A double Landau–de Gennes mathematical model of smectic A liquid crystals

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Numerical Analysis Group Internal Seminar
October 20, 2020

Outline

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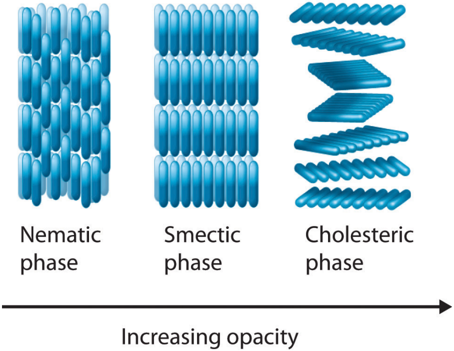
What are liquid crystals?

- Liquid crystals (LC) are an intermediate state of matter between isotropic liquid and solid crystals.
- LC flow like liquids, but the constituent molecules retain orientational order.
- LC are of many different types, the main related classes being nematic, smectic and cholesteric.



(Averill and Eldredge, 2011)

Three continuum models for nematic LC

	Oseen–Frank (OF)	Ericksen	Landau–de Gennes (LdG)
variables	vector n	scalar s vector n	tensor Q
constraints	$\|n\| = 1$	$\|n\| = 1$	$Q = Q^\top$ $\mathrm{tr}(Q) = 0$
energy density	$W_{of}(n)$	$W_e(s, n)$	$W_{ldg}(Q)$

Examples of energy density:

$$2W_{of}(n) = K_1 |\nabla \cdot n|^2 + K_2 |n \cdot \nabla \times n|^2 + K_3 \left| n \times (\nabla \times n) \right|^2,$$

$$2W_e(s, n) = -\frac{s^2}{2} - \frac{s^3}{3} + \frac{s^4}{4} + 2s^2 W_{of}(n) + K_5 |\nabla s|^2 + K_6 |\nabla s \cdot n|^2,$$

$$W_{ldg}(Q) = \frac{K}{2} |\nabla Q|^2 + \frac{a}{2} \mathrm{tr}\left(Q^2\right) - \frac{b}{3} \mathrm{tr}\left(Q^3\right) + \frac{c}{4} \left(\mathrm{tr}\left(Q^2\right)\right)^2.$$

Q tensor

Degrees of freedom of tensor Q

$$\text{Symmetric and traceless } Q \Longleftrightarrow \begin{cases} (q_1, q_2) & \text{in 2D} \\ (q_1, q_2, q_3, q_4, q_5) & \text{in 3D.} \end{cases}$$

$$Q = \begin{bmatrix} q_1 & q_2 \\ q_2 & -q_1 \end{bmatrix} \quad \text{or} \quad Q = \begin{bmatrix} q_1 & q_3 & q_4 \\ q_3 & q_2 & q_5 \\ q_4 & q_5 & -(q_1 + q_2) \end{bmatrix}.$$

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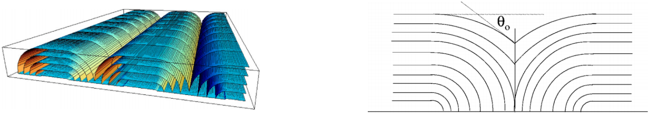
Uniaxial Q

One preferred alignment direction of LC molecules:

$$Q = s\left(n \otimes n - \frac{I_d}{d}\right), \; d \in \{2, 3\}.$$

Two typical defects in smectic A

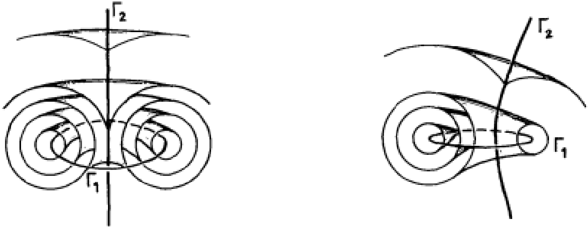
Oily streaks (OS)



(Michel et al., 2004)

Left: flattened hemi-cylinders; right: defect wall.

Focal Conic Domains (FCD)



(Williams and Kléman, 1975)

Left: Toroidal Focal Conic Domains (TFCD); right: FCD.

This work

A new model for smectic A LC

Smectic order parameter is characterized by *real-valued* u.
Nematic order parameter is characterized by *tensor* Q.

Novel applications

Two typical smectic A defects, OS and (T)FCD, are captured numerically for the first time.

Outline

de Gennes model

Smectic order parameter $\psi : \Omega \to \mathbb{C}$.
Nematic order parameter $n : \Omega \to \mathbb{R}^d$, $|n| = 1$.

de Gennes model (Gennes, 1972)

$$\begin{aligned} \min \quad & J(n,\psi) = \int_\Omega \left(F_S(n,\psi) + W_{of}(n) \right), \\ \text{subject to} \quad & |n| = 1 \text{ a.e. in } \Omega, \end{aligned}$$

where $F_S(n,\psi) = |\nabla\psi - iqn\psi|^2 + r|\psi|^2 + \frac{g}{2}|\psi|^4$ with $i = \sqrt{-1}$, $q > 0, r = r_0(T - T_{ns}) < 0, g > 0$.

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Issues

- $\mathrm{Im}(\psi)$ does not relate to anything physical;
- this description is based on *coarse-grained* length, and hence cannot model dislocations in smectic layers.

Pevnyi–Selinger–Sluckin (PSS) model

Smectic order parameter $\delta\rho : \Omega \to \mathbb{R}$.
Nematic order parameter $n : \Omega \to \mathbb{R}^d$, $|n| = 1$.

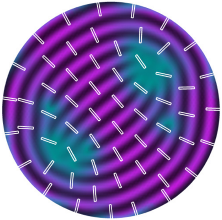
PSS model (Pevnyi, Selinger, and Sluckin, 2014)

$$\begin{aligned} \min \quad & J(\delta\rho, n) = \int_\Omega \left(\frac{a}{2}(\delta\rho)^2 + \frac{b}{3}(\delta\rho)^3 + \frac{c}{4}(\delta\rho)^4 \right. \\ & \qquad \left. + B \left| \mathcal{D}^2 \delta\rho + q^2 \left(n \otimes n\right) \delta\rho \right|^2 + \frac{K}{2} |\nabla n|^2 \right), \\ \text{subject to} \quad & |n| = 1 \text{ a.e. in } \Omega, \end{aligned}$$

where $a < 0$ and $c, B, q, K > 0$.

PSS model

An example of $+\frac{1}{2}$ defects illustrated in (Pevnyi, Selinger, and Sluckin, 2014):



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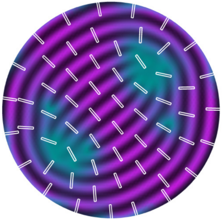

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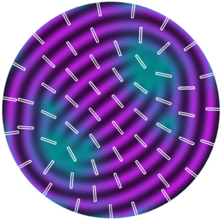

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You can't represent half charge defects by a unit vector field n?

In fact ...

They use *tensor* $\mathrm{n} \otimes \mathrm{n}$ instead in their implementations.

Ball–Bedford (BB) model

BB model (Ball and Bedford, 2015)

Directly replacing $n \otimes n$ by $Q/s + I_3/3$ in the PSS model:

$$\min \; I(u, Q) = \int_\Omega \left(\frac{1}{2}|\nabla Q|^2 + K \left| \mathcal{D}^2 u + \frac{q^2}{3s} \left(3Q + sI_3\right) u \right|^2 + \frac{a}{2}u^2 + \frac{b}{3}u^3 + \frac{c}{4}u^4 \right),$$

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Issues

- Choice of the scalar order parameter s?
- Numerical singularities caused by $s \approx 0$.
- No provided implementations.

Our proposed model (double LdG)

Smectic order parameter $u : \Omega \to \mathbb{R}$.

Nematic order parameter $Q : \Omega \to \mathbb{R}^{d\times d}$, symmetric and traceless.

Double LdG model (a unified framework)

$$\begin{aligned}\min\ \mathcal{J}(u,Q) = \int_\Omega \Bigg(& \frac{a}{2}u^2 + \frac{b}{3}u^3 + \frac{c}{4}u^4 \\ & + B\left|\mathcal{D}^2 u + q^2\left(Q + \frac{I_d}{d}\right)u\right|^2 \\ & + \frac{K}{2}|\nabla Q|^2 + f_n^b(Q)\Bigg),\end{aligned} \tag{1}$$

where the nematic bulk term is defined as

$$f_n^b(Q) := \begin{cases} \left(-l\left(\mathrm{tr}(Q^2)\right) + l\left(\mathrm{tr}(Q^2)\right)^2\right), & \text{if } d=2, \\ \left(-\frac{l}{2}\left(\mathrm{tr}(Q^2)\right) - \frac{l}{3}\left(\mathrm{tr}(Q^3)\right) + \frac{l}{2}\left(\mathrm{tr}(Q^2)\right)^2\right), & \text{if } d=3. \end{cases}$$

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$$

$f_n^b(Q)$ is chosen so that its global minimizer is a uniaxial tensor Q with $s = 1$. (Majumdar and Zarnescu, 2010, Proposition 15)

Existence of minimizers

Define the admissible set

$$\mathcal{A} = \Big\{ u \in H^2(\Omega, \mathbb{R}),\ \ Q \in H^1(\Omega, S_0) :$$

$$Q = s\left(n \otimes n - \frac{I_d}{d}\right) \text{ for some } s \in [0,1] \text{ and } n \in H^1(\Omega, \mathcal{S}^{d-1}),$$

$$Q = Q_b \text{ on } \partial\Omega \Big\},$$

with Dirichlet boundary data $Q_b \in H^{1/2}(\partial\Omega, S_0)$.

Theorem (existence of minimizers)

Let $\mathcal{J}$ be of the form (1) with positive parameters c, B, q, K, l. Then there exists a pair (u^*, Q^*) that minimizes $\mathcal{J}$ over the admissible set $\mathcal{A}$.

Proof: by the direct method of calculus of variations.
(Davis and Gartland, 1998, Theorem 4.3) & (Bedford, 2014, Theorem 5.19)

Finite element approximations

Essentially...

we are solving a *second order* PDE and *fourth order* PDE, coupled together.

- For the second order PDE $\Leftarrow$ common continuous Lagrange elements ✓
- For the fourth order PDE $\Leftarrow$ a practical choice of finite elements?

Use continuous Lagrange elements for $u \in H^2$

By adding the following penalty term in the total energy:

$$\frac{\gamma}{2h^3}\left(\sum_{e_{ij}\in\mathcal{E}_I}\int_{e_{ij}}\left([\![\nabla u]\!]\right)^2\right).$$

(Engel et al., 2002; Brenner and Sung, 2005)

Convergence tests via MMS

Exact solutions:

$$q_1^{exact} = \left(\cos\left(\frac{\pi(2y-1)(2x-1)}{8}\right)\right)^2 - \frac{1}{2},$$
$$q_2^{exact} = \cos\left(\frac{\pi(2y-1)(2x-1)}{8}\right)\sin\left(\frac{\pi(2y-1)(2x-1)}{8}\right),$$
$$u^{exact} = 10\left((x-1)x(y-1)y\right)^2$$

Manufactured equations to be solved:

$$4Bq^4u^2q_1 + 2Bq^2u\left(\partial_x^2 u - \partial_y^2 u\right) - 2K\Delta q_1 - 4lq_1 + 16lq_1\left(q_1^2+q_2^2\right) = f_1,$$
$$4Bq^4u^2q_2 + 4Bq^2u\left(\partial_x\partial_y u\right) - 2K\Delta q_2 - 4lq_2 + 16lq_2\left(q_1^2+q_2^2\right) = f_2,$$
$$au + bu^2 + cu^3 + 2B\Delta^2 u + Bq^4\left(4\left(q_1^2+q_2^2\right)+1\right)u + 2Bq^2(t_1+t_2) = f_3,$$

here, f_1, f_2, f_3 are source terms derived from substituting the exact solutions to the left hand sides.

Convergence tests via MMS: settings

- $(u, q_1, q_2) \xLeftarrow{FEM} (\mathbb{Q}_3 \times \mathbb{Q}_2 \times \mathbb{Q}_2)$ + interior penalty
- Mesh size $h = \frac{1}{N}$ with $N = 5$, 10, 20, 40, 80.
- Define numerical errors in L^2 and H^1 norms as

$$\|e_u\|_0 = \|u^{exact} - u_h\|_0,$$

$$\|e_u\|_1 = \|u^{exact} - u_h\|_1,$$

$$\|e_Q\|_0 = \|(q_1^{exact}, q_2^{exact}) - (q_{1,h}, q_{2,h})\|_0,$$

$$\|e_Q\|_1 = \|(q_1^{exact}, q_2^{exact}) - (q_{1,h}, q_{2,h})\|_1.$$

- Order of convergence:

$$\log_2\left(\frac{\text{error}_{i+1}}{\text{error}_i}\right), i = 1, 2, 3, 4.$$

- Choose parameters used in experiments later
$a = -10,\ b = 0,\ c = 10,\ B = 10^{-5},\ K = 0.3,\ l = 30.$

Convergence tests: $\gamma = 1$

$(u, Q) \xleftarrow{FEM} \mathbb{Q}_3 \times (\mathbb{Q}_2)^2$

Decoupled case $q = 0$:

$N = \frac{1}{h}$	$\|e_u\|_0$	rate	$\|e_u\|_1$	rate	$\|e_Q\|_0$	rate	$\|e_Q\|_1$	rate
5	6.06e-05	–	1.71e-03	–	4.90e-05	–	1.62e-03	–
10	1.24e-06	5.61	7.82e-05	4.45	6.65e-06	2.88	3.92e-04	2.05
20	7.69e-08	4.01	9.73e-06	3.01	8.63e-07	2.95	9.69e-05	2.02
40	4.81e-09	4.00	1.22e-06	3.00	1.10e-07	2.98	2.41e-05	2.00
80	3.01e-10	4.00	1.52e-07	3.00	1.38e-08	2.99	6.03e-06	2.00

Coupled case with $q = 40$:

$N = \frac{1}{h}$	$\|e_u\|_0$	rate	$\|e_u\|_1$	rate	$\|e_Q\|_0$	rate	$\|e_Q\|_1$	rate
5	1.74e-05	-	5.74e-04	-	9.80e-05	-	3.24e-03	-
10	1.97e-06	3.15	9.42e-05	2.61	1.33e-05	2.88	7.83e-04	2.05
20	1.66e-07	3.57	1.11e-05	3.08	1.73e-06	2.95	1.94e-04	2.02
40	2.01e-08	3.04	1.43e-06	2.95	2.20e-07	2.97	4.83e-05	2.00
80	1.63e-09	3.62	1.64e-07	3.13	2.76e-08	2.99	1.21e-05	2.00

Outline

Introduction

Modeling of smectic A LC

Numerical results

Conclusions and future work

Oily streaks: problem settings

- Let $\Omega = [-1, 1] \times [0, 1]$ with boundary labels

$$\Gamma_l = \{(x, y) : x = -1\}\,, \qquad \Gamma_r = \{(x, y) : x = 1\}\,,$$
$$\Gamma_b = \{(x, y) : y = 0\}\,, \qquad \Gamma_t = \{(x, y) : y = 1\}\,.$$

- Discretize the domain Ω into 90×30 quads
- $(u, q_1, q_2) \xLeftarrow{FEM} (\mathbb{Q}_3 \times \mathbb{Q}_2 \times \mathbb{Q}_2) +$ interior penalty
- Choose parameters

$$a = -10,\ b = 0,\ c = 10,\ B = 10^{-5},\ K = 0.3,$$
$$q = 30,\ l = 30,\ w = 10.$$

Oily streaks: problem settings

- Weakly enforcing boundary conditions via

$$f_s(Q) = \int_{\Gamma_b} \frac{w}{2} \left| Q - Q_{planar} \right|^2 + \int_{\Gamma_t \cup \Gamma_l \cup \Gamma_r} \frac{w}{2} \left| Q - Q_{homeotropic} \right|^2 .$$

  - w is the weak anchoring weight;
  - prescribed configuration at the bottom surface:

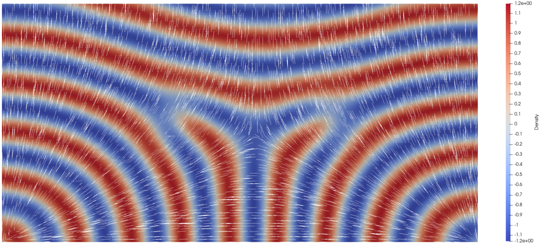
$$Q_{planar} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix}$$

    gives horizontally aligned directors;
  - prescribed configuration at the top/left/right surfaces:

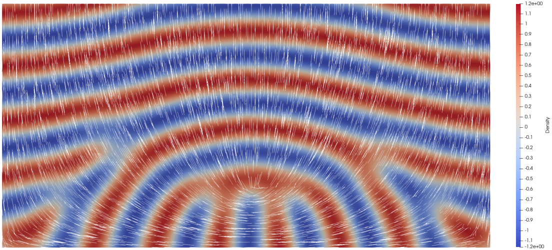
$$Q_{homeotropic} = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

    gives vertical aligned directors.

Oily streaks: two solution examples



(a) A $-\frac{1}{2}$-charge defect.



(b) A $+\frac{1}{2}$-charge defect.

TFCDs: problem settings

- Let $\Omega = [-1.5, 1.5] \times [-1.5, 1.5] \times [0, 2]$.
- Discretize the domain Ω into $6 \times 6 \times 5$ hexahedra.
- $(u, Q) \xLeftarrow{\mathit{FEM}} (\mathbb{Q}_3 \times (\mathbb{Q}_2)^5)$ + interior penalty
- Choose parameters

$$a = -10,\ b = 0,\ c = 10,\ B = 10^{-3},\ K = 0.03,$$
$$q = 10,\ l = 30,\ w = 10.$$

TFCDs: problem settings

- Weakly enforcing top-bottom surfaces boundary conditions via

$$f_s(Q) = \int_{\Gamma_{bottom}} \frac{w}{2} \left|Q - Q_{radial}\right|^2 + \int_{\Gamma_{top}} \frac{w}{2} \left|Q - Q_{vertical}\right|^2,$$

  - w denotes the weak anchoring weight;
  - prescribed configuration at the bottom surface:

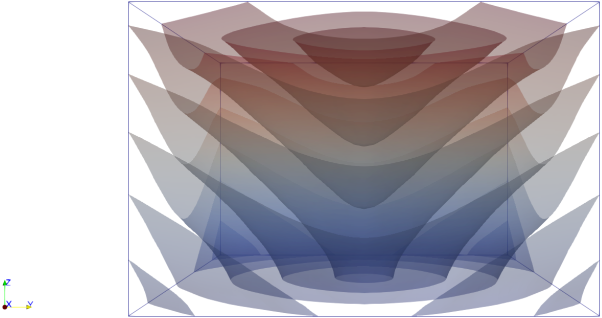
$$Q_{radial} = \begin{bmatrix} \frac{x^2}{\sqrt{x^2+y^2}} - \frac{1}{3} & \frac{xy}{\sqrt{x^2+y^2}} & 0 \\ \frac{xy}{\sqrt{x^2+y^2}} & \frac{y^2}{\sqrt{x^2+y^2}} - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix}$$

    represents the in-plane (x-y plane) radial configuration of the director;
  - prescribed configuration at the top surface:

$$Q_{vertical} = \begin{bmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix}$$

    gives the vertical (along the z-axis) alignment of directors.

TFCD solution



Zero iso-surfaces of the density variation u, colored by height.

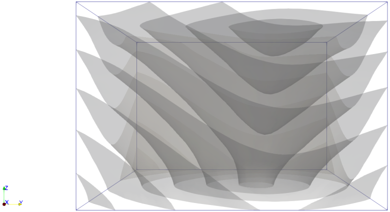
FCD solutions

- Replace the top boundary configuration $Q_{vertical}$ by a slightly tilted configuration Q_{tilt}:

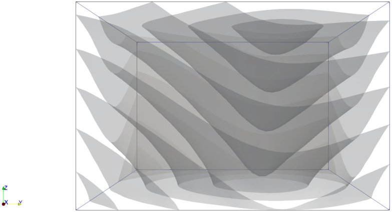
$$Q_{tilt} = \begin{bmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & (\sin(\theta))^2 - \frac{1}{3} & \sin(\theta)\cos(\theta) \\ 0 & \sin(\theta)\cos(\theta) & (\cos(\theta))^2 - \frac{1}{3} \end{bmatrix}, \qquad (3)$$

- θ (to be specified in experiments) is the zenith angle between the director and the z-axis.

Taking $\theta = \frac{\pi}{8}$



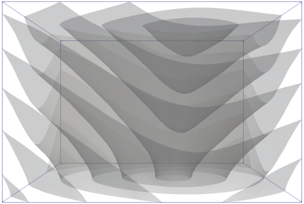
FCD



FCD

FCDs

Taking $\theta = \frac{\pi}{10}$



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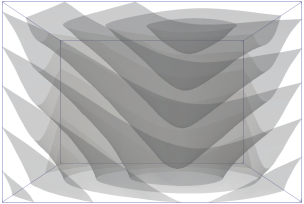
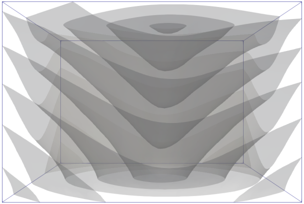
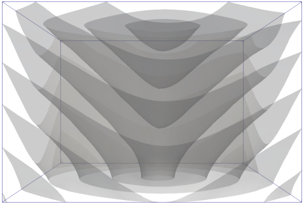


FCD

Taking $\theta = \frac{\pi}{12}$



FCD



FCD

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Conclusions

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Future work

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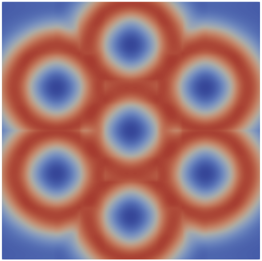
- Hexagonal packing of TFCDs?



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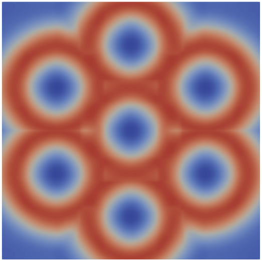
- Extension to simultaneously describe isotropic, nematic, smectic A and smectic C phases.
- Hexagonal packing of TFCDs?



Thank you for your attention!