Continuum Theories of active liquid crystalline fluids

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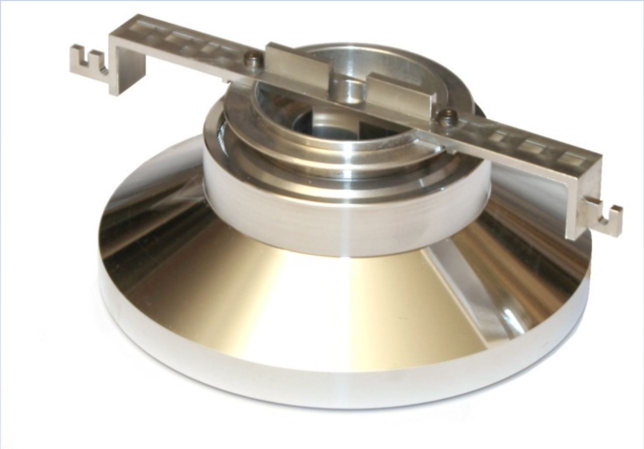
Scope of today's talk

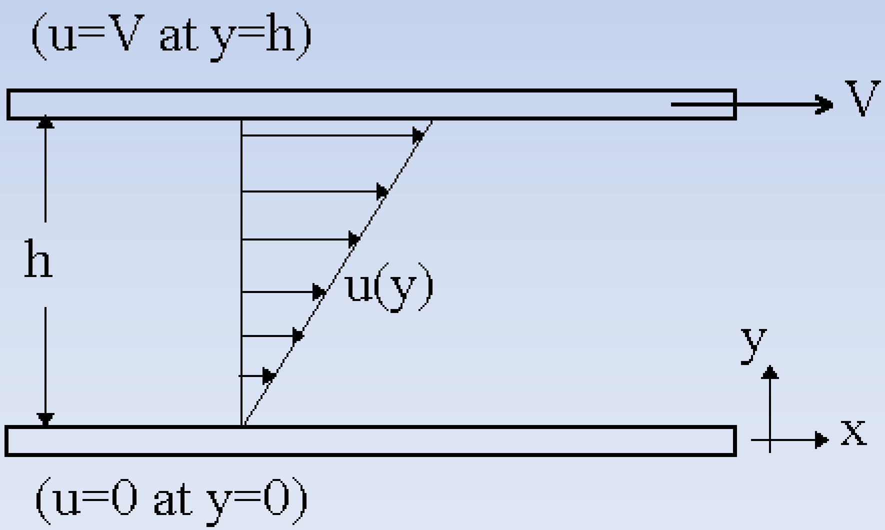
- **Pedagogical theory talk**
  –literature, experimental systems not detailed
- Active fluids: World view and context
- Story 1: active polar fluid (solitary waves)
- Story 2: active nematic fluid (defect ordered nematic)
- Things to be done, coming attractions….

Introduction and Context

Traditional non-equilibrium materials

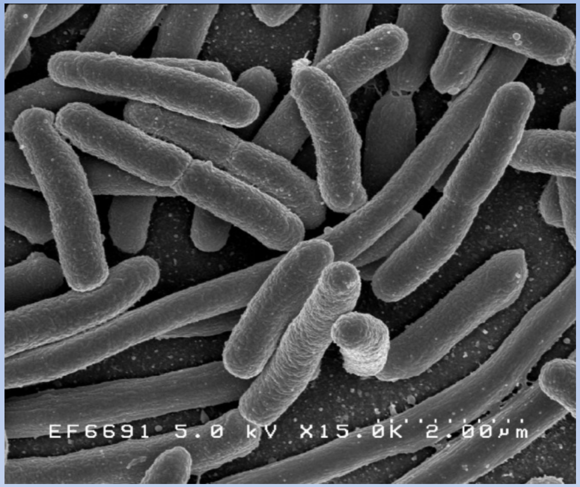
- Driven at the boundary : Macroscopic Drive
- Energy cascades down to the microscale – dissipation/temperature
- Thermodynamics gives me a theoretical handle on what happens

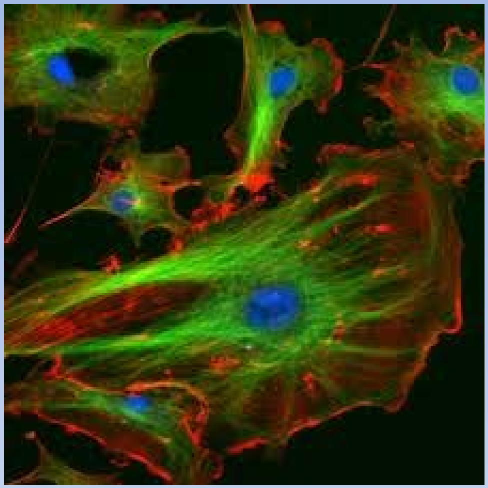




Introduction and Context

Active Materials

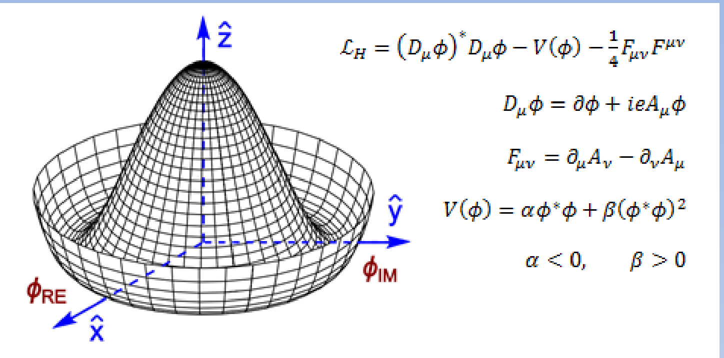




- Driven at the microscale
- Energy cascades up to the macroscale
- Rules of the game ? Design principles ?

Introduction and Context

Why should I care?



Interesting from a fundamental point of view :

- Liberation from the constraints of equilibrium

- Need to invent theory – Fluctuation-dissipation, regression etc out the window.

- New Physics : Long range order in 2D, Anamolous fluctuations, Novel instabilities and pattern formation,

Introduction and Context

Why should I care?

Interesting from a more real world point of view :

- Physical Scaffold of Biological Systems

- Properties dynamically changed by coupling to regulation

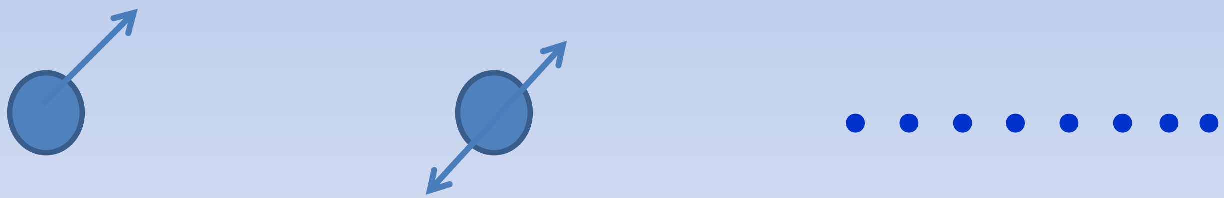
Introduction and Context

Theoretical paradigm-Symmetry and Hydrodynamics

- Prototype active fluid : Particles that consume fuel from environment and produce forces

- Classify fluids based on symmetry

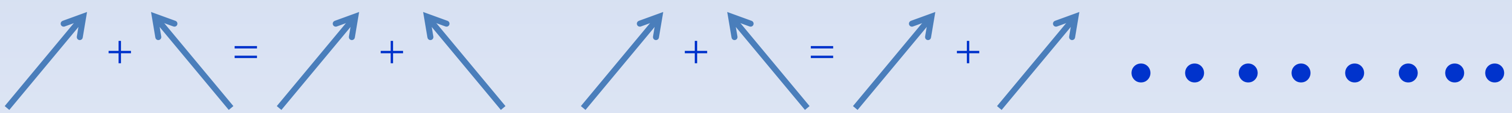
- Symmetry of activity



Polar

Dipolar/Nematic

- Symmetry of interactions

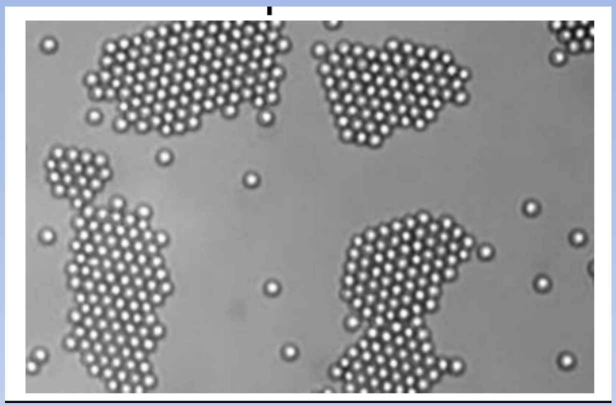


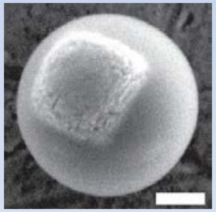
Don’t care/isotropic

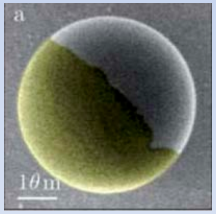
Polar

Introduction and Context

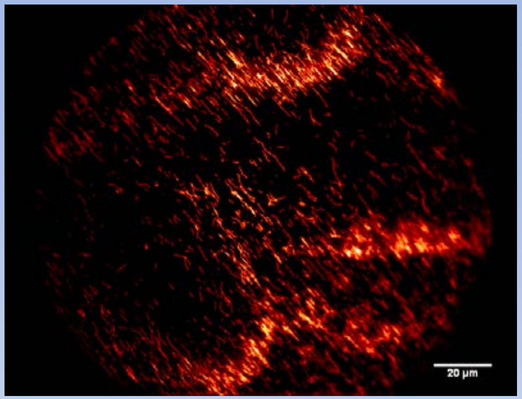
Examples

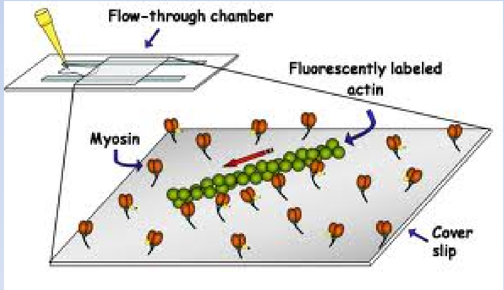




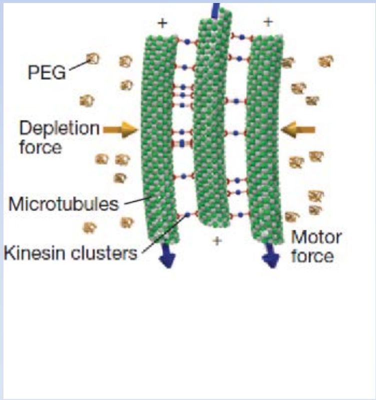


Polar drive
/isotropic interactions





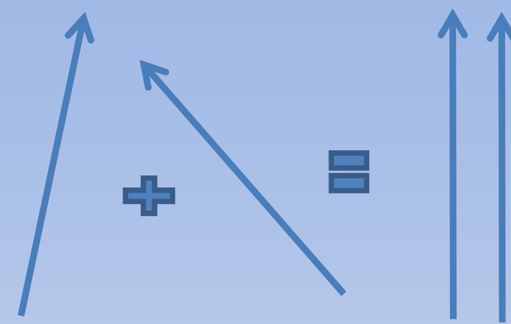
Polar drive
/Polar interactions



Nematic drive
/Nematic interactions

Story 1: Active Polar Fluid

- Polar activity and polar interactions
- Move through a medium – Force=velocity
- Macroscopic theory – Hydrodynamics



Dynamics of Conserved Quantities and Broken Symmetry Variables

Density of Particles

$$\rho\left(\mathbf{r},t\right)$$

Polarization (Velocity)

$$\mathbf{P}\left(\mathbf{r},t\right) \quad \left(w_0\mathbf{P} \right)$$

$$\partial_t\mathbf{P}+\lambda_1(\mathbf{P}\cdot\nabla\mathbf{P}) = -D_{\mathrm{R}}\left(a_2+P^2a_4\right)\mathbf{P} - w_0\nabla\rho + (D_s - D_b)\nabla(\nabla\cdot\mathbf{P})$$

$$+ D_b\nabla^2\mathbf{P} + \lambda_2\mathbf{P}(\nabla\cdot\mathbf{P}) + \frac{\lambda_3}{2}\nabla P^2$$

Toner and Tu 1995

Active Polar Fluid

- Start with an equilibrium polar fluid

$$\partial_t \mathbf{P} = -\frac{\delta F}{\delta \mathbf{P}}$$

- Gradient descent dynamics on some free energy landscape

- Under some imposed inhomogeneous flow

$$\partial_t \mathbf{P} + \lambda_1 (\mathbf{P}\cdot\nabla\mathbf{P}) = \ldots D_b)\nabla(\nabla\cdot\mathbf{P})$$

$$\partial_t \mathbf{P} + \mathbf{u}\cdot\nabla\mathbf{P} + \boldsymbol{\omega}\times\boldsymbol{P} + \overleftrightarrow{E}\cdot\mathbf{P} = -\frac{\delta F}{\delta \mathbf{P}}$$

- Active fluid has self generated flow

$$\mathbf{u} = \mu_T \mathbf{F}_{act} = \lambda\mathbf{P}$$

$$\boldsymbol{\omega} = \mu_R \boldsymbol{\tau}_{act} = \lambda'\nabla\times\mathbf{P}$$

$$\overleftrightarrow{E} \sim \mu_S \nabla\mathbf{F}_{act} \sim \nabla\mathbf{P}$$

Story 1: Active Polar Fluid

- Extensively studied equation that has rich phenomenology

Toner PRL 1995, Bertin PRE 2006, J.Phys A 2009, Solon PRL 2012 …many many others,

- Applicable to self propelled particle systems with "Vicsek" like interactions – Actin filament motility assay, quinke rotors, chemotactic bacteria, self-propelled rods….

- Focus on one particular phenomenon – solitary waves

Story 1: Active Polar Fluid

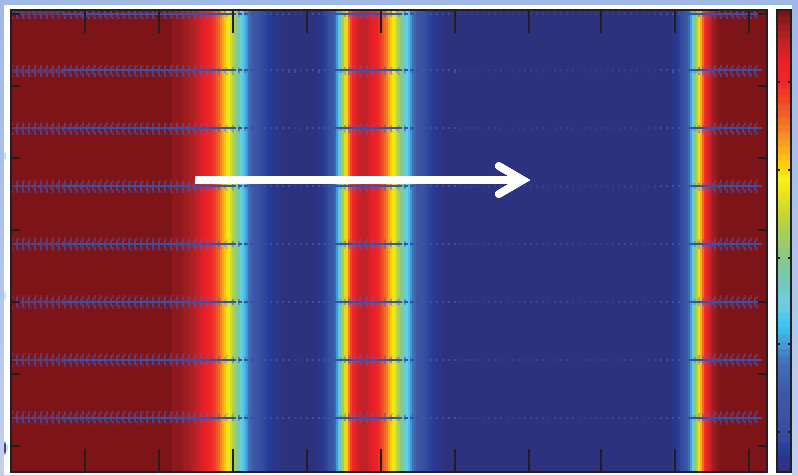
$$\partial_t \rho = -\underline{\nabla \cdot (w_0 \rho \mathbf{P}} - D\nabla \rho)$$

$$\partial_t \mathbf{P} + \qquad = -\underline{D_{\mathrm{R}} \left(a_2 + P^2 a_4\right)} \mathbf{P} -$$

Low density a2 >0 and P = 0

High density a2<0 and P $= \sqrt{\dfrac{-a_2(\rho)}{a_4(\rho)}}$

Story 1: Active Polar Fluid



$$\partial_t \rho = -\nabla \cdot w_0 \rho \mathbf{P}$$

$$\partial_t \rho \mathbf{P} = \qquad - w_0 \nabla \rho$$

Stripe Phase

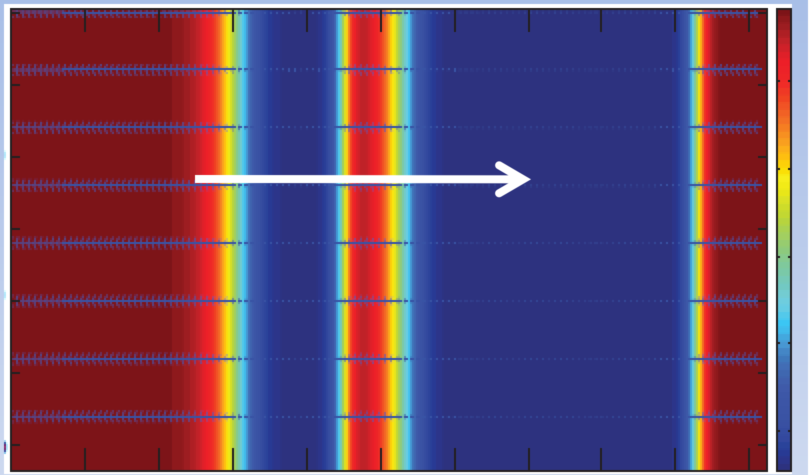
- Not a pattern but rather solitonic wave trains

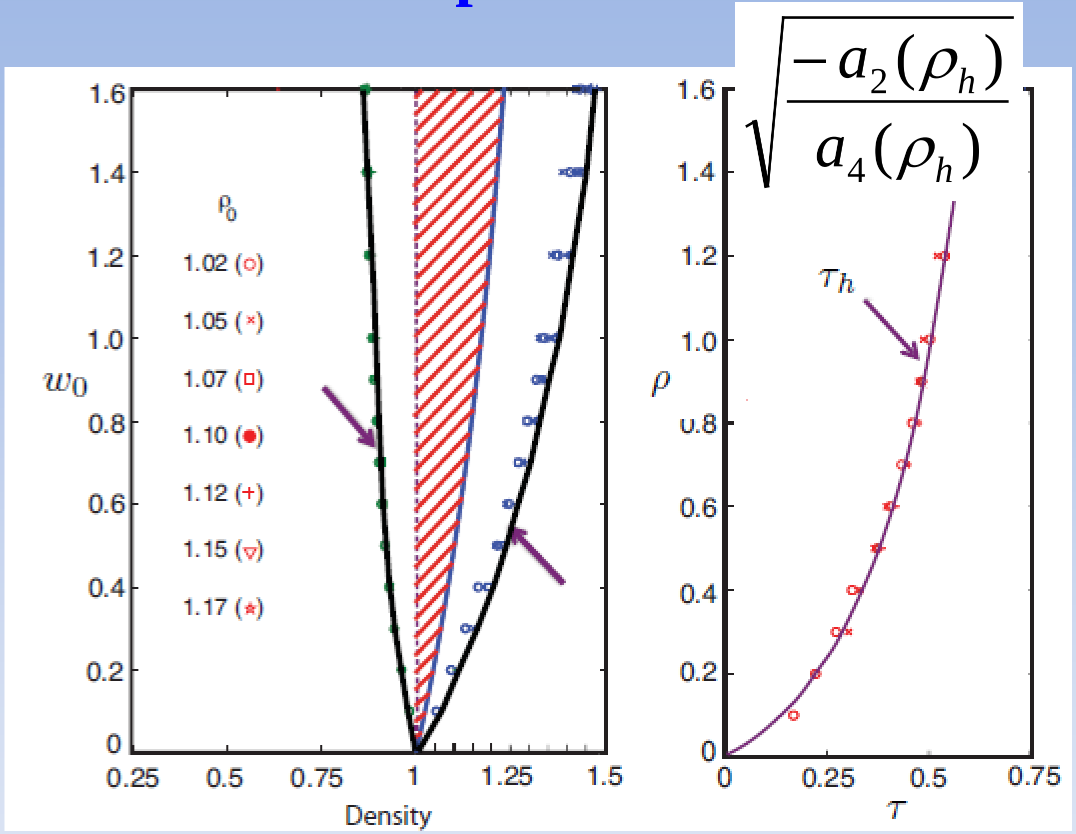
- Initial conditions determine widths/number of stripes

Recent work along these lines: Solon PRL 2014

Story 1: Active Polar Fluid

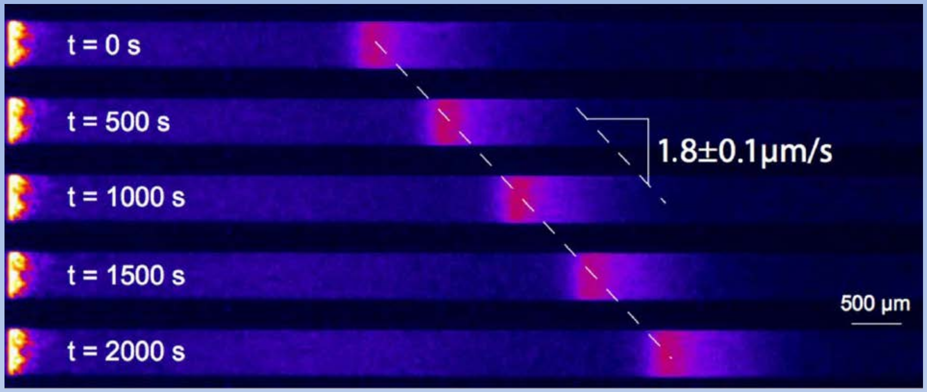
Stripe Phase

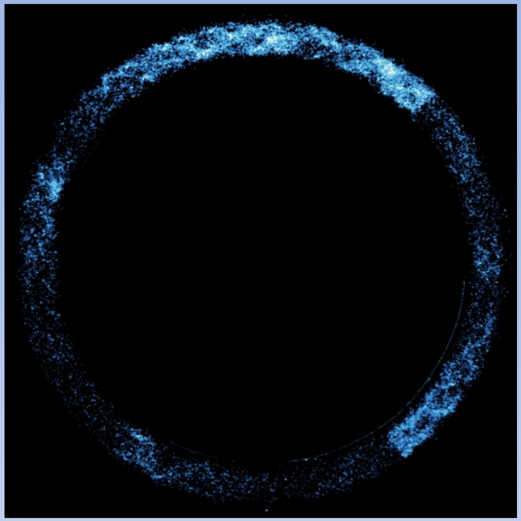


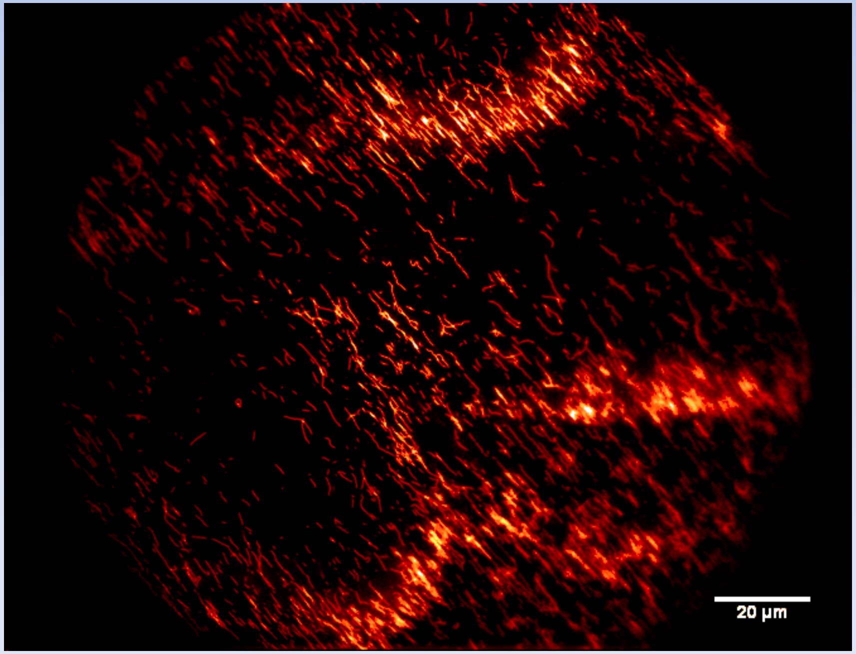


NB : Not a complete story, works only close to the critical point

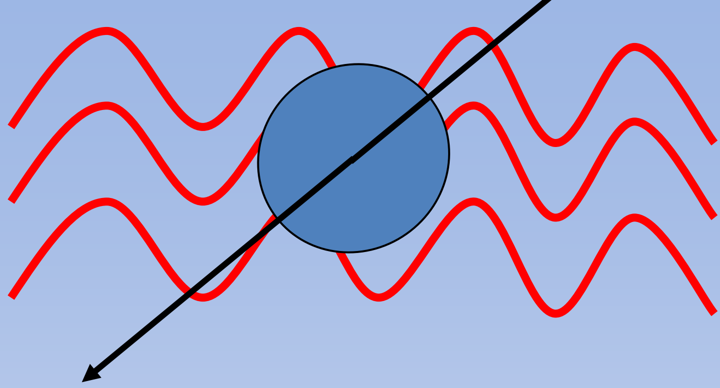
Story 1: Active Polar Fluid

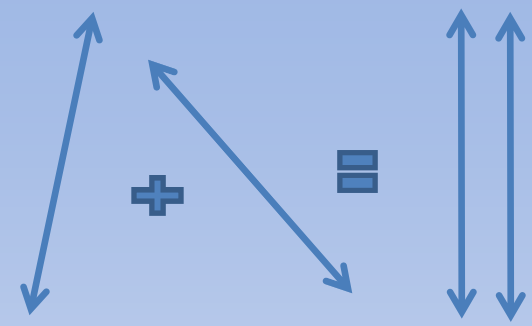






Story 2 : Active Nematic Fluid





Dynamics of Conserved Quantities and Broken Symmetry Variables

Density of Particles

$$\rho\left(\mathbf{r},t\right)$$

Nematic Order Parameter

$$Q_{\alpha\beta}\left(\mathbf{r},t\right)=\left\langle \hat{u}_{\alpha}\hat{u}_{\beta}-\frac{1}{2}\delta_{\alpha\beta}\right\rangle$$

Story 2 : Active Nematic Fluid

- Start with an equilibrium nematic fluid

$$\partial_t Q_{\alpha\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}}$$

- Gradient descent dynamics on some free energy landscape

$$\partial_t Q_{\alpha\beta} + \mathbf{u} \cdot \nabla Q_{\alpha\beta} + \Omega_{\alpha\gamma} Q_{\gamma\beta} - Q_{\alpha\gamma}\Omega_{\gamma\beta} + E_{\alpha\gamma}Q_{\gamma\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}}$$

$$\Omega_{\alpha\beta} = \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\omega_\gamma$$

- Active fluid has self generated flow

$$\mathbf{u} = \mu_T \mathbf{F}_{act} = \lambda_C \nabla \cdot \overleftrightarrow{Q}$$

$$\boldsymbol{\omega} = \mu_R \boldsymbol{\tau}_{act} = \lambda_R \nabla \times \nabla \cdot \overleftrightarrow{Q}$$

$$E_{\alpha\beta} \propto \mu_E \lambda \partial_\gamma F_\beta$$

Story 2 : Active Nematic Fluid

- The dynamical equation of interest

$$\partial_t Q_{ij} = -\gamma \frac{\delta F}{\delta Q} + \frac{\lambda_C}{\rho}[\partial_k Q_{kl}]\partial_l Q_{ij}$$

$$-\frac{\lambda_R}{2\rho}\left(Q_{ik}\partial_k\partial_l Q_{jl} - Q_{ik}\partial_j\partial_l Q_{kl} - Q_{kj}\partial_i\partial_l Q_{kl} + Q_{kj}\partial_k\partial_l Q_{il}\right)$$

- Need dynamics for the density

Active Convection

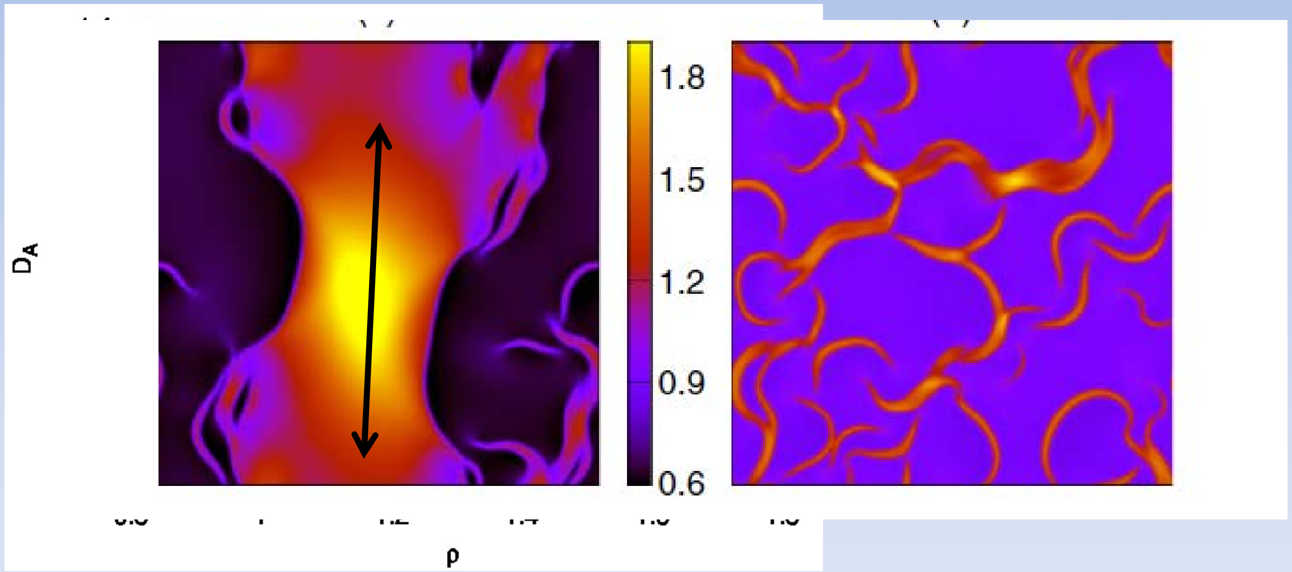
Active

$$\partial_t \rho = D\nabla^2\rho + D_Q \nabla\nabla : \mathbf{Q}$$

Active Convection

Story 2 : Active Nematic Fluid

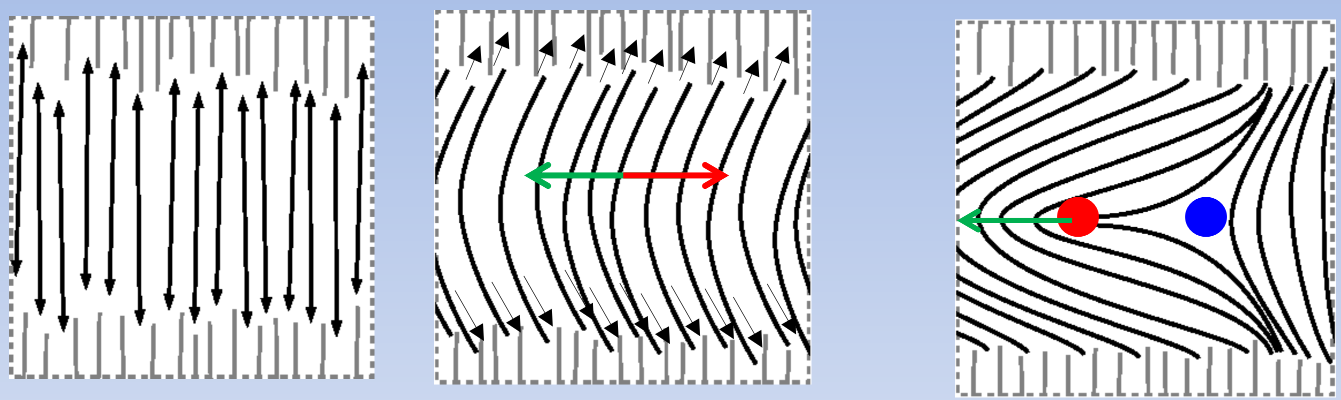
- Close to the critical density – “similar phenomenology”
    - Symmetry does not allow for propagating waves
    - Instead you get bands of nematic high density regions



Recent work : Ngo PRL 2014 Bertin New J.Phys 2013…

Story 2 : Active Nematic Fluid

- What happens to the homogeneous nematic state at high densities?



- Onset controlled by the active torque

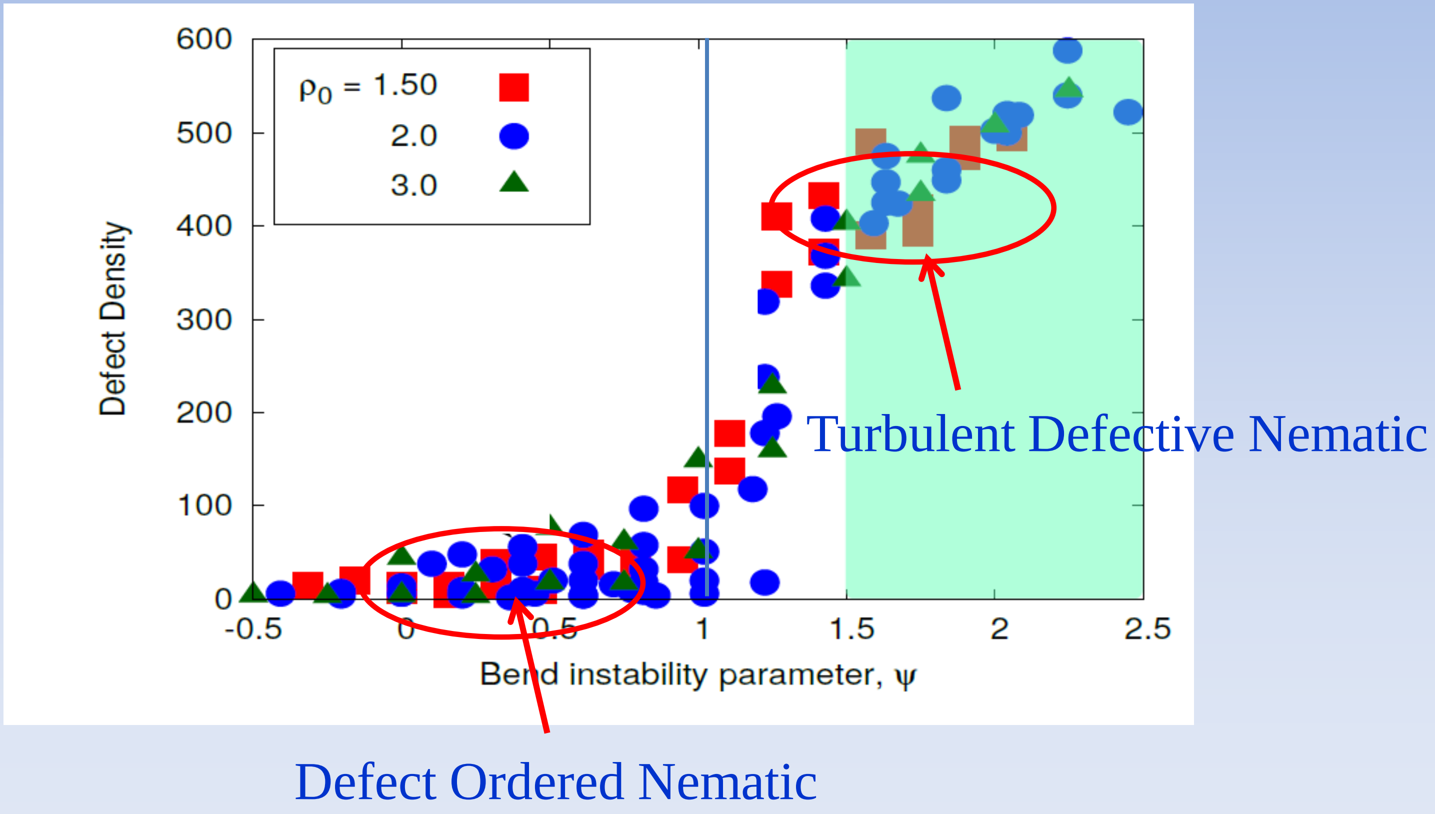
$$\psi = \frac{\lambda_R - 2D_\delta}{D_E \cdot f(\rho_0)} > 1$$

Active torque - (bend-splay)

Goes to zero at the critical point

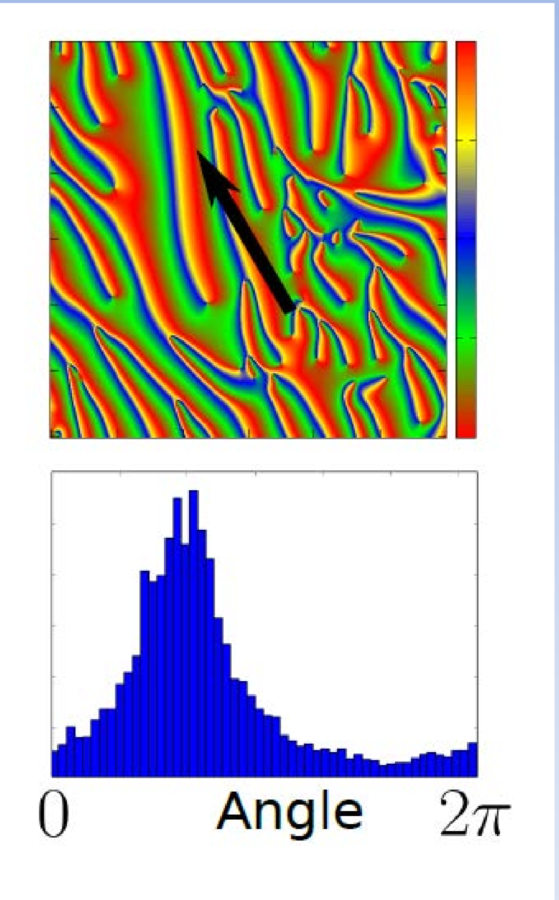
Story 2 : Active Nematic Fluid

- What happens to Random Initial Conditions?
- Initialize in an isotropic state and integrate the equations



Story 2 : Active Nematic Fluid

- Defect Ordered Nematic

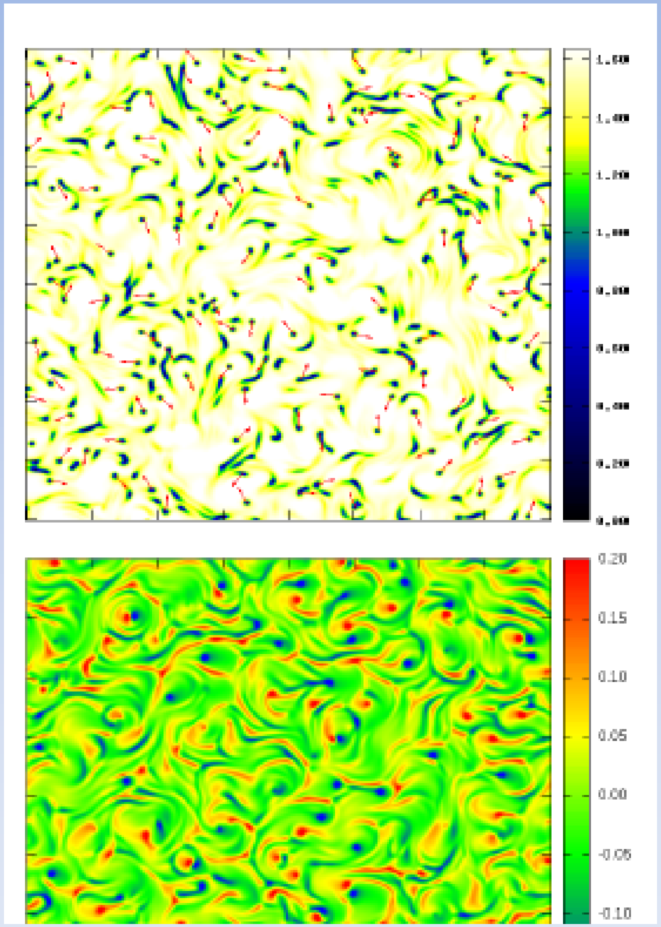


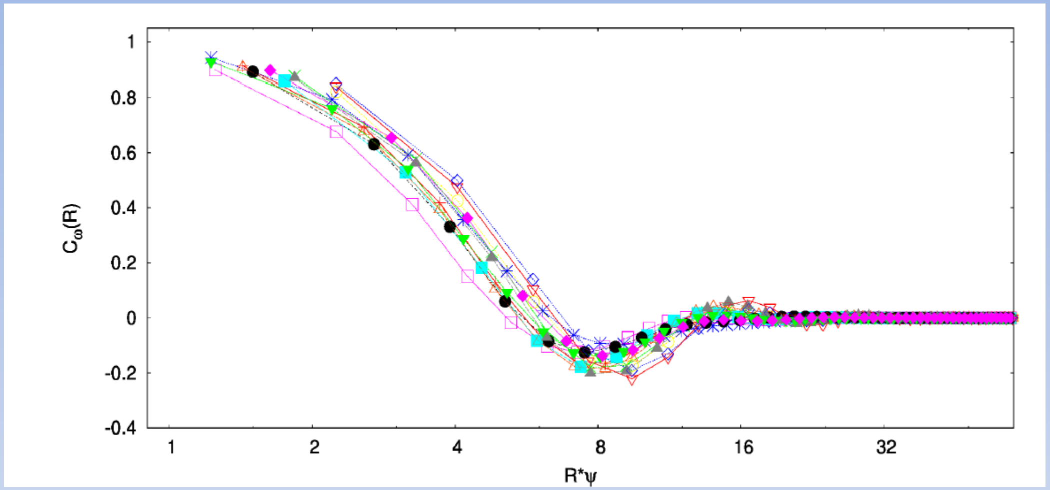
Movie 1

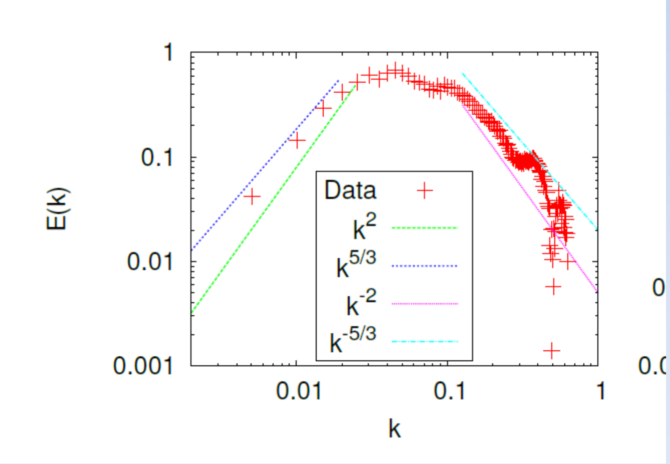
Movie 2

Story 2 : Active Nematic Fluid

- Turbulent Defective nematic

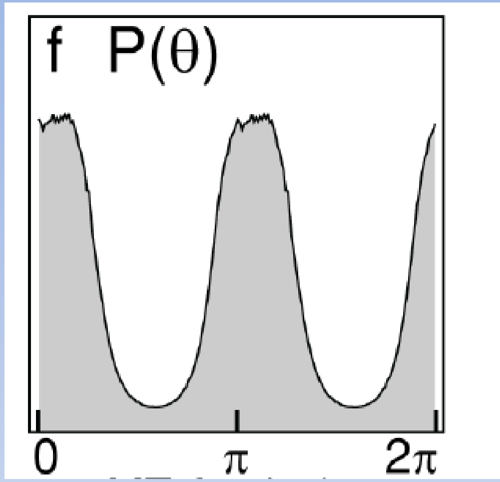






Coming Attractions/Weird things that real systems do

- The defect order in the experimental system is nematic



- Confinement does weird things : Movie

Summary

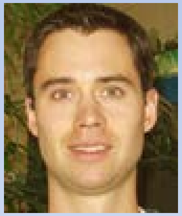
- Active fluids sorted by symmetry
- Two stories
- Solitary waves in polar systems
- Defective states in nematic systems
- More things to understand than understood

Students

Elias Putzig

Gabe Redner

Collaborators



Mike Hagan

Arvind Baskaran

Cristina Marchetti

Gopinath et al PRE 2012

Baskaran et al EPJE 2012

Putzig et al Phys Rev E 2014

DeCamp et al Nature Materials 2015

Putzig et al arXiv:1506.03501

Active Nematic Fluid – Context

Active nematic suspension

$$\partial_t Q_{\alpha\beta} + \mathbf{u}\cdot\nabla Q_{\alpha\beta} + \Omega_{\alpha\gamma}Q_{\gamma\beta} - Q_{\alpha\gamma}\Omega_{\gamma\beta} + E_{\alpha\gamma}Q_{\gamma\beta} = -\frac{\delta F}{\delta Q_{\alpha\beta}}$$

$$\nabla^2 \mathbf{u} = \nabla\cdot\sigma^{act}$$

$$\sigma_{ij}^{act} = \alpha Q_{ij}$$

$$\nabla^2 \mathbf{u} + \zeta\mathbf{u} = \nabla\cdot\sigma^{act}$$

- Same director dynamics
- Stokes equation
- Same active stress
- Screening/damping
- Same theory with $\lambda_C = \lambda_R$

Many experts in the audience : Marchetti et al, Yeomans et al…

Active Nematic Fluid – Context

Dry Active nematic

$$\partial_t Q_{ij} = -\left(\alpha + \beta Tr\left(Q^2\right)\right) Q_{ij} + \nabla^2 Q_{ij} + \partial_i \partial_j \rho$$

$$\partial_t \rho = \nabla^2 \rho + \partial_i \partial_j Q_{ij}$$

- This theory with
  $\lambda_C = \lambda_R = 0$
  $D_\delta = 0$
- Valid close to critical density
- Phase separation, chaos giant number fluctuations
- Unchanged here

Many experts in the audience : Ramaswamy et al, Toner et al, Bertin et al, Aranson et al
Shi et al, Chate et al…