Hydrodynamics of Active Nematic Fluids

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Supported by the NSF
Brandeis MRSEC
(NSF-DMR 0820492)

Introduction

Active materials are a new class of soft material maintained out of equilibrium by internal energy sources. There are many example in biological contexts, including bacterial colonies, purified extracts of cystoskeletal filaments and motor proteins and the cell cytoskeleton. The key property that distinguishes active matter from more familiar non-equilibrium systems, such as fluid under shear, is that the energy input that maintains the system out of equilibrium comes from each constituent, rather than from the boundaries. Each active particle consumes and dissipates energy going through a cycle that fuels internal changes, generally (but not necessarily) leading to collective motion.

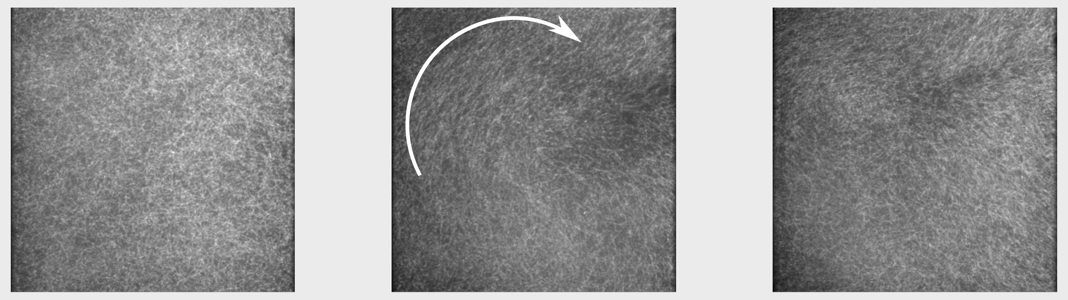
Active suspensions can exist in various liquid crystalline states. Apolar particles are fore-aft symmetric and can form nematic phases, characterized by a macroscopic axis of mean orientation identified by a unit vector $\mathbf{n}$ (the director field) and the global symmetry $\mathbf{n} \to -\mathbf{n}$.

Motivations

This work is motivated by the experimental work currently carried on in the Dogic Lab on active suspensions of microtubules and kinesin.

Microtubules are one of the essential building block of the cytoskeleton of eukaryotic cells. Being the most rigid filaments in the cytoskeleton, they are responsible for the elasticity and the structural integrity of the whole cell. Microtubules are polymers composed of α- and β-tubulin dimers. These dimers polymerize in protofilaments which then bundle in hollow cylindrical filaments of 25 nm in diameters and 100 nm to 10 μm in length.

Kinesin is a molecular motor. It is powered by the ATP hydrolysis and can "walk" along the external wall of a microtubule and serve in a variety of cellular functions, including mitosis and the transport of cargos inside the cell. As other motor proteins, kinesin is composed of a motor-head, where the ATP cycle takes place, and a long tail that bind to cargos or other kinesins. The head has two binding-sites: one for the microtubule and the other for ATP. ATP binding and hydrolysis as well as the release of ADP produces a conformational change of the microtubule-binding domain that results in a motion of the kinesin.



(a) (b) (c)

Confined solution of length-stabilized microtubles and kinesin. (a) The system appears isotropic, but the different shades of grey reveal small concentration gradients. (b) In this snapshot the fluid is rapidly moving. There is a net vorticity in the system with a current that rotates clockwise (here highlited with a white arrow). (c) After the motion the fluid recovers a temporary state of rest. Courtesy of Tim Sanchez (Dogic Lab).

Methods

Active filaments are modeled as rigid rods crosslinked by two-headed motor clusters that can exert forces on the filaments by converting the chemical energy of the ATP hydrolysis into mechanical work. Their dynamics is investigated in the framework of a phenomenological hydrodynamic theory. The theory is constructed to account for:

- Macroscopic density variations.
- Non-homogeneous orientational order.
- Hydrodynamic coupling between local orientations and flow.

Hydrodynamic variables

- Filaments concentration: c
- Flow velocity: $\mathbf{v} = (v_x,\, v_y)$
- Nematic tensor: $Q_{ij} = S(n_i n_j - \frac{1}{2}\delta_{ij})$

Density Equation

We consider a concentration c of active particles in a solvent. The fluid is incompressible, thus the total density is constant:

$$\rho = \rho_{\text{solvent}} + Mc = \text{constant}$$

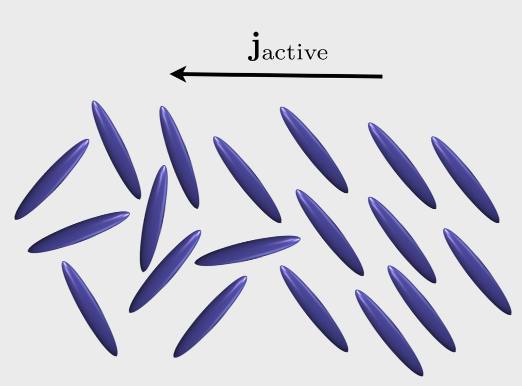
Concentration equation:

anisotropic diffusion

$$[\partial_t + \mathbf{v}\cdot\nabla]c = \nabla\cdot[(D_1\boldsymbol{\delta} + D_2\mathbf{Q})\nabla c + \alpha_1 c\,\nabla\cdot\mathbf{Q}]$$

advection — active currents

Like diffusive currents are driven by spatial variations in the concentration, active currents in a nematic fluid are driven by variations in the alignment.



$$\mathbf{j}_{\text{active}} \sim c\,\nabla\cdot\mathbf{Q}$$

Methods

Nematic Tensor Equation

The dynamics of the nematic tensor consists of two processes: a relaxation toward the equilibrium configuration and the coupling with the macroscopic flow. The later is associated with the fact that, due to their elongated shape, particles can rotate in a shear-flow.

coupling orientation/flow

$$[\partial_t + \mathbf{v}\cdot\nabla]Q_{ij} = \lambda u_{ij} + Q_{ik}\omega_{kj} - \omega_{ik}Q_{kj} + \gamma^{-1}H_{ij}$$

advection — relaxational dynamics

Strain-rate and vorticity:

$$u_{ij} = \tfrac{1}{2}(\partial_i v_j + \partial_j v_i) \qquad \omega_{ij} = \tfrac{1}{2}(\partial_i v_j - \partial_j v_i)$$

Molecular tensor:

Frank elasticity

$$H_{ij} = -\frac{\delta F}{\delta Q_{ij}} = -[A(c) + \tfrac{1}{2}B(c)S^2]Q_{ij} + L\nabla^2 Q_{ij}$$

isotropic/nematic transition (Landau-de Gennes)

Flow-velocity equation

liquid crystalline elasticity

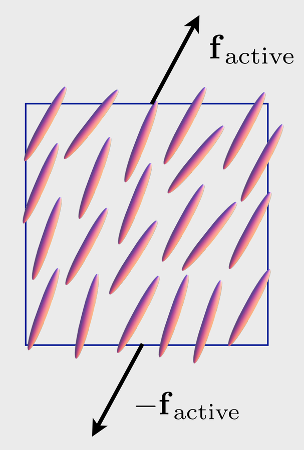
$$\rho[\partial_t + \mathbf{v}\cdot\nabla]\mathbf{v} = \eta\nabla^2\mathbf{v} - \nabla p + \nabla\cdot(\boldsymbol{\sigma}_{\text{elastic}} + \boldsymbol{\sigma}_{\text{active}})$$

Navier-Stokes — active forces

Elastic stress:

$$\boldsymbol{\sigma}_{\text{elastic}} = -\lambda\mathbf{H} + \mathbf{QH} - \mathbf{HQ}$$

Active stress:



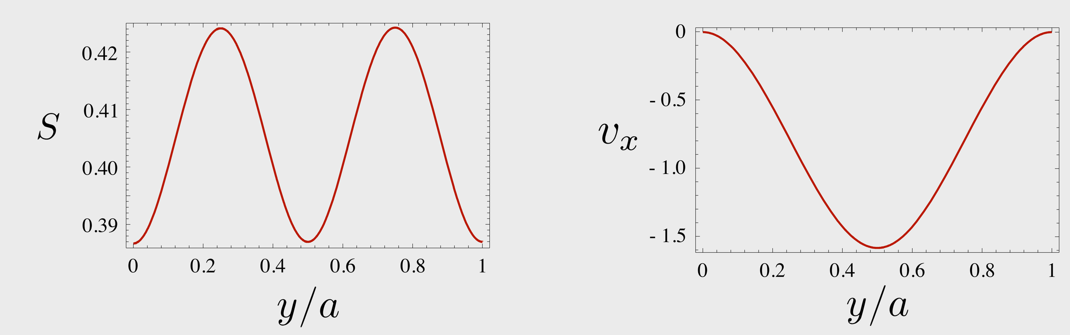
Each active particle exerts a force on the solvent with a resulting tensile/contractile stress:

$$\boldsymbol{\sigma}_{\text{active}} \sim \alpha_2\mathbf{Q}$$

Results

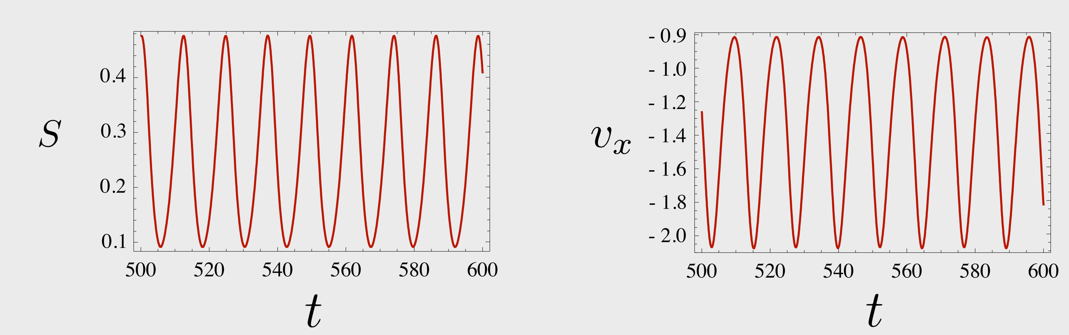
Spontaneous and Oscillatory Flow in *quasi*-1D

Active nematic fluid in an infinitely long 2D channel with no-slipping walls. At large active stresses the system undergoes a transition to a state of non-uniform orientation and spontaneous flow.



Nematic order parameter (left) and longitudinal velocity (right) across the channel. For intermediate values of the activity parameter $\alpha = \alpha_1 = \alpha_2$, the system undergoes a transition from a stationary homogeneous state, to a state of non-uniform nematic order and flow.

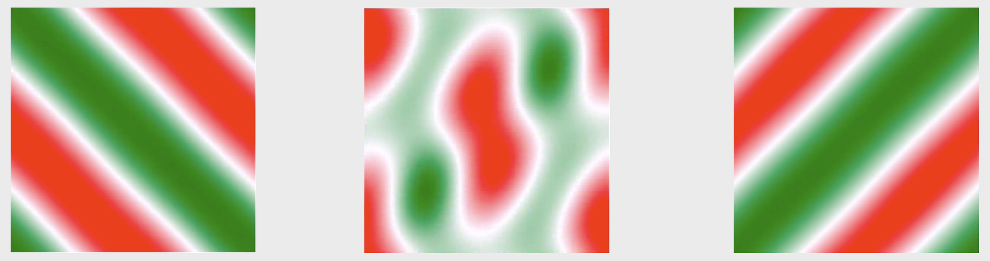
At even larger activities, the former state becomes unstable to an oscillatory flow.



Nematic order parameter (left) and longitudinal velocity (right) as a function of time in the oscillatory regime.

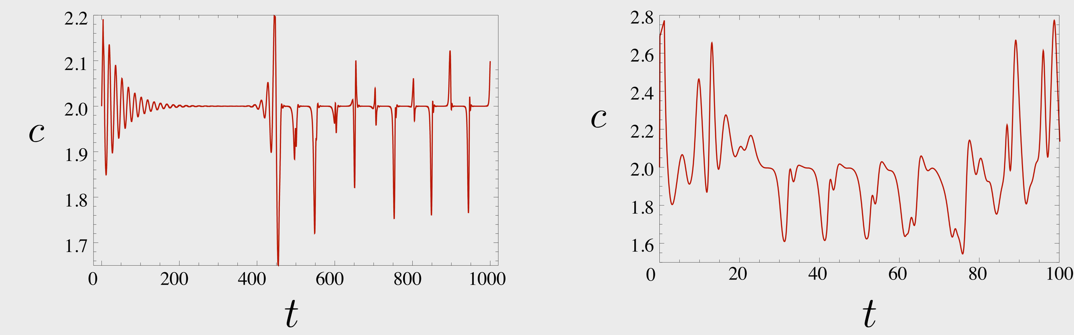
Intermittency and Chaos in 2D

At low activities the fluid is homogeneous. The nematic order parameter is constant throughout the system and the director field uniform.



Concentration of the active nematogens in the intermittent regime. The colors green/red denotes region of high/low concentration. The system consists of a square box with periodic boundary. The hydrodynamic equations are integrated numerically through a finite-difference scheme.

Upon raising the activity the system undergoes a transition to a chaotic regime. The route to chaos appears to take place via an "on-off" intermittency.



Concentration of the active nematogens in the center of the box. For intermediate values of the activity parameter $\alpha = \alpha_1 = \alpha_2$ (left), the fluid exhibit an "on-off" intermittent dynamics consisting of periods of laminar flow separated by chaotic "bursts". Upon increasing the activity (right) the dynamics becomes completely chaotic.