Ericksen–Leslie and Q-tensor models of spontaneous flow transitions in active nematic liquid crystals

Josh Walton
Supervised by Prof. Nigel Mottram and Dr Geoff McKay

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University of Strathclyde
Department of Mathematics and Statistics

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Pioneering research and skills

Outline

From nematic to active nematic liquid crystals

Continuum modelling of active nematics

Geometry and the Ericksen-Leslie equations

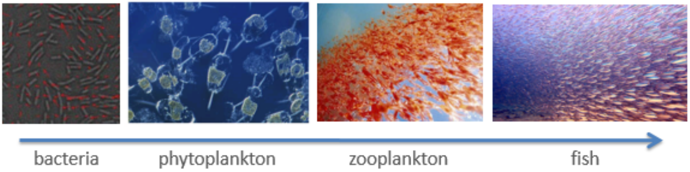
Spontaneous flow transitions due to activity

Conclusions

From isotropic fluids to (active) nematic liquid crystals

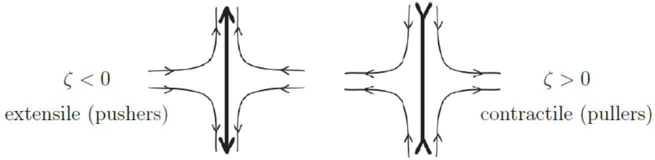
- **Isotropic fluids** flow through external influences (i.e. shear, pressure, gravity). Such fluids are governed by the **Navier-Stokes equations**.
- **Nematic liquid crystals** induce flow, but only when out of equilibrium (i.e. backflow and kickback in a **Freedericksz transition**). Such fluids are governed by the **Ericksen-Leslie equations**.
- **Active nematic liquid crystals** (ANLC) consist of objects (i.e. living organisms not molecules) which form a nematic phase and also have the ability to continuously produce and expend energy internally.

This normally means they can generate forces on each other as well as the surrounding fluid and hence induce flow.



Continuum modelling of active nematics

- Continuum hydrodynamic models based on liquid crystal theory have been used to describe dynamic self-organising systems such as bacterial swarms.
- The velocity at a point in space is taken to be the average velocity of a large number of swimmers.
- We think of the “swimming” organisms as either **pushers** or **pullers**. We only consider flow aligning organisms.



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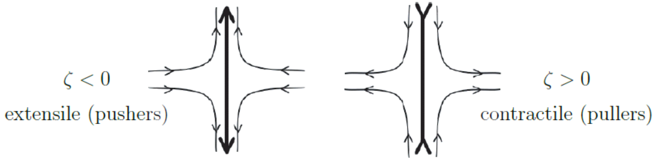
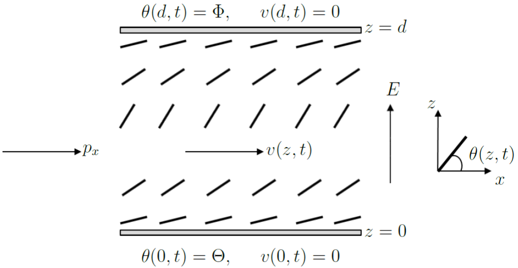


- One model uses the **Ericksen-Leslie theory** with an extra active stress term σ_{ij}^{ζ} where the activity "strength" is governed by ζ.

$$\boxed{\sigma_{ij}^{\zeta} = \zeta n_i n_j.}$$

Geometry and the Ericksen-Leslie equations



The Ericksen-Leslie equations for this set-up are (in the absence of fluid inertia, pressure gradient and an electric field)

$$\gamma_1\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3-K_1)\sin\theta\cos\theta(\theta_z)^2 - m(\theta)v_z,$$
$$0 = (g(\theta)v_z + m(\theta)\theta_t + \zeta\cos\theta\sin\theta)_z,$$

where

$$m(\theta) = \alpha_3\cos^2\theta - \alpha_2\sin^2\theta,$$
$$g(\theta) = \frac{1}{2}\left(\alpha_4 + (\alpha_5-\alpha_2)\sin^2\theta + (\alpha_3+\alpha_6)\cos^2\theta\right) + \alpha_1\sin^2\theta\cos^2\theta.$$

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$$\boxed{\begin{aligned}\left(\gamma_1 - \frac{m^2(\theta)}{g(\theta)}\right)\theta_t &= (K_1 \cos^2\theta + K_3 \sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2 \\ &\quad - \frac{m(\theta)\mathcal{A}}{g(\theta)\mathcal{B}} + \frac{\zeta m(\theta)}{g(\theta)}\left[\cos\theta\sin\theta - \mathcal{K}_2 - \frac{\mathcal{C}}{\mathcal{B}}\right],\end{aligned}}$$

where

$$\mathcal{A} = \int_0^d \frac{m(\theta)[(K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2]}{\gamma_1 g(\theta) - m^2(\theta)}\,\mathrm{d}z,$$

$$\mathcal{B} = \int_0^d \frac{\gamma_1}{\gamma_1 g(\theta) - m^2(\theta)}\,\mathrm{d}z,$$

$$\mathcal{C} = \int_0^d \frac{m^2(\theta)\cos\theta\sin\theta}{g(\theta)(\gamma_1 g(\theta) - m^2(\theta))}\,\mathrm{d}z - \mathcal{K}_2\int_0^d \frac{m^2(\theta)}{g(\theta)(\gamma_1 g(\theta) - m^2(\theta))}\,\mathrm{d}z,$$

$$\mathcal{K}_2 = \int_0^d \frac{\cos\theta\sin\theta}{g(\theta)}\,\mathrm{d}z \Bigg/ \int_0^d \frac{1}{g(\theta)}\,\mathrm{d}z.$$

The effects due to flow appear in three terms in the governing equation for θ.

$$\Big(\underbrace{\gamma_1 - \frac{m^2(\theta)}{g(\theta)}}_{\text{rotational viscosity}}\Big)\theta_t = (K_1\cos^2\theta + K_3\sin^2\theta)\theta_{zz} + (K_3 - K_1)\sin\theta\cos\theta(\theta_z)^2$$

$$- \underbrace{\frac{m(\theta)\mathcal{A}}{g(\theta)\mathcal{B}}}_{\text{director-flow coupling}} + \underbrace{\frac{\zeta m(\theta)}{g(\theta)}\left[\cos\theta\sin\theta - \mathcal{K}_2 - \frac{\mathcal{C}}{\mathcal{B}}\right]}_{\text{activity}}.$$

- $\theta = 0$ is a solution of this equation (and leads to $v = 0$).
- The activity term in this equation is similar to a magnetic/electric field term in a **Freedericksz transition** but a **non-local** version.
- This term introduces the possibility that $\theta = 0$ could be **unstable**. At a **critical value of activity**, a **Freedericksz-like transition** will occur from a trivial state.

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- **What are the non-trivial steady state solutions?**
- **What are the stabilities of these solution?**

Spontaneous flow transitions due to activity

Considering the stability of the state $\theta = 0$ we find there are modes of instability

$$\text{Mode 1}: \theta(z,t) = \Theta\left[\cos\left(\frac{2q}{d}\left(z - \frac{d}{2}\right)\right) - \cos q\right]\exp(\sigma t),$$

$$\text{Mode 2}: \theta(z,t) = \Theta\sin\left(\frac{2n\pi z}{d}\right)\exp(\sigma t),$$

where $n \in \mathbb{Z}$. Mode 1 is a symmetric solution, whereas Mode 2 is anti-symmetric.

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$$\eta_{\text{splay}}\theta_t = K_1\theta_{zz} - \frac{K_1\alpha_3^2}{\gamma_1\eta_1 d}\int_0^d \theta_{zz}\,\mathrm{d}z + \frac{\zeta\alpha_3}{\eta_1}\left[\theta - \frac{1}{d}\int_0^d \theta\,\mathrm{d}z\right],$$

where $\eta_{\text{splay}} = \gamma_1 - \alpha_3^2/\eta_1$.

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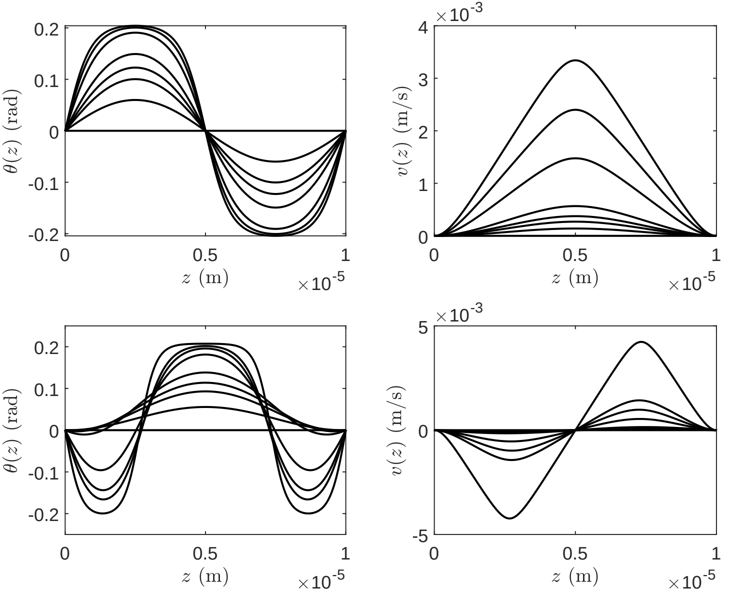
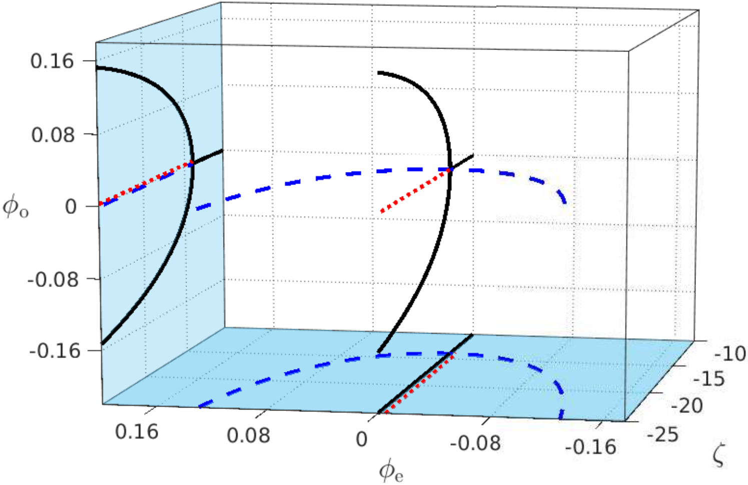
where $\eta_{\text{splay}} = \gamma_1 - \alpha_3^2/\eta_1$. These modes lead to instability when (with $q = n\pi$)

$$\boxed{\zeta_c = \frac{4n^2\pi^2 K_1\eta_1}{\alpha_3 d^2}.}$$

Non-trivial solutions for extensile swimmers



Bifurcation diagram for extensile swimmers



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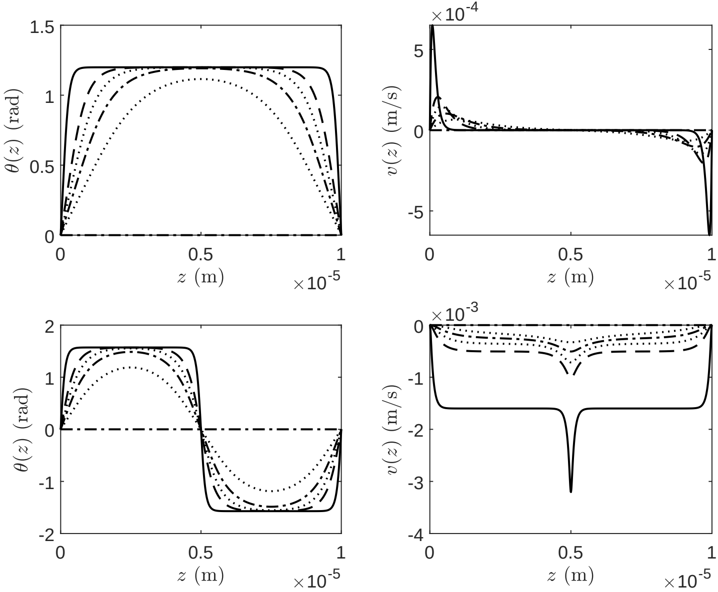

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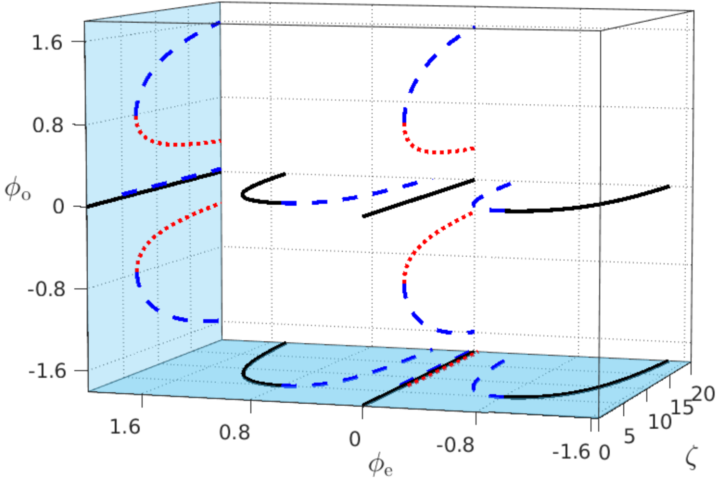

How does temperature effect the critical activities?

- We consider an order parameter model of active nematics based on $\mathbf{Q}$-tensor theory.
- The critical activity can be determined analytically in the same manner as done in the Ericksen-Leslie model.

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$$\boxed{\zeta_c(S_{\mathrm{eq}}) = \frac{4n^2\pi^2 K_1(S_{\mathrm{eq}})\eta_1(S_{\mathrm{eq}})}{\alpha_3(S_{\mathrm{eq}})d^2} \times \frac{\bar{S}}{S_{\mathrm{eq}}}.}$$

- $\bar{S} = 0.6$ (the uniaxial order parameter of the liquid crystal when the experimental measurements were taken).
- S_{eq} are the values of S which satisfy the minimisation of the Landau-de Gennes potential

$$\frac{2\alpha\Delta T}{3}S^2 + \frac{4b}{27}S^3 + \frac{2c}{9}S^4 = 0.$$

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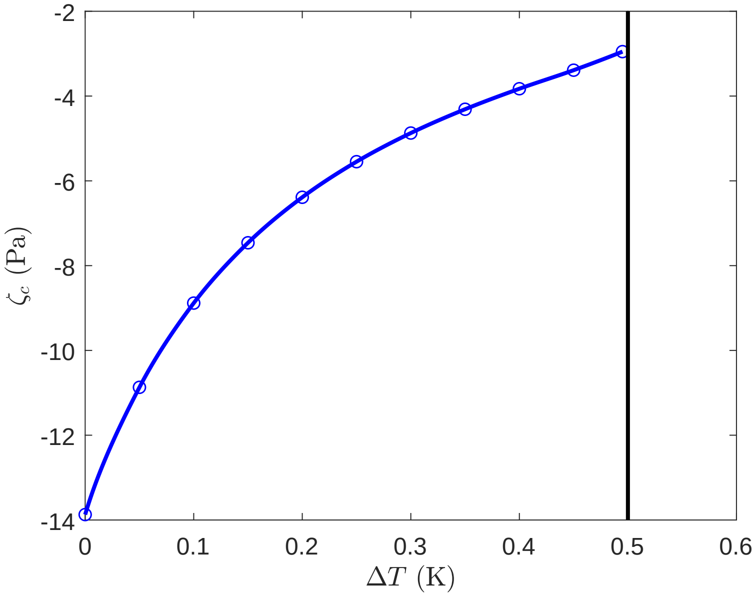
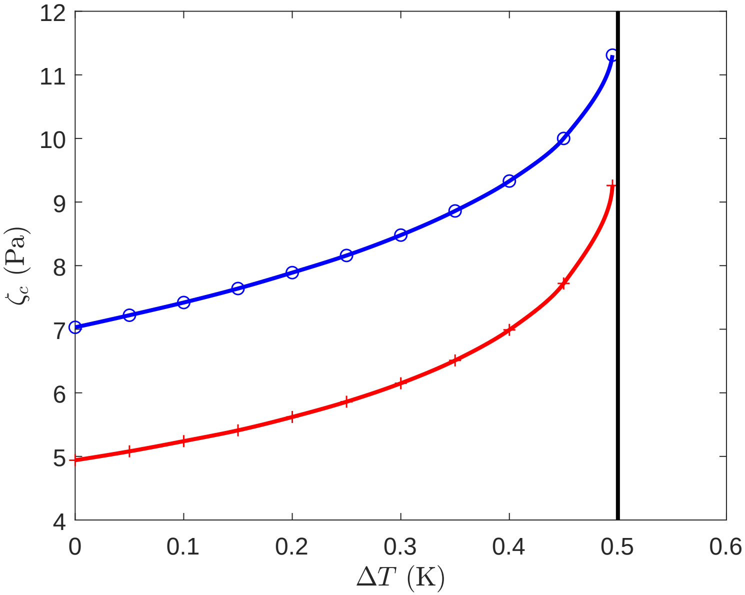
- For the choice of parameter values, the nematic phase disappears at critical temperature $\Delta T = 0.5\,\mathrm{K}$.
- At temperature $\Delta T = 0\,\mathrm{K}$, we recover the results from the Ericksen-Leslie model.



-2
-4
-6
-8
-10
-12
-14
0
0.1
0.2
0.3
0.4
0.5
0.6
ζ_c (Pa)
ΔT (K)


12
11
10
9
8
7
6
5
4
ζ_c (Pa)
0
0.1
0.2
0.3
0.4
0.5
0.6
ΔT (K)

Conclusions

- We have used the Ericksen-Leslie and $\mathbf{Q}$-tensor theories of liquid crystals to explain flow generation in active fluids.
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What else have we looked at?

- Pressure driven active nematics.
- The influence of external orienting fields.
- Flow of active fluids in 2D geometries.

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Future questions

- What alternative terms can be used to model the activity?
- Most marine based organisms are polar; how does this break in nematic symmetry change the results?
- What happens in 3D?

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