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

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Motivation

- 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.

Liquid crystal model: $\mathbf{Q}$-tensor theory

- Describe the orientation of each molecule in a uniaxial nematic liquid crystal by a single vector $\mathbf{u}$ in direction of its main axis.
- Represent average orientation by symmetric traceless order tensor

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

- Use orthogonal eigenframe $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ to write

$$\mathbf{Q} = S\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right) + T(\mathbf{m} \otimes \mathbf{m} - \mathbf{l} \otimes \mathbf{l})$$

  where S and T are uniaxial and biaxial order parameters.
- Consider a uniaxial molecular distribution ($T = 0$) where the (unit) eigenvector $\mathbf{n}$ is known as the liquid crystal director

$\mathbf{Q}$-tensor representation

- Symmetric traceless tensor $\mathbf{Q}$ has 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

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

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

- With strong anchoring (Dirichlet boundary conditions), there is no contribution from the surface energy.

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

Bulk energies

- Elastic: induced by distorting the **Q**-tensor in space

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

- Thermotropic: potential function which dictates which preferred state (uniaxial, biaxial or isotropic)

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

- Electrostatic: due to an applied electric field **E** (electric potential U with $\mathbf{E} = -\nabla U$).

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

Derivation of time-dependent PDEs

- Use a dissipation function with viscosity coefficient ν:

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

- Obtain **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 $\mathbf{D}$.

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SUMMARY

- Final time-dependent physical PDEs (PPDEs) are

$$\begin{aligned} \frac{\partial q_i}{\partial t} &= \nabla \cdot \boldsymbol{\Gamma}_i - f_i, \qquad i = 1, \ldots, 5, \\ \nabla \cdot \mathbf{D} &= 0. \end{aligned}$$

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

Adaptive finite element methods

- Three common forms of grid adaptivity in finite elements:
  - *h*-refinement: uniform mesh locally coarsened or refined, normally based on *a posteriori* error estimates;
  - *p*-refinement: order of local polynomial approximation is increased or decreased in accordance with solution error;
  - *r*-refinement: original mesh points are moved to areas where high resolution is needed.

- Advantages of moving meshes:
  - retaining fixed number of mesh points and connectivity;
  - interpolation from old to new mesh unnecessary for time-dependent problems.

- Focus here on Moving Mesh PDE model.

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

Adapt PPDEs for mesh movement

- Define physical domain Ω and computational domain Ω_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

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

- Additional convection-like term due to the mesh movement

Finite elements for the physical PDEs

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

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

- 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 ($i = 1, \ldots, 5$)

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

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 2×2 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 τ;
  - 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

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

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

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

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

Additional details for MMPDE

- Discretise in space using linear finite elements.
- Discretise in time using a backward Euler scheme.
- Boundary conditions obtained using a 1D MMPDE.
- To avoid solving nonlinear algebraic systems, at $t = t^{n+1}$ evaluate coefficients a, b, c, d, e at the time $t = t^n$.
- Solve resulting linear systems using iterative method BiCGSTAB with Incomplete LU preconditioner.
- Adaptive time-stepping based on computed solutions of PPDEs and MMPDE.

Overview of full algorithm

Set an initial uniform mesh Δ_N^0. Set the initial guess $\mathbf{q}_i^0$.
Select an initial Δt^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 Δ_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

- Choose input function $\mathcal{T}(\mathbf{x}, t)$.
- Three different forms of monitor function.
  - AL. Based on a measure of the **arc-length** of $\mathcal{T}$:

$$w(\mathcal{T}(\mathbf{x}, t)) = \left(1 + |\nabla \mathcal{T}(\mathbf{x}, t)|^2\right)^{\frac{1}{2}}$$

  - BM1: Based on **first-order partial derivatives** of $\mathcal{T}$:

$$w(\mathcal{T}(\mathbf{x}, t)) = \alpha(\mathbf{x}, t) + |\nabla \mathcal{T}(\mathbf{x}, t)|^{\frac{1}{m}}$$

  - BM2: Based on **second-order partial derivatives** of $\mathcal{T}$:

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

- Scaling parameters α and m regulate mesh clustering.

Choosing the input function

- Two different forms of input function.
  - Scalar order parameter. Based on the trace of $\mathbf{Q}^2$:

$$\mathcal{T}(\mathbf{x}, t) = \mathrm{tr}(\mathbf{Q}^2)$$

$\mathrm{tr}(\mathbf{Q}^2) = S^2$ for a uniaxial state with scalar order parameter S

  - Biaxiality. Based on a direct invariant measure of biaxiality

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

which takes values ranging from 0 (uniaxial) to 1 (fully biaxial).

- Both have extrema at the centre of a defect and vary rapidly in the immediate neighbourhood of the defect centre.

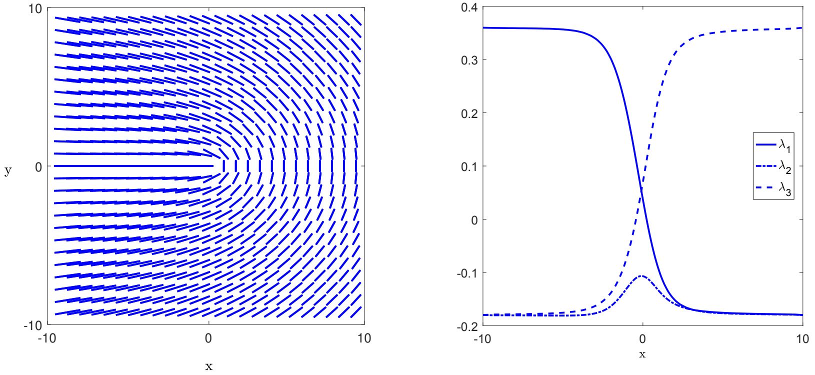
Numerical experiments

- PPDEs non-dimensionalised with respect to lengths and energies.
- Use triangular grid with quadratic basis functions for PPDEs, linear basis functions for MMPDE.
- Monitor/input function combinations:

Method name	AL	BM1a	BM1b	BM2b
Monitor function	AL	BM1	BM1	BM2
Input function	$\mathrm{tr}(\mathbf{Q}^2)$	$\mathrm{tr}(\mathbf{Q}^2)$	biaxiality	biaxiality

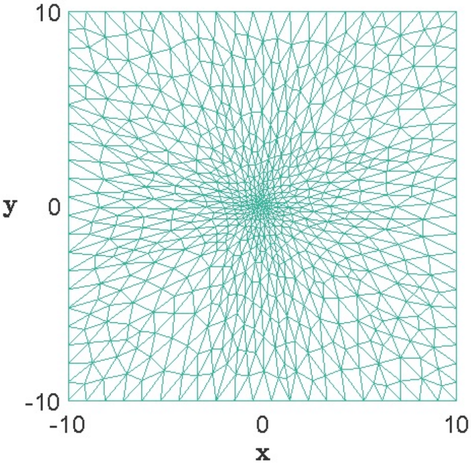
- All experiments in MATLAB.

Test problem 1: stationary defect



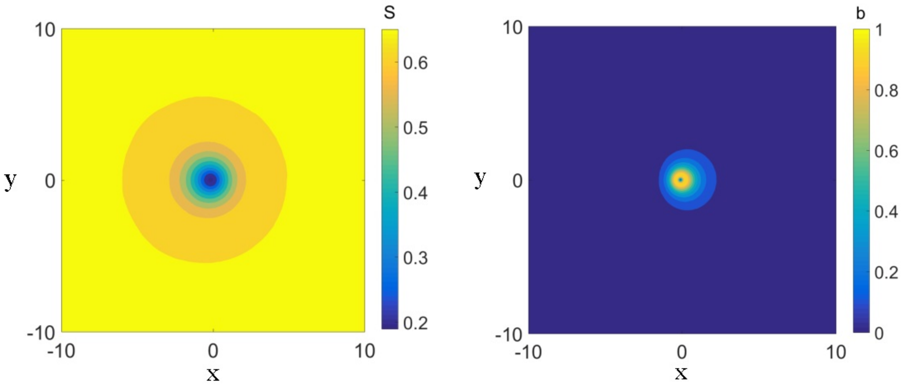
Director field of $1/2$ defect and eigenvalue exchange along $y = 0$.

Typical adapted grid



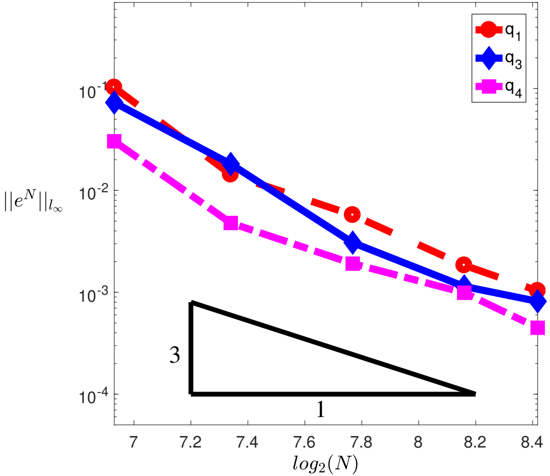
Sample adapted grid with 1388 quadratic elements.

Typical solutions



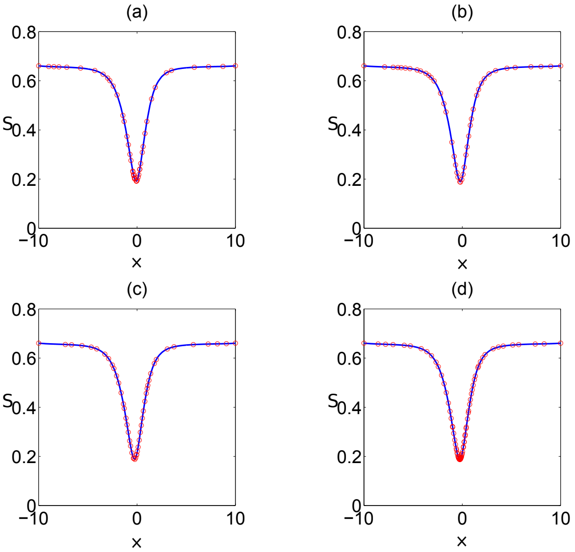
Scalar order parameter S and biaxiality.

Estimated rate of spatial convergence



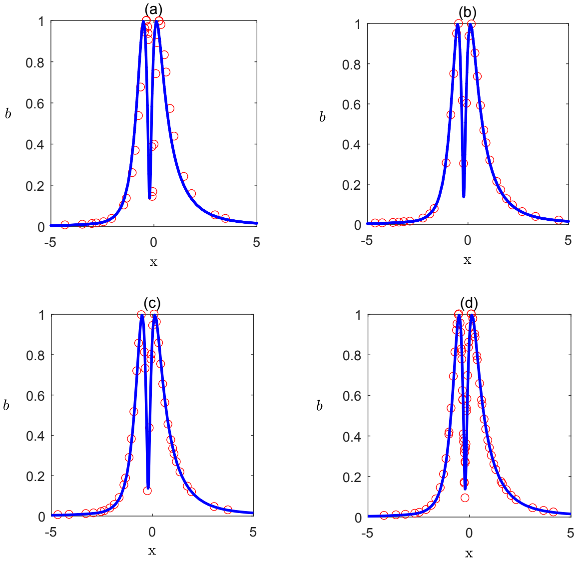
ℓ_∞ error compared with reference solution is $O(N^{-3})$.

Scalar order parameter along line $y = 0$



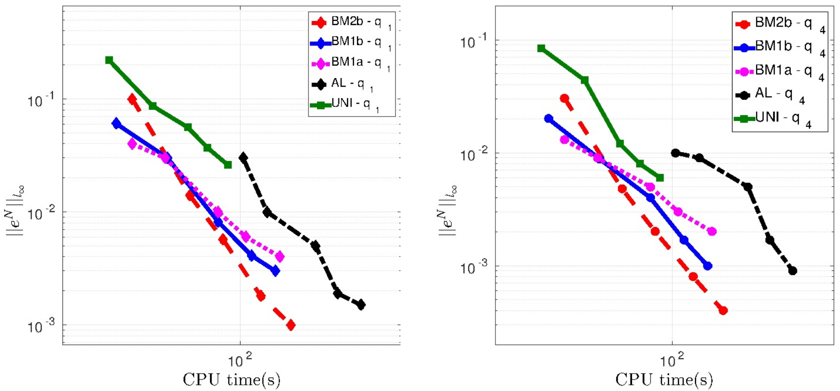
(a) AL (b) BM1a (c) BM1b (d) BM2b

Biaxiality along line $y = 0$



(a) AL (b) BM1a (c) BM1b (d) BM2b

Comparing computational costs



CPU time versus ℓ_∞ error for different grid sizes

- BM2b established as combination of choice.

Test problem 2: 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 at time $t = 0$.

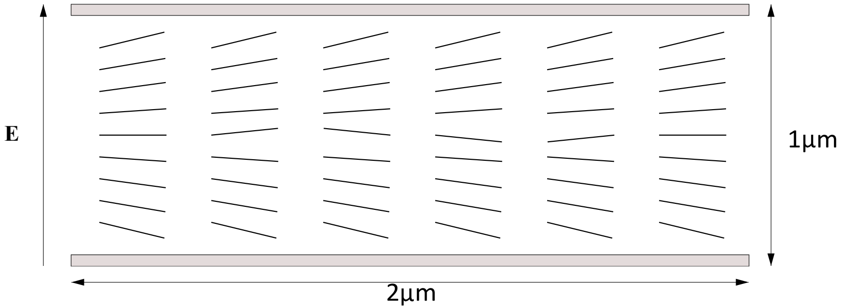
- Inhomogeneous transition mediated by the nucleation of defect pairs moving and annihilating each other.

- Initial director angle across cell centre follows $\sin(2\pi x/p)$ for cell width p.

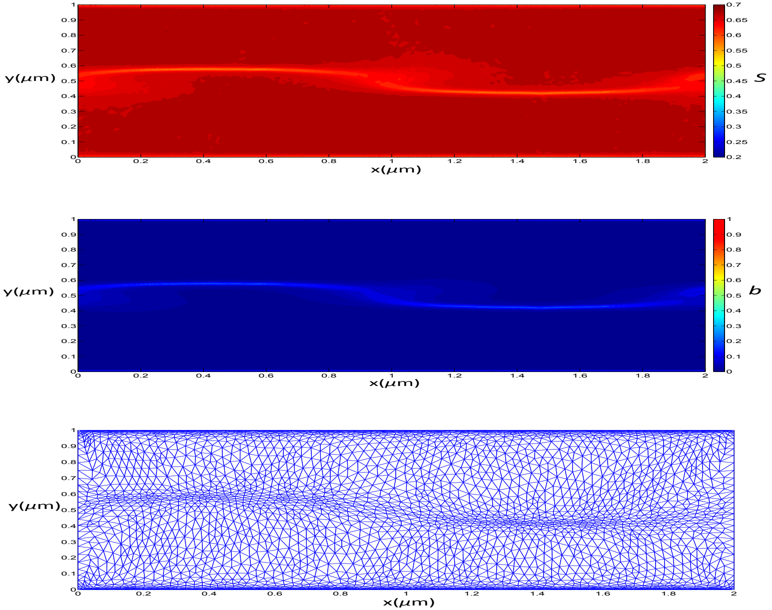
- Perturbation fixed only at $t = 0$ for one time step, but introduces solution gradients in two dimensions.

Pi-cell geometry

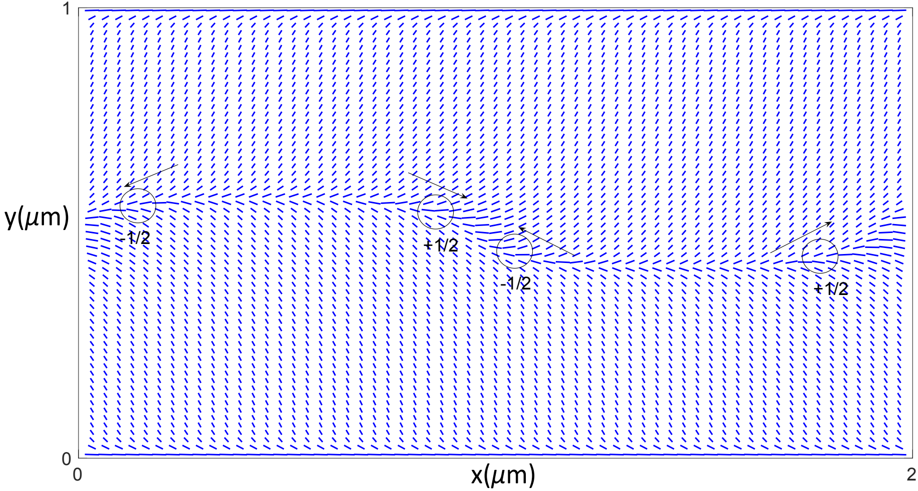
- Pre-tilt angle $\theta = \pm 6^\circ$ at boundaries.
- Electric field strength $18V\mu\mathrm{m}^{-1}$.



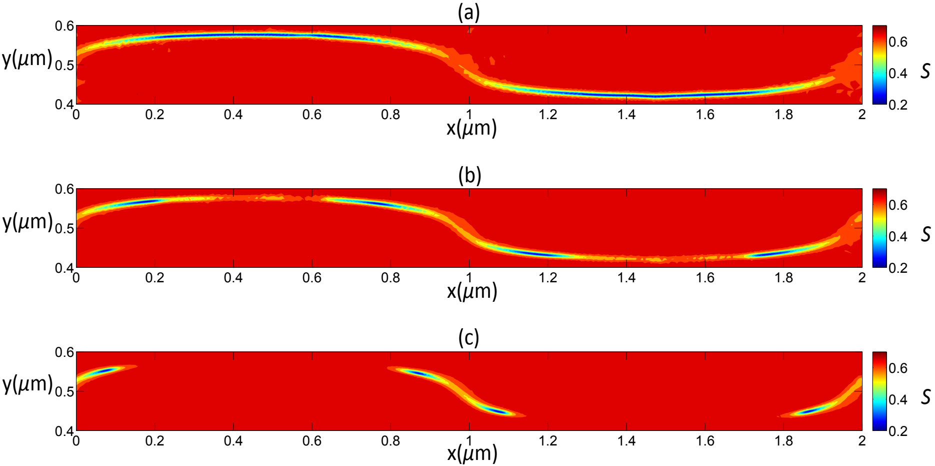
S, biaxiality and mesh after 12μs



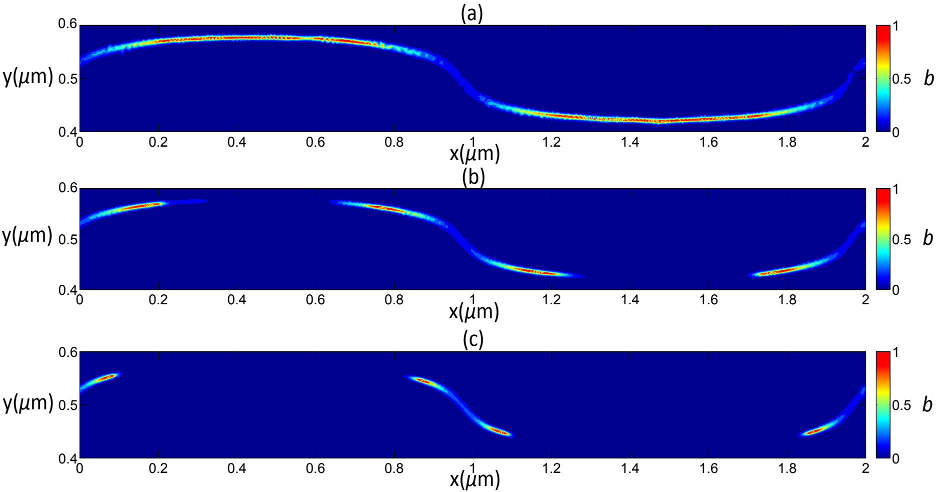
Director field after 15.5μs



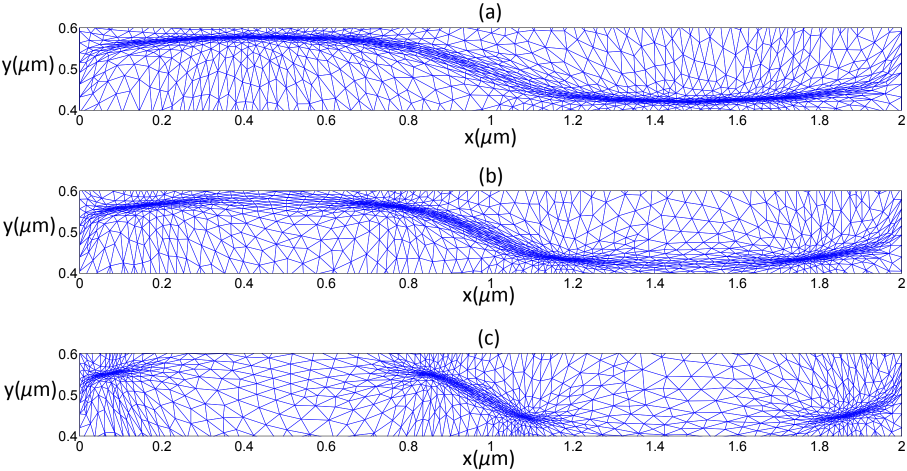
Order parameter S after (a) 15.5μs (b) 16μs and (c) 17μs



Biaxiality after (a) 15.5μs (b) 16μs and (c) 17μs



Adaptive mesh after (a) 15.5μs (b) 16μs and (c) 17μs



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.