Finite Element Analysis of a Nematic Liquid Crystal Landau-de Gennes Model with Quartic Elastic Terms

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Outline

Background
- Measures of orientational order
- Biaxial nematics
- The tensor order parameter Q

Phenomenontological theory
- Landau-de Gennes energy model
- Oseen-Frank energy model
- Golovaty et al. energy model

Numerical model
- Reformulation
- Finite element discretization
- Numerical results

What are liquid crystals?

- Rod-like or disc-like molecules: orientation matters
- Intermediate phase of matter between crystalline solid and isotropic liquid

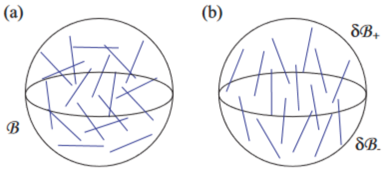

Figure 1: Molecules in a small ball within an isotropic fluid (left) and a liquid crystal (right). Source: [2]

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Orientational order

- Director $\vec{n}(\vec{x}, t)$
- Molecular orientation angle θ_m
- Scalar order parameter $S = \frac{1}{2} \int_{\mathcal{B}} (3\cos^2\theta_m - 1) f(\theta_m)\, d\vec{x}$
- Crystal: $S = 1$. Isotropic: $S = 0$. Randomly oriented perpendicular to $\vec{n}$: $S = -\frac{1}{2}$ (unusual).

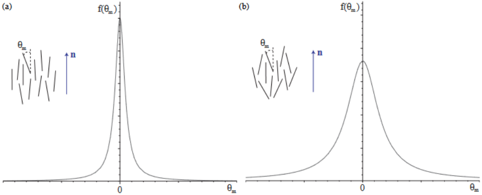

Figure 2: Probability distribution function for the angle between a molecule and the director, when the system has high (left) or low (right) orientational order. Source: [2]

Types of liquid crystals

- Nematic (what we'll be talking about today): No positional order
- Smectic: Layers, either perpendicular to director (Smectic A) or skew (Smectic C)
- Cholesterolic: Director field spirals in a helix
- etc.

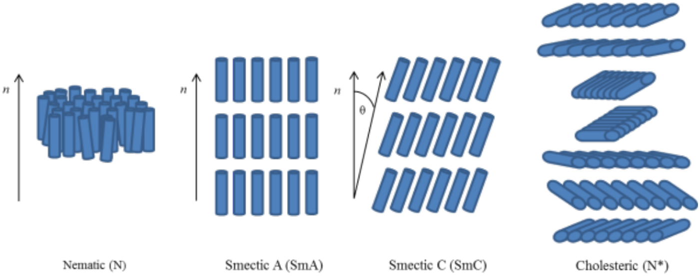

Figure 3: Molecular arrangements for different types of liquid crystals. Source: [3]

Uniaxial nematic arrangement

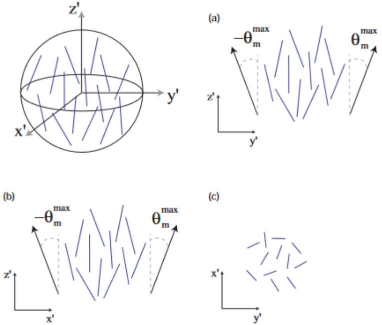

Figure 4: A uniaxial distribution of molecules with director z', viewed along each axis. Source: [2]

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Biaxial nematic arrangement

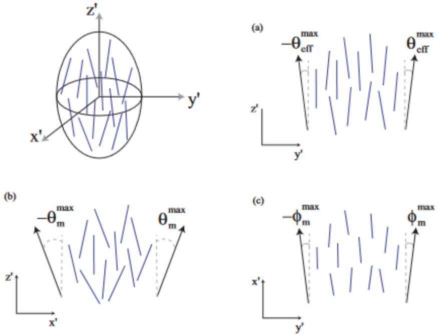

Figure 5: A biaxial distribution of molecules with primary director z' and secondary director x', viewed along each axis. Source: [2]

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Constructing a theory

- $\vec{n} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$
- $\vec{m} = (\sin\phi\cos\psi - \cos\phi\sin\psi\sin\theta, -\sin\phi\sin\psi\sin\theta - \cos\phi\cos\psi, \sin\psi\cos\theta)$
- Theory depends on five (dependent) variables: θ, ϕ, ψ, S_1, S_2
- Issue: Degenerate when $\theta = \frac{\pi}{2}$

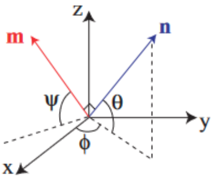

Figure 6: The directors n and m in terms of Euler angles. Source: [2]

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The tensor order parameter **Q**

$$Q = S_1(\vec{n} \otimes \vec{n}) + S_2(\vec{m} \otimes \vec{m}) - \frac{1}{3}(S_1 + S_2)I$$

- Symmetric and traceless
- No problems with degeneracies
- Uniaxial when two eigenvalues are the same:

$$\begin{aligned}
\lambda_1 &= (2S_1 - S_2)/3 \\
\lambda_2 &= -(S_1 + S_2)/3 \\
\lambda_3 &= (2S_2 - S_1)/3
\end{aligned}$$

The nitty-gritty details

$$Q = \begin{pmatrix} q_1 & q_2 & q_3 \\ q_2 & q_4 & q_5 \\ q_3 & q_5 & -q_1 - q_4 \end{pmatrix}$$

$$\begin{aligned}
q_1 &= S_1 \cos^2\theta \cos^2\phi + S_2(\sin\phi\cos\psi - \cos\phi\sin\psi\sin\theta)^2 - \frac{1}{3}(S_1 + S_2) \\
q_2 &= S_1 \cos^2\theta \sin\phi\cos\phi - S_2(\cos\phi\cos\psi + \sin\phi\sin\psi\sin\theta) \\
&\qquad * (\sin\phi\cos\psi - \cos\phi\sin\psi\sin\theta) \\
q_3 &= S_1 \sin\theta\cos\theta\cos\phi + S_2\sin\psi\cos\theta(\sin\psi\cos\psi - \cos\phi\sin\psi\sin\theta) \\
q_4 &= S_1 \cos^2\theta\sin^2\phi + S_2(\cos\phi\cos\psi + \sin\phi\sin\psi\sin\theta)^2 - \frac{1}{3}(S_1 + S_2) \\
q_5 &= S_1 \cos\theta\sin\theta\sin\phi - S_2\sin\psi\cos\theta(\cos\phi\cos\psi + \sin\phi\sin\psi\sin\theta)
\end{aligned}$$

Free energy of a liquid crystal sample

Components include (quoting Mottram [2]):

- "the elastic energy of any **distortion** to the structure of the material"
- "**thermotropic** energy which dictates the preferred phase of the material"
- "**electric and/or magnetic** energy from an externally applied electric or magnetic field and, in polar materials, the internal self-interaction energy of the polar molecules"
- "**surface** energy terms representing the interaction energy between the bounding surface and the liquid crystal molecules at the surface"

$$\begin{aligned}\mathcal{F} &= \mathcal{F}_{distortion} + \mathcal{F}_{thermotropic} + \mathcal{F}_{electromagnetic} + \mathcal{F}_{surface} \\ &= \int_{\Omega} (F_d + F_t + F_e)\, d\vec{x} + \int_{\partial\Omega} F_s\, ds\end{aligned}$$

Landau-de Gennes thermotropic energy

- Describes what state the material would prefer to be in
- High temperatures: Minimum at $Q = 0$ (isotropic)
- Low temperatures: Minimum at three uniaxial states ($S_1 = 0$, $S_2 = 0$, or $S_1 = S_2$)
- For temperature-dependent a, b, and c, the Landau-de Gennes energy is defined as

$$F_t = a\,\mathrm{tr}(Q^2) + \frac{2b}{3}\,\mathrm{tr}(Q^3) + \frac{c}{2}\,\mathrm{tr}^2(Q^2)$$

- When $a < \frac{b^2}{27c}$, minimizers of F_t are uniaxial
- Golovaty et al. [1] make this assumption, define the minimal set

$$\mathcal{N} = \left\{ s_0 \left(\vec{n} \otimes \vec{n} - \frac{1}{3} I \right) : \vec{n} \in \mathbb{S}^2 \right\}$$

and add an ignorable constant such that $F_t(\mathcal{N}) = 0$

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Landau-de Gennes elastic energy

- Mottram [2] again: "It is, generally, energetically favourable for Q to be constant throughout the material and any gradients in Q would lead to an increase in distortional energy. F_d therefore depends on the spatial derivatives of Q."

$$\mathcal{F}_{LdG}(Q) = \int_\Omega \sum_{i,j,k=1}^{3} \left(\frac{L_1}{2} Q_{ij,k}^2 + \frac{L_2}{2} Q_{ij,j} Q_{ik,k} + \frac{L_3}{2} Q_{ik,j} Q_{ij,k} \right) d\vec{x}$$

- L_i's are material constants

Oseen-Frank energy

- Director-based, not Q-tensor-based
- For some $\vec{n} : \Omega \to \mathbb{S}^2$, we have

$$\mathcal{F}_{OF}(\vec{n}) = \int_\Omega \left(\frac{K_1}{2}(\operatorname{div}\vec{n})^2 + \frac{K_2}{2}((\operatorname{curl}\vec{n})\cdot\vec{n})^2 + \frac{K_3}{2}|(\operatorname{curl}\vec{n})\times\vec{n}|^2 + \frac{K_2+K_4}{2}(\operatorname{tr}(\nabla\vec{n})^2 - (\operatorname{div}\vec{n})^2) \right) d\vec{x}$$

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Correspondence between OF and LdG

- Motivation: Find a Q-tensor-based model which corresponds smoothly to $\mathcal{F}_{d,OF}$
- Previous attempts have added another term to $\mathcal{F}_{d,LdG}$:

$$\int_{\Omega} Q_{lk} Q_{ij,k} Q_{ij,l} \, d\vec{x}$$

- Problem: Cubic term means energy is unbounded from below

Golovaty et al. energy model

- Solution: Define model with quartic terms instead

$$\mathcal{F}_{GNS}(Q) = \int_\Omega \Bigg(\frac{L_1}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{curl} Q \right|^2 + \frac{L_3}{2} \left| \left(\frac{2 s_0}{3} I - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2 s_0}{3} I - Q \right) \operatorname{curl} Q \right|^2 + F_t(Q) \Bigg) \, d\vec{x}$$

- s_0 is the scalar order parameter of the uniaxial tensors which minimize F_t
- $s_0^4 L_4 = K_2 + K_4$ and $s_0^4 (L_i + L_4) = K_i$ for $i = 1, 2, 3$

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Divergence and curl of tensor fields

$$\operatorname{div} A = \sum_{j=1}^{3} (\operatorname{div} A_j)\vec{e}_j = \begin{bmatrix} A_{11,1} + A_{12,2} + A_{13,3} \\ A_{21,1} + A_{22,2} + A_{23,3} \\ A_{31,1} + A_{32,2} + A_{33,3} \end{bmatrix}$$

$$(\operatorname{curl} A)\vec{v} = \operatorname{curl}(A^\top \vec{v}) \qquad \forall \vec{v} \in \mathbb{R}^3$$

$$\operatorname{curl} A = \sum_{i,j,k,m=1}^{3} \varepsilon_{ijk} A_{mj,i} \vec{e}_k \otimes \vec{e}_m$$

Relevant property of curl:

$$\operatorname{curl}\left(\vec{m} \otimes \vec{m}\right) = \begin{bmatrix} \operatorname{curl}\left(m_1 \vec{m}\right) & \operatorname{curl}\left(m_2 \vec{m}\right) & \operatorname{curl}\left(m_3 \vec{m}\right) \end{bmatrix}$$

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Golovaty et al.'s proposition

- Let $Q \in H^1(\Omega; \mathcal{N})$, such that $Q = s_0(\vec{n} \otimes \vec{n} - I/3)$ for $\vec{n} \in H^1(\Omega; \mathbb{S}^2)$. Then

$$\mathcal{F}_{GNF}(Q) = \mathcal{F}_{OF}(\vec{n}).$$

- Proof: Too long for this talk. I've cited the paper in the references
- After proving this result, Golovaty et al. relax the condition $Q \in \mathcal{N}$ to $Q \in \mathbb{S}^2$ to allow for biaxial states, then proves a Γ-convergence result as nematic correlation length divided by domain size tends to zero

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A slightly modified energy

$$
\begin{aligned}
\mathcal{F}(Q) = \int_\Omega \Bigg(&\frac{L_1}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{curl} Q \right|^2 \\
&+ \frac{L_3}{2} \left| \left(\frac{2s_0}{3} I - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} I - Q \right) \operatorname{curl} Q \right|^2 \\
&+ \frac{L_5}{2} |Q|^2 |\nabla Q|^2 + F_t(Q) \Bigg) \, d\vec{x}
\end{aligned}
$$

- Adding a fifth quartic term to make a Γ-convergence result later on possible
- This model also reduces to Oseen-Frank in the uniaxial case for suitable L_i's

Dissipation law

- Formal definition of symmetric traceless tensor space:

$$\mathcal{S} = \{Q : Q \in \mathbb{R}^{3\times 3},\, Q = Q^\top,\, \mathbf{tr}\,(Q) = 0\}$$

- Projection operator:

$$\mathscr{P}(A) = \frac{1}{2}(A + A^\top) - \frac{\mathbf{tr}\,(A)}{3} I$$

- Gradient descent:

$$\frac{\partial Q}{\partial t} = -M\mathscr{P}\left(\frac{\delta \mathcal{F}}{\delta Q}\right)$$

- Dissipation law from chain rule:

$$\frac{d\mathcal{F}}{dt} = \int_\Omega \mathscr{P}\left(\frac{\delta \mathcal{F}}{\delta Q}\right) : \frac{\partial Q}{\partial t}\, d\vec{x} = \left\|\frac{\partial Q}{\partial t}\right\|^2$$

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Energy components

$$S_1(Q) = \frac{s_0}{3} I + Q \qquad S_2(Q) = \frac{2s_0}{3} I - Q$$

$$\mathcal{F}_1(Q) = \frac{L_1}{2} \left\| S_1 \operatorname{div} Q \right\|^2 \qquad \mathcal{F}_2(Q) = \frac{L_2}{2} \left\| S_1 \operatorname{curl} Q \right\|^2$$

$$\mathcal{F}_3(Q) = \frac{L_3}{2} \left\| S_2 \operatorname{div} Q \right\|^2 \qquad \mathcal{F}_4(Q) = \frac{L_4}{2} \left\| S_2 \operatorname{curl} Q \right\|^2$$

$$\mathcal{F}_5(Q) = \frac{L_5}{2} \left\| Q |\nabla Q| \right\|^2$$

$$\mathcal{F}_6(Q) = \int_\Omega \left(a \operatorname{tr}(Q^2) + \frac{2b}{3} \operatorname{tr}(Q^3) + \frac{c}{2} \operatorname{tr}^2(Q^2) \right) \, d\vec{x}$$

$$\mathcal{F}(Q) = \mathcal{F}_1(Q) + \mathcal{F}_2(Q) + \mathcal{F}_3(Q) + \mathcal{F}_4(Q) + \mathcal{F}_5(Q)$$

Derivatives of energy components

$$\frac{\delta \mathcal{F}_1}{\delta Q} = L_1 \left(-\nabla (S_1^2 \operatorname{div} Q) + S_1 \operatorname{div} Q \, (\operatorname{div} Q)^\top \right)$$
$$\frac{\delta \mathcal{F}_2}{\delta Q} = L_2 \left(\operatorname{curl} (S_1^2 \operatorname{curl} Q)^\top + S_1 \operatorname{curl} Q \, (\operatorname{curl} Q)^\top \right)$$
$$\frac{\delta \mathcal{F}_3}{\delta Q} = L_3 \left(-\nabla (S_2^2 \operatorname{div} Q) + S_2 \operatorname{div} Q \, (\operatorname{div} Q)^\top \right)$$
$$\frac{\delta \mathcal{F}_4}{\delta Q} = L_4 \left(\operatorname{curl} (S_2^2 \operatorname{curl} Q)^\top + S_2 \operatorname{curl} Q \, (\operatorname{curl} Q)^\top \right)$$
$$\frac{\delta \mathcal{F}_5}{\delta Q} = L_5 \left(-\nabla (|Q|^2 \nabla Q) + |\nabla Q|^2 Q \right)$$
$$\frac{\delta \mathcal{F}_6}{\delta Q} = 2aQ - 2bQ^2 + 2c \operatorname{tr}(Q^2) Q$$

Finite elements

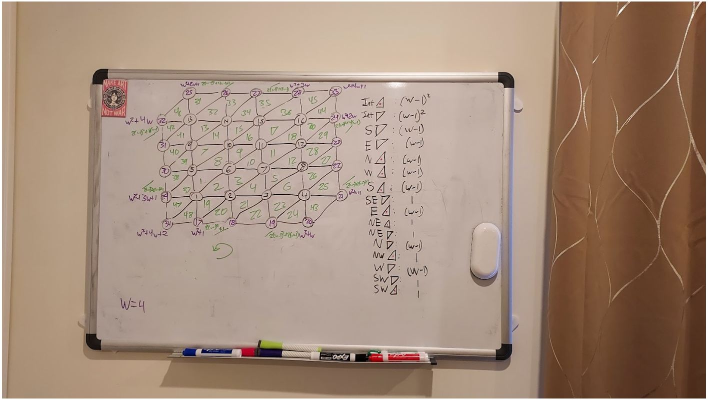

Figure 7: A whiteboard drawing demonstrating the partition of a square into finite elements

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Weak solutions

- Given a tetrahedral mesh $\{\Omega_\ell\}$ of Ω with element diameter h, define

$$\mathcal{T}_h^0 = \{\varphi : \Omega \to \mathcal{S} : \varphi \text{ continuous}, \varphi|_{\Omega_\ell} \text{ linear}, \varphi|_{\partial\Omega} = 0\}$$
$$\mathcal{T}_h^g = \{\varphi + g : \varphi \in \mathcal{T}_h^0\}$$

  where g is a Dirichlet boundary condition
- Basis functions: Multiply basis of $\mathcal{S}$ by “hat” functions, which are zero on all nodes except one
- The discrete formulation is to find $Q_h \in \mathcal{T}_h^g$ such that

$$\left\langle \frac{Q_h^{n+1} - Q_h^n}{\Delta t}, \varphi \right\rangle = -MH^{n+\frac{1}{2}}(\varphi) \qquad \forall \varphi \in \mathcal{T}_h^0$$

  where $H^{n+\frac{1}{2}}(\varphi)$ represents “$\left\langle \frac{\delta \mathcal{F}}{\delta Q_h^{n+\frac{1}{2}}}, \varphi \right\rangle$”

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Discretization

The discrete value of $(\cdot)(\vec{x}, t)$ at time t^n is denoted $(\cdot)^n(\vec{x})$.
The average of $(\cdot)^n$ and $(\cdot)^{n+1}$ is denoted $(\cdot)^{n+\frac{1}{2}}$.

$$H_1^{n+\frac{1}{2}}(\varphi) = L_1 \left\langle (S_{1,h} \operatorname{div} Q_h)^{n+\frac{1}{2}}, S_{1,h} \operatorname{div} \varphi + \varphi \operatorname{div} Q_h^{n+\frac{1}{2}} \right\rangle$$

$$H_2^{n+\frac{1}{2}}(\varphi) = L_2 \left\langle (S_{1,h} \operatorname{curl} Q_h)^{n+\frac{1}{2}}, S_{1,h} \operatorname{curl} \varphi + \varphi \operatorname{curl} Q_h^{n+\frac{1}{2}} \right\rangle$$

$$H_3^{n+\frac{1}{2}}(\varphi) = L_3 \left\langle (S_{2,h} \operatorname{div} Q_h)^{n+\frac{1}{2}}, S_{2,h} \operatorname{div} \varphi - \varphi \operatorname{div} Q_h^{n+\frac{1}{2}} \right\rangle$$

$$H_4^{n+\frac{1}{2}}(\varphi) = L_4 \left\langle (S_{2,h} \operatorname{curl} Q_h)^{n+\frac{1}{2}}, S_{2,h} \operatorname{curl} \varphi - \varphi \operatorname{curl} Q_h^{n+\frac{1}{2}} \right\rangle$$

$$H_5^{n+\frac{1}{2}}(\varphi) = L_5 \left(\left\langle (|\nabla Q_h|^2)^{n+\frac{1}{2}} Q_h^{n+\frac{1}{2}}, \varphi \right\rangle + \left\langle (|Q_h|^2)^{n+\frac{1}{2}} \nabla Q_h^{n+\frac{1}{2}}, \nabla \varphi \right\rangle \right)$$

$$H_6^{n+\frac{1}{2}}(\varphi) = \left\langle 2a Q_h^{n+\frac{1}{2}} - \frac{2b}{3}(2(Q_h^2)^{n+\frac{1}{2}} + Q_h^{n+1} Q_h) + 2c(\operatorname{tr}(Q_h^2))^{n+\frac{1}{2}} Q_h^{n+\frac{1}{2}}, \varphi \right\rangle$$

$$H^{n+\frac{1}{2}} = H_1^{n+\frac{1}{2}} + H_2^{n+\frac{1}{2}} + H_3^{n+\frac{1}{2}} + H_4^{n+\frac{1}{2}} + H_5^{n+\frac{1}{2}} + H_6^{n+\frac{1}{2}}$$

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Discrete dissipation law

- The scheme on the previous two slides satisfies the semi-discrete dissipation law

$$\frac{\mathcal{F}(Q_h^{n+1}) - \mathcal{F}(Q_h^n)}{\Delta t} = -\frac{1}{M}\left\| \frac{Q_h^{n+1} - Q_h^n}{\Delta t} \right\|^2$$

- Q_h^{n+1} is uniquely defined and can be found by fixed-point iteration (due to Banach's theorem)

Numerical results: Convergence tests

- Domain: $\Omega = [0,2]^2$
- Initial and boundary conditions:

$$Q_0 = \vec{n}_0 \vec{n}_0^\top - \frac{|\vec{n}_0|^2}{2} I_2,$$

where

$$\vec{n}_0 = \begin{pmatrix} x(2-x)y(2-y) \\ \sin(\pi x)\sin(\pi y/2) \end{pmatrix}$$

- Max time: $T = 0.8$
- Grid size and number of time steps vary between experiments

Numerical results: Spatial refinement

1600 time steps per experiment. Reference solution Q_{ref} calculated with $h = 0.005$ using 25000 time steps.

h	$\|Q_h - Q_{\text{ref}}\|$	Order	$\|\mathcal{F}(Q_h) - \mathcal{F}(Q_{\text{ref}})\|$	Order
0.2	4.3506×10^{-2}	$-$	9.7867×10^{-4}	$-$
0.1	1.5921×10^{-2}	1.4503	3.2908×10^{-4}	1.5724
0.05	3.5480×10^{-3}	2.1659	7.3880×10^{-5}	2.1552
0.025	8.3939×10^{-4}	2.0796	1.7793×10^{-5}	2.0539

Numerical results: Time refinement

$h = 2/30$ for all experiments. Reference solution Q_{ref} taken with the same h and 80000 time steps.

Δt	$\|Q_h - Q_{\text{ref}}\|$	Order	$\lvert\mathcal{F}(Q_h) - \mathcal{F}(Q_{\text{ref}})\rvert$	Order
4×10^{-3}	4.2744×10^{-6}	–	4.7072×10^{-7}	–
2×10^{-3}	1.0684×10^{-6}	2.0002	1.1767×10^{-7}	2.0001
1×10^{-3}	2.6708×10^{-7}	2.0001	2.9415×10^{-8}	2.0001
5×10^{-4}	6.6771×10^{-8}	2.0000	7.3541×10^{-9}	1.9999
2.5×10^{-4}	1.6684×10^{-8}	2.0007	1.8377×10^{-9}	2.0006

Numerical results: Maximum Δt

For each h, we find the maximum Δt for which the fixed-point iteration converges for at least 100 time steps

h	Max convergent Δt	Order
0.2	7.9801×10^{-2}	–
0.1	2.2379×10^{-2}	1.8342
0.05	7.7537×10^{-3}	1.5292
0.025	2.0005×10^{-3}	1.9545
0.0125	4.0707×10^{-4}	2.2970
0.00625	9.1601×10^{-5}	2.1518

Numerical results: Tactoid simulations

- Ω is the unit circle, discretized by a Delaunay triangulation with 5809 nodes and 11366 elements
- Time step: $\Delta t = 0.01$
- Initial and boundary conditions:

$$Q_0 = \sqrt{\frac{-2a}{c}} \left(\vec{n}_0(\theta) \vec{n}_0^\top(\theta) - \frac{1}{2} I_2 \right) \chi_{r^2 \geq 0.3}$$

  where $\vec{n}_0 : [0, 2\pi) \to \mathbb{S}^1$ depends on the experiment
- Isotropic tactoid surrounded by a nematic sample
- Cue the animations!

References

[1] DMITRY GOLOVATY, MICHAEL NOVACK, and PETER STERNBERG. "A novel Landau-de Gennes model with quartic elastic terms". In: *European Journal of Applied Mathematics* 32.1 (Mar. 2020), pp. 177–198. ISSN: 1469-4425. DOI: 10.1017/s095679252000008x. URL: http://dx.doi.org/10.1017/S095679252000008X.

[2] Nigel J. Mottram and Christopher J. P. Newton. *Introduction to Q-tensor theory*. 2014. arXiv: 1409.3542 [cond-mat.soft].

[3] UKEssays. *Classifications of Liquid Crystals*. URL: https://om.ukessays.com/essays/chemistry/classifications-liquid-crystals-7625.php?vref=1. (accessed: 04.25.2024).

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