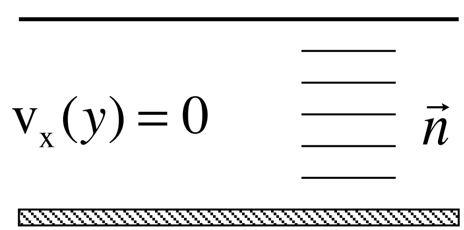
$\sigma_{xy}(0) = \sigma_{xy}(L) = 0$

$\rightarrow \sigma_{xy}(y) = 0$

Only solution is aligning and homogeneous

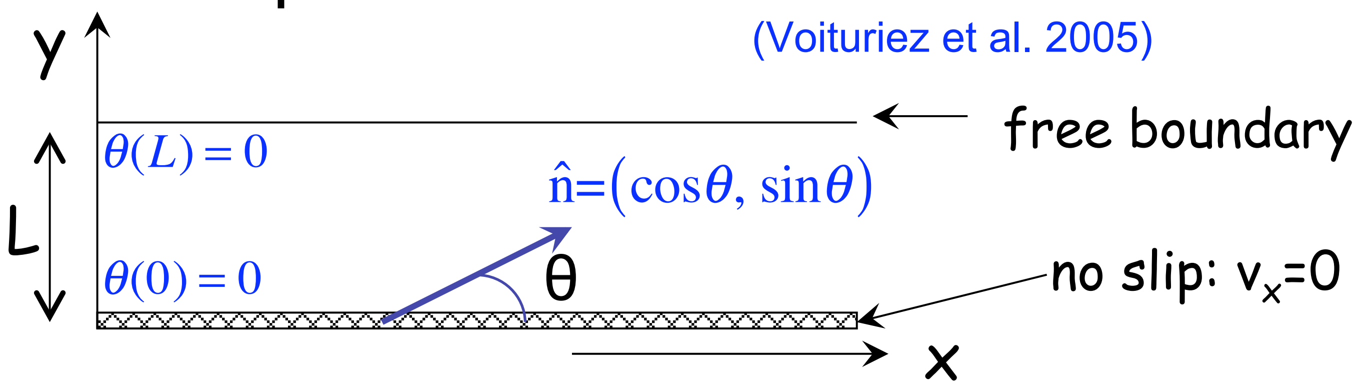
$\theta(y) = 0$ anchoring

$\mathrm{v}_x(y) = 0$ no flow



"Spontaneous flow" in confined active nematic

(Voituriez et al. 2005)



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

Active Nematic

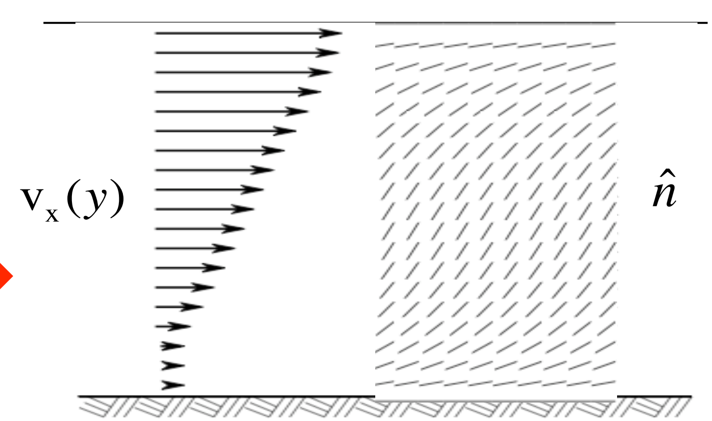
$$\left.\begin{aligned} \partial_t\theta &= K\partial_y^2\theta - (1-\lambda\cos 2\theta)\partial_y v_x \\ \sigma_{xy} &= \eta\partial_y v_x + K(1-\lambda\cos 2\theta)\partial_y^2\theta + \alpha\sin 2\theta \end{aligned}\right\} \rightarrow \partial_y^2\theta \simeq -\frac{1}{l_\alpha^2}\sin 2\theta$$

steady state

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

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

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



“Spontaneous flow” in polar active film

(Giomi, MCM & Liverpool, PRL 2008)

Variations in filament concentration cannot be neglected → two-fluid description needed

Hydrodynamics of active suspensions

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

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

"self-propulsion": only in polar systems

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

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

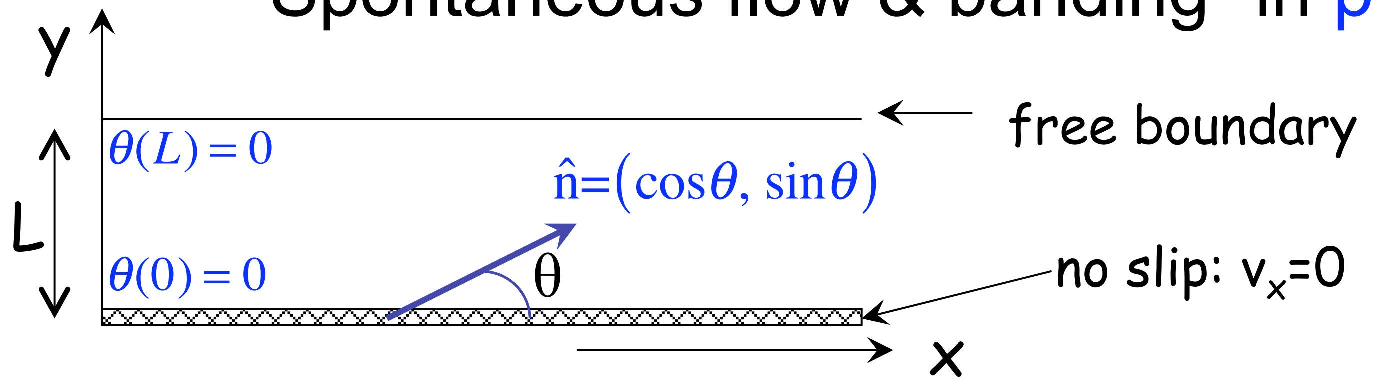
mechanical stresses

active contractile\tensile stresses in polar & nematic

active polar stresses

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

"Spontaneous flow & banding" in polar films



$\rho = \text{constant}$

$\sigma_{xy}(y) = 0$

$$\partial_y j_y = \partial_y(\beta n_y - D\, \partial_y c) = 0 \quad \rightarrow \quad \partial_y c = \beta \sin\theta / D$$

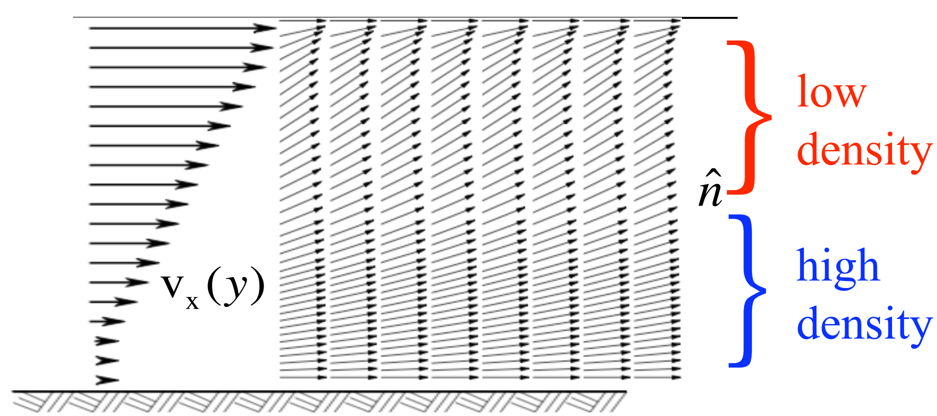
$$K\partial_y^2\theta = (1 - \lambda\cos 2\theta)\partial_y v_x$$

$$\sigma_{xy} = \eta\partial_y v_x + \alpha \sin 2\theta = 0$$

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

spontaneous flow & concentration bands

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



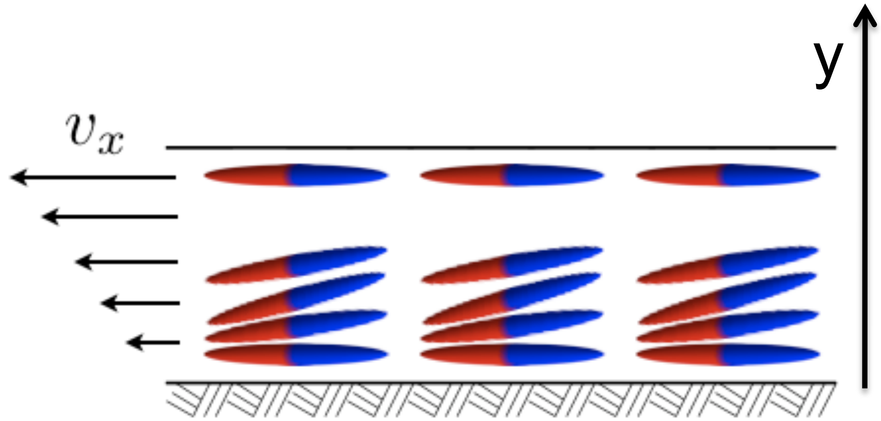
Spontaneous Flow in Active Polar Fluids

Giomi, MCM & Liverpool, PRL 2008

Active currents across the channel balanced by diffusion yield additional concentration gradients

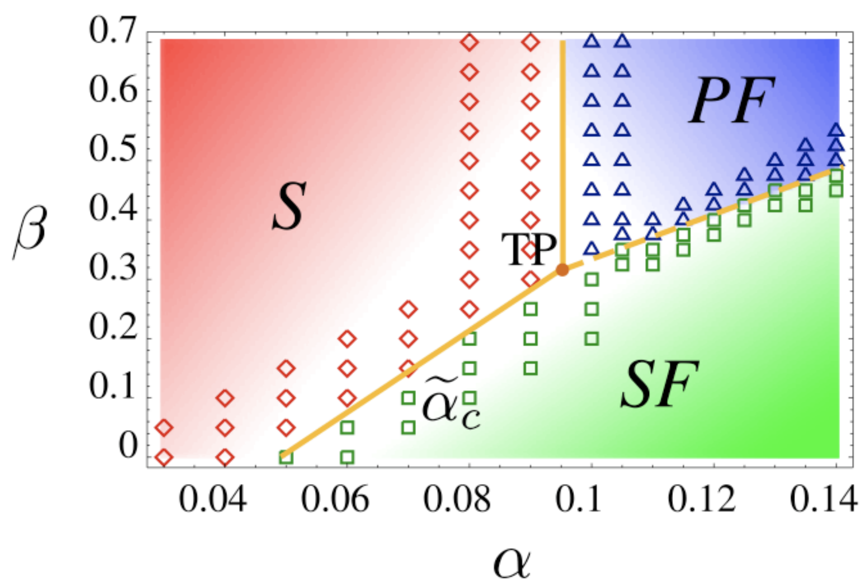
$$\partial_t c + \partial_y j_y = 0$$

$$\rightarrow \quad j_y = \beta c \sin\theta - D\partial_y c = 0$$



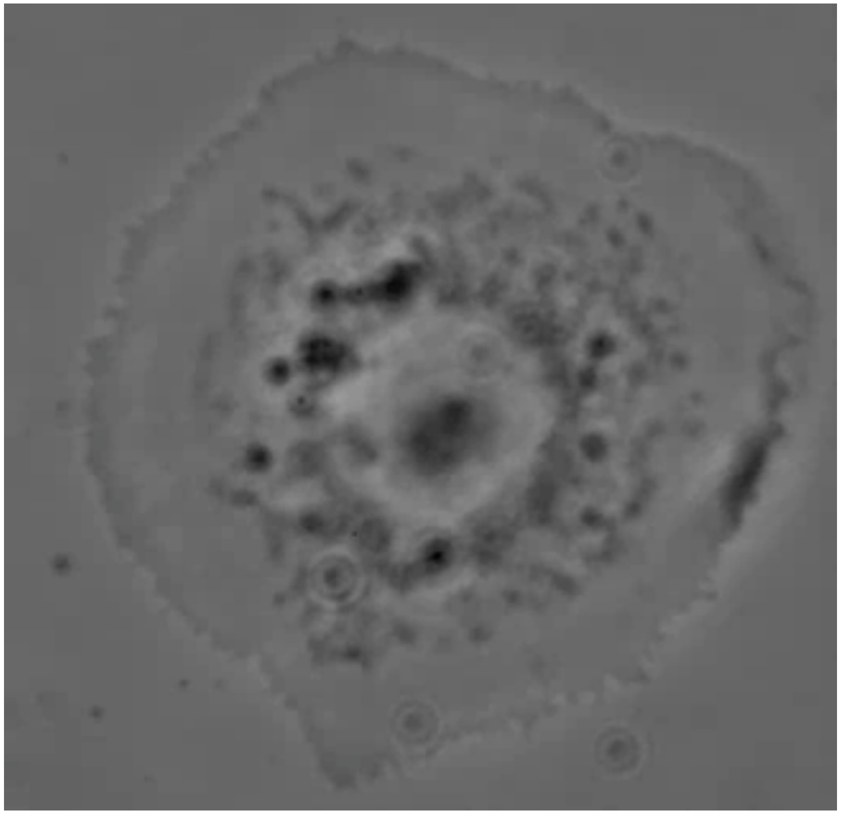
Steady Spontaneous Flow (SF) for $\alpha > \alpha_c(\beta)$

PF=Periodic or Oscillating Flow



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 β_c, as seen in experiments

β~ treadmilling rate

α~ myosin contractility

Lesson:

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