# A Moving Mesh Finite Element Method for Modelling Defects in Liquid Crystals

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# Motivation

- Liquid crystals may have different equilibrium configurations: can force switching between stable states by altering applied voltage, magnetic field, boundary conditions, . . .
- Understanding the formation and dynamics of defects is important in the design and control of liquid crystal devices.
- Defects typically induce distortion over very small length scales as compared to the size of the cell.
- This poses significant challenges for standard numerical modelling techniques.
- In this talk we present a finite-element based adaptive moving mesh model designed to track defect movement.

# Q-tensor representation

- Represent average molecular orientation by symmetric traceless order tensor

$$\mathbf{Q} = \sqrt{\frac{3}{2}} \left\langle \mathbf{u} \otimes \mathbf{u} - \frac{1}{3}\mathbf{I} \right\rangle$$

with five degrees of freedom.

- Represent $\mathbf{Q}$ using a (non-unique) basis of five linearly-independent tensors, e.g.

$$\mathbf{Q} = \begin{bmatrix} q_1 & q_2 & q_3 \\ q_2 & q_4 & q_5 \\ q_3 & q_5 & -q_1 - q_4 \end{bmatrix}.$$

- Five unknowns for PDE model: $q_1,\ q_2,\ q_3,\ q_4,\ q_5$.

# Q-tensor equations

- Minimise the free energy

$$F = \int_V F_{bulk}(\mathbf{Q}, \nabla \mathbf{Q})\, dv$$

$$F_{bulk} = F_{elastic} + F_{thermotropic} + F_{electrostatic}$$

$$F_{elastic} = \frac{1}{2} L_1 (\mathrm{div}\ \mathbf{Q})^2 + \frac{1}{2} L_2 |\nabla \times \mathbf{Q}|^2$$

$$F_{thermotropic} = \frac{1}{2} A(T - T^*)\ \mathrm{tr}\ \mathbf{Q}^2 - \frac{\sqrt{6}}{3} B\ \mathrm{tr}\ \mathbf{Q}^3 + \frac{1}{4} C (\mathrm{tr}\ \mathbf{Q}^2)^2$$

$$F_{electrostatic} = -\frac{1}{2} \epsilon_0 \mathbf{E} \cdot \boldsymbol{\epsilon} \mathbf{E} - (\bar{e}\ \mathrm{div}\ \mathbf{Q}) \cdot \mathbf{E}$$

- Solutions with least energy are physically relevant: solve Euler-Lagrange equations.

# Derivation of time-dependent PDEs

- Use a dissipation function with viscosity coefficient $\nu$:

$$\mathcal{D} = \frac{\nu}{2}\mathrm{tr}\left[\left(\frac{\partial \mathbf{Q}}{\partial t}\right)^2\right] = \nu(\dot{q}_1\dot{q}_4 + \dot{q}_1^2 + \dot{q}_2^2 + \dot{q}_3^2 + \dot{q}_4^2 + \dot{q}_5^2).$$

- Obtain $\mathbf{Q}$-tensor PDEs (for $i = 1, \ldots, 5$ and $j = 1, 2, 3$):

$$\frac{\partial \mathcal{D}}{\partial \dot{q}_i} = \nabla \cdot \hat{\mathbf{\Gamma}}_i - \hat{f}_i,$$

$$(\hat{\mathbf{\Gamma}}_i)_j = \frac{\partial F_{bulk}}{\partial q_{i,j}}, \qquad q_{i,j} = \frac{\partial q_i}{\partial x_j}, \qquad \hat{f}_i = \frac{\partial F_{bulk}}{\partial q_i}.$$

- Combining equations and manipulating terms we can write

$$\frac{\partial q_i}{\partial t} = \nabla \cdot \mathbf{\Gamma}_i - f_i, \qquad i = 1, \ldots, 5.$$

# Coupling with electric field

- Additional unknown $U$ such that $\mathbf{E} = -\nabla U$.
- Assuming no free charges, solve the Maxwell equation $\nabla \cdot \mathbf{D} = 0$ for electric displacement $\mathbf{D}$.

**SUMMARY**

- Final time-dependent physical PDEs (PPDEs) are

$$\frac{\partial q_i}{\partial t} = \nabla \cdot \mathbf{\Gamma}_i - f_i, \qquad i = 1, \ldots, 5,$$

$$\nabla \cdot \mathbf{D} = 0.$$

- 6 PDEs in 6 unknowns $(q_1, q_2, q_3, q_4, q_5, U)$

# Adapt PPDEs for mesh movement

- Focus here on Moving Mesh PDE model.

  **Huang and Russell**, *Adaptive Moving Mesh Methods*, Springer (2011)

- Define physical domain $\Omega$ and computational domain $\Omega_c$.

- Map $\boldsymbol{\xi} = (\xi, \eta) \subset \Omega_c$ to $\mathbf{x} = (x, y) \subset \Omega$ using bijective mappings $\mathcal{A}_t : \Omega_c \to \Omega$ such that

$$\mathbf{x}(\boldsymbol{\xi}, t) = \mathcal{A}_t(\boldsymbol{\xi}).$$

- Define a mesh velocity

$$\dot{\mathbf{x}}(\mathbf{x}, t) = \left.\frac{\partial \mathbf{x}}{\partial t}\right|_{\boldsymbol{\xi}} (\mathcal{A}_t^{-1}(\mathbf{x}))$$

  and apply the Chain Rule to get

$$\left.\frac{\partial q}{\partial t}\right|_{\boldsymbol{\xi}} = \left.\frac{\partial q}{\partial t}\right|_{\mathbf{x}} + \dot{\mathbf{x}} \cdot \nabla q.$$

# Finite elements for the physical PDEs

- PPDEs in computational domain($i = 1, \dots, 5$):

$$\left.\frac{\partial q_i}{\partial t}\right|_{\boldsymbol{\xi}} - \dot{\mathbf{x}} \cdot \nabla q = \nabla \cdot \Gamma_i - f_i, \qquad \nabla \cdot \mathbf{D} = 0.$$

- Find $q_{ih}(t)$, $U_h$ such that, for test functions $v_h$,

$$\frac{d}{dt}\int_\Omega q_{ih} v_h \, \mathrm{d}\mathbf{x} - \int_\Omega (\nabla \cdot (\dot{\mathbf{x}} q_{ih}))\, v_h \, \mathrm{d}\mathbf{x} = \int_\Omega \Gamma_{ih} \cdot \nabla v_h \, \mathrm{d}\mathbf{x} - \int_\Omega f_{ih} v_h \, \mathrm{d}\mathbf{x},$$

$$\int_\Omega \mathbf{D}_h \cdot \nabla v_h \, \mathrm{d}\mathbf{x} = 0.$$

- Non-linear differential algebraic system $(i = 1, \dots, 5)$

$$\frac{d}{dt}(M(t)\mathbf{q}_i(t)) = \mathbf{G}_i(t, \mathbf{q}_i(t), \mathbf{u}(t)), \qquad \mathbf{C}(\mathbf{q}_i(t), \mathbf{u}(t)) = \mathbf{0}.$$

# Moving Mesh PDEs

- Avoid mesh crossings by evolving the inverse mapping

$$\mathcal{A}_t^{-1}(\mathbf{x}) = \boldsymbol{\xi}(\mathbf{x}, t).$$

- Choose mapping $\boldsymbol{\xi}(\mathbf{x})$ for a fixed $t$ to minimise

$$I[\boldsymbol{\xi}] = \frac{1}{2}\int_{\Omega_t} [(\nabla\xi)^T G^{-1}(\nabla\xi) + (\nabla\eta)^T G^{-1}(\nabla\eta)]\,\mathrm{d}\mathbf{x}$$

  with $2 \times 2$ symmetric positive definite monitor matrix $G$.

- For robustness, evolve mesh via gradient flow equations

$$\frac{\partial\xi}{\partial t} = \frac{P}{\tau}\nabla\cdot(G^{-1}\nabla\xi), \qquad \frac{\partial\eta}{\partial t} = \frac{P}{\tau}\nabla\cdot(G^{-1}\nabla\eta).$$

- User-specified parameters:
  - positive temporal smoothing parameter $\tau$;
  - positive spatial balancing function $P(\mathbf{x}, t)$.

# Final form of MMPDE

- Use Winslow monitor matrix with monitor function $w(\mathbf{x}, t)$:

$$G = \begin{bmatrix} w & 0 \\ 0 & w \end{bmatrix}.$$

- In practice, interchange variable roles in MMPDE to obtain

$$\tau \frac{\partial \mathbf{x}}{\partial t} = P(a\mathbf{x}_{\xi\xi} + b\mathbf{x}_{\xi\eta} + c\mathbf{x}_{\eta\eta} + d\mathbf{x}_{\xi} + e\mathbf{x}_{\eta}).$$

$$a = \frac{1}{w}\frac{x_\eta^2 + y_\eta^2}{J^2}, \quad b = -\frac{2}{w}\frac{(x_\xi x_\eta + y_\xi y_\eta)}{J^2}, \quad c = \frac{1}{w}\frac{x_\xi^2 + y_\xi^2}{J^2},$$

$$d = \frac{1}{(wJ)^2}[w_\xi(x_\eta^2 + y_\eta^2) - w_\eta(x_\xi x_\eta + y_\xi y_\eta),$$

$$e = \frac{1}{(wJ)^2}\left[-w_\xi(x_\xi x_\eta + y_\xi y_\eta) + w_\eta(x_\xi^2 + y_\xi^2)\right].$$

# Overview of full algorithm

Set an initial uniform mesh $\Delta_N^0$. Set the initial guess $\mathbf{q}_i^0$.
Select an initial $\Delta t^0$. Set $n = 0$.
**while** $(t^n < t^{\max})$;
    Evaluate monitor function at time $t^n$.
    Integrate MMPDE forward in time to obtain new grid $\Delta_N^{n+1}$.
    Integrate PPDEs forward using SDIRK2 to obtain $\mathbf{q}_i^{n+1}$, $\mathbf{u}^{n+1}$.
    $n := n + 1$.
**end while**.

# Choice of monitor function

- BM2: Based on **second-order partial derivatives** of $\mathcal{T}(\mathbf{x}, t)$:

$$w(\mathcal{T}(\mathbf{x},t)) = \alpha(\mathbf{x},t) + \left(\sqrt{\left(\frac{\partial^2\mathcal{T}}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2\mathcal{T}}{\partial x \partial y}\right)^2 + \left(\frac{\partial^2\mathcal{T}}{\partial y^2}\right)^2}\right)^{\frac{1}{m}}$$

- Scaling parameters $\alpha$ and $m$ regulate mesh clustering.

- Input function based on a direct invariant measure of biaxiality

$$\mathcal{T}(\mathbf{x},t) = \left[1 - \frac{6\,\mathrm{tr}(\mathbf{Q}^3)^2}{\mathrm{tr}(\mathbf{Q}^2)^3}\right]^{\frac{1}{2}}.$$

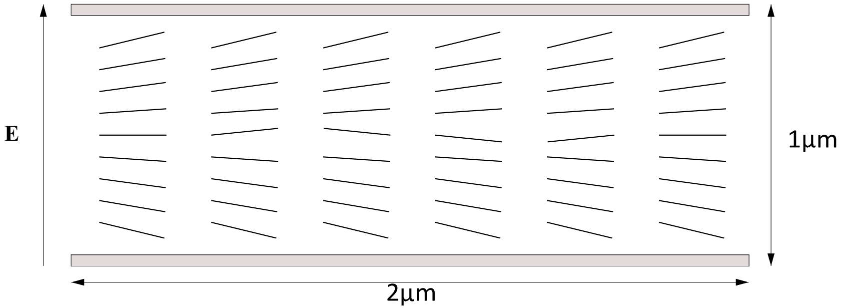
- This has an extremum at the centre of a defect and varies rapidly in the immediate neighbourhood of the defect centre.

# Test problem: 2D Pi-cell

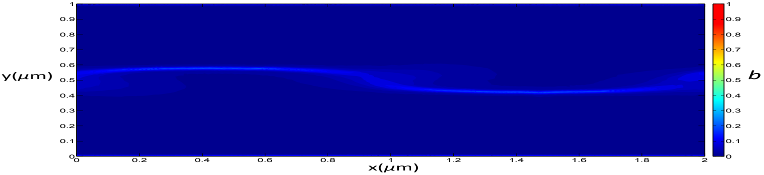
- Two-dimensional Pi-cell geometry.
  **Zhang, Chung, Wang and Bos**, *Liquid Crystals* 34(2), 2007
- Electric field applied parallel to the cell thickness.
- Inhomogeneous transition mediated by the nucleation of defect pairs moving and annihilating each other.
- Initial director angle across cell centre follows $\sin(2\pi x/p)$ for cell width $p$ at $t = 0$ for one time step.
- Use triangular grid with quadratic basis functions for PPDEs, linear basis functions for MMPDE.

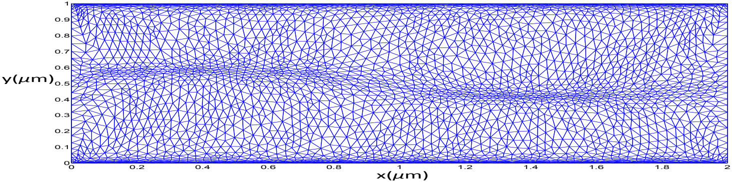
# Pi-cell geometry

- Pre-tilt angle $\theta = \pm 6^\circ$ at boundaries.
- Electric field strength $18 V \mu\mathrm{m}^{-1}$.

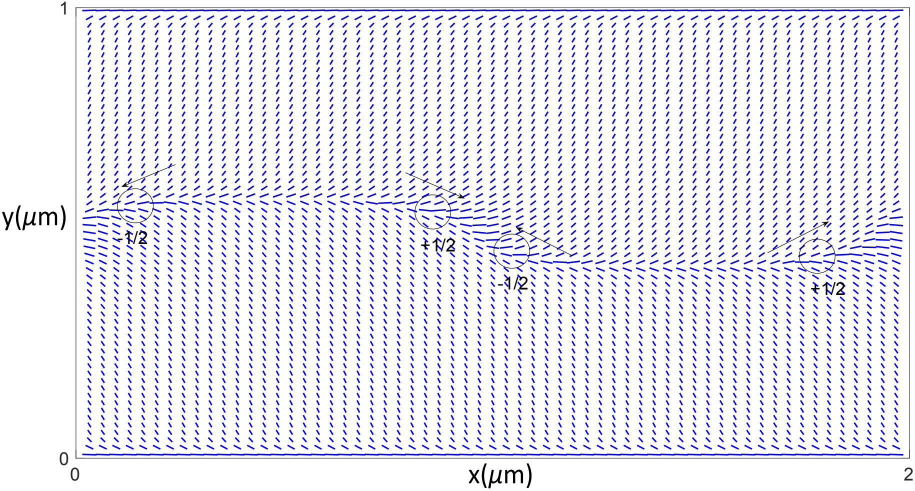


# Biaxiality and mesh after 12$\mu$s

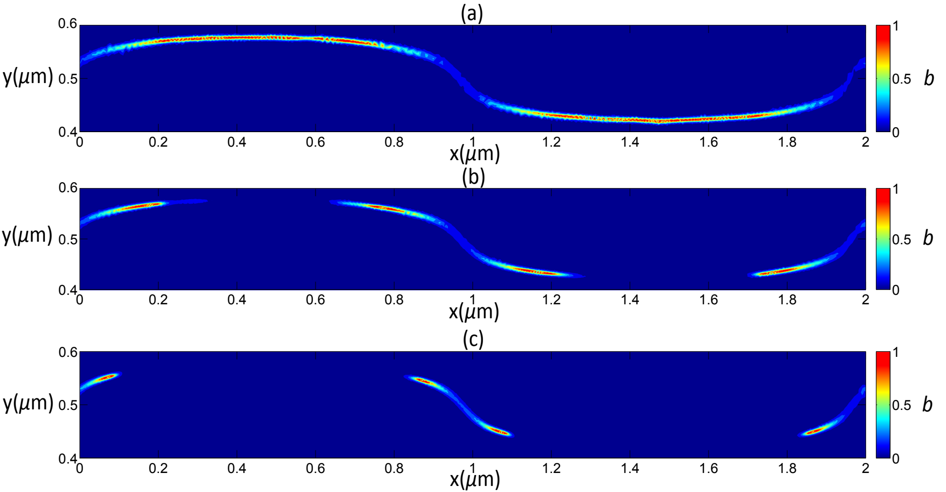


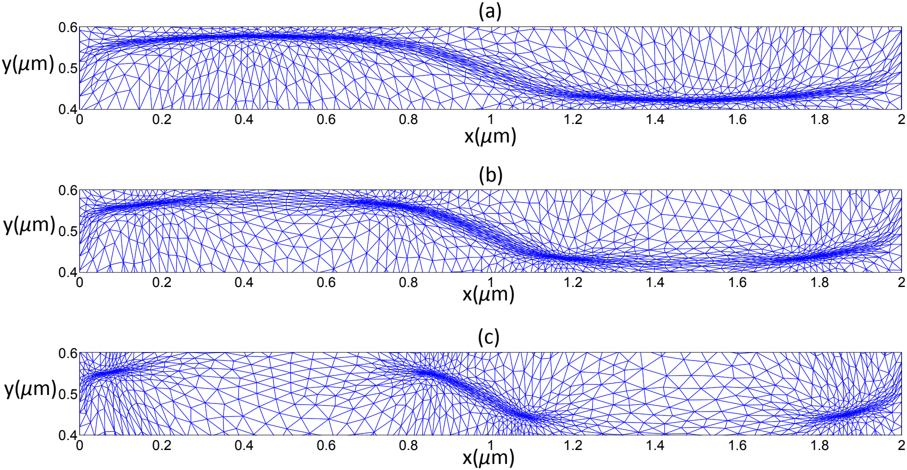
# Director field after 15.5$\mu$s



# Biaxiality after (a) 15.5$\mu$s (b) 16$\mu$s and (c) 17$\mu$s



# Adaptive mesh after (a) 15.5$\mu$s (b) 16$\mu$s and (c) 17$\mu$s



# Summary and future work

- New efficient moving mesh method for **Q**-tensor models of liquid crystal cells.
- Found biaxiality to be a good choice for the monitor input function.
- Demonstrated optimal spatial convergence for a model of a static $+1/2$ defect.
- Method resolved the movement and core details of defects (including creation and annihilation) in a time-dependent Pi-cell problem.

  **MacDonald, Mackenzie and Ramage**, *JCP:X* 8, 2020
- Future challenges involve the extension to more irregular geometries (e.g. the ZBD) and three dimensions.