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

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Motivation

- Defects in a liquid crystal can arise due to external factors such as applied electric or magnetic fields, or the constraining geometry of the liquid crystal cell.
- 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 for tracking defect movement.

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

- most common nematic LC consists of effectively uniaxial molecules: describe orientation of each molecule by a single vector $\mathbf{u}$ in direction of its main axis
- represent average orientation by symmetric and traceless order tensor

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

- with orthogonal eigenframe $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$:

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

S, T uniaxial and biaxial order parameters

- we consider uniaxial molecular distribution ($T = 0$) where the (unit) eigenvector $\mathbf{n}$ is known as the liquid crystal director

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

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

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

- we can derive expressions for individual energy contributions in terms of $\mathbf{Q}$, $\nabla\mathbf{Q}$

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

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

Bulk energies

- elastic energy: 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 energy: 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 energy: 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 gives

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

Coupling with electric field

- additional unknown U such that $\mathbf{E} = -\nabla U$
- assuming no free charges, solve the Maxwell equation

$$\nabla \cdot \mathbf{D} = 0, \qquad \text{electric displacement } \mathbf{D}$$

$$\boxed{\textbf{SUMMARY}}$$

- final time-dependent physical PDEs (PPDEs) are

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

- 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: initially uniform mesh is locally coarsened or refined by inclusion or deletion of mesh points, 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.

Adapt PPDEs for mesh movement

- physical domain Ω, computational domain Ω_c
- bijective mappings $\mathcal{A}_t : \Omega_c \to \Omega$ map $\boldsymbol{\xi} = (\xi, \eta) \subset \Omega_c$ to $\mathbf{x} = (x, y) \subset \Omega$:

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

- define 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

- final set of six coupled PDEs ($i = 1, \ldots, 5$):

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

- 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 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

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

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 function spatial balancing parameter $P(\mathbf{x}, t)$

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

- boundary conditions obtained using a 1D MMPDE
- discretise in space using linear finite elements
- discretise in time using a backward Euler scheme
- 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.

Choosing the 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

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

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

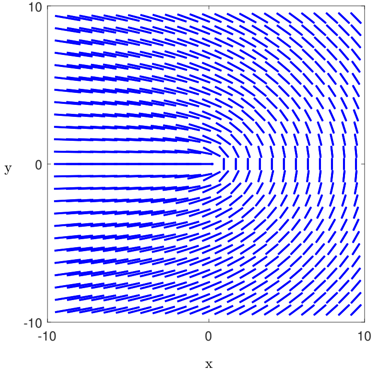
- PPDEs non-dimensionalised with respect to lengths and energies
- use quadratic triangular finite elements for PPDEs, linear finite elements for MMPDE
- Monitor/input function combinations:

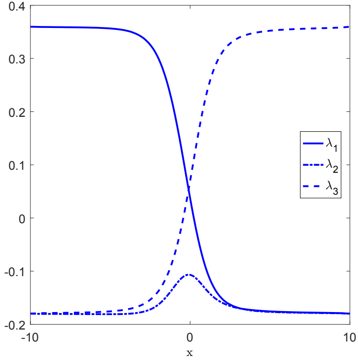
Method name	AL	BM1a	BM1b	BM2b
Monitor function	AL	BM1	BM1	BM2
Input function	$\mathrm{tr}(\mathbf{Q}^2)$	$\mathrm{tr}(\mathbf{Q}^2)$	biaxiality	biaxiality

- all experiments in MATLAB

Test problem 1: stationary defect

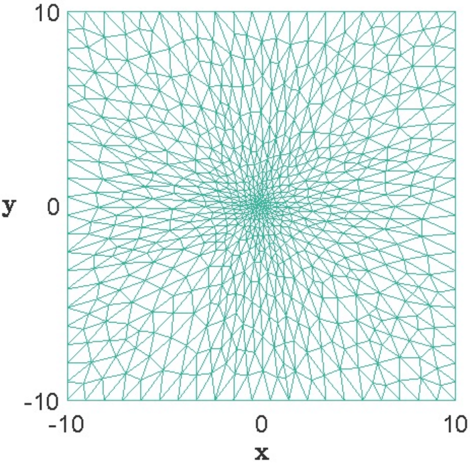
- director field of 1/2 defect and eigenvalue exchange along $y = 0$



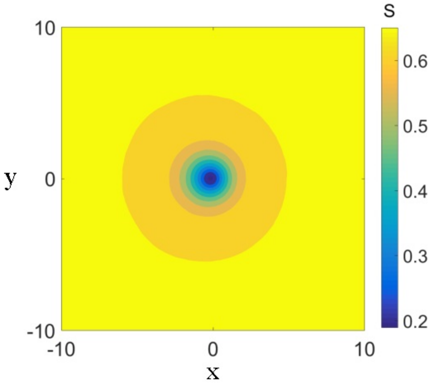


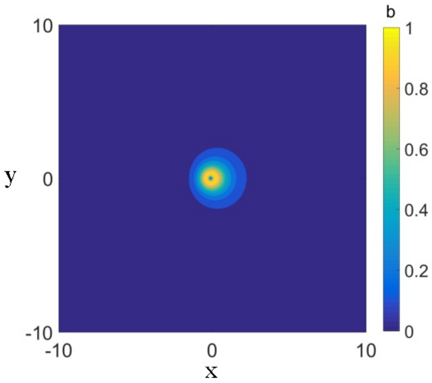
Typical adapted grid

- sample adapted grid with 1388 quadratic elements



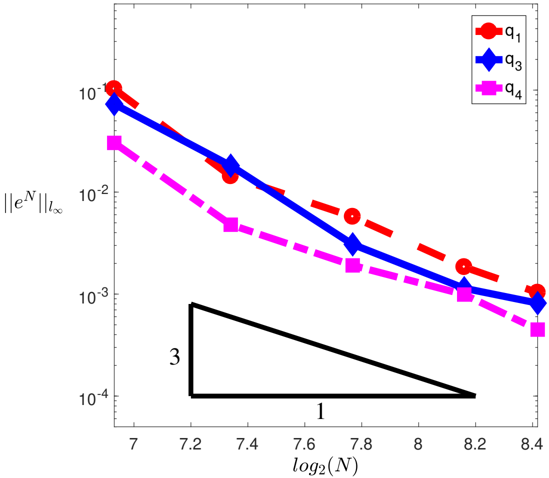
- scalar order parameter S and biaxiality





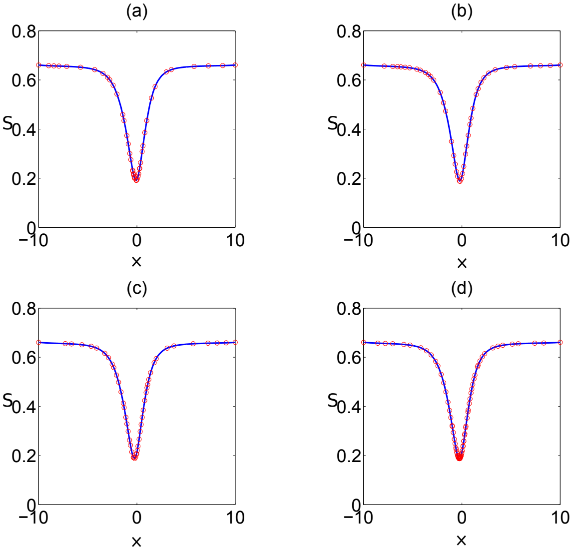
Estimated rate of spatial convergence

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



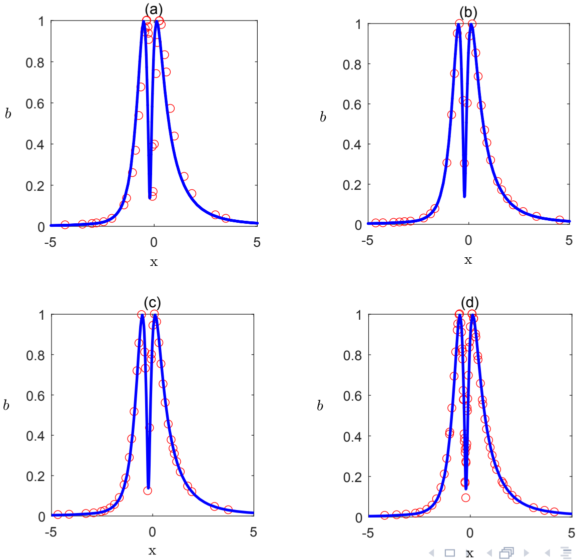
Scalar order parameter along line $y = 0$

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



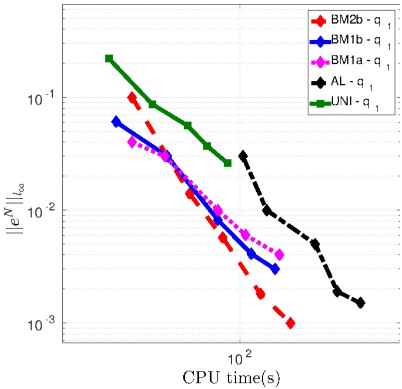
Biaxiality along line $y = 0$

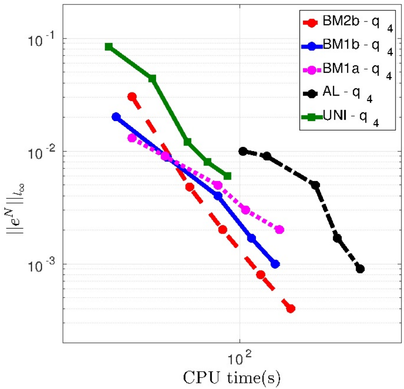
- (a) AL; (b) BM1a; (c) BM1b; (d) BM2b



Comparing computational costs

- CPU time versus ℓ_∞ error for different grid sizes



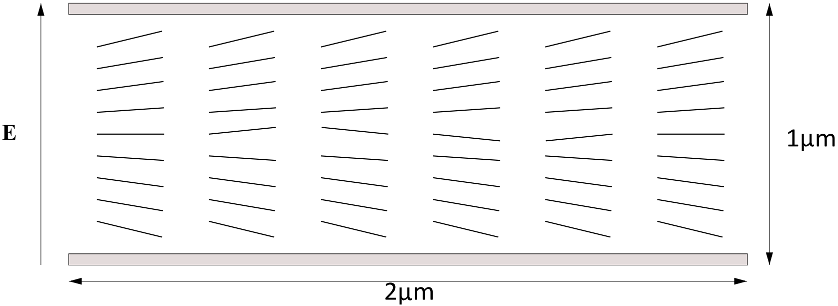


- BM2b established as combination of choice

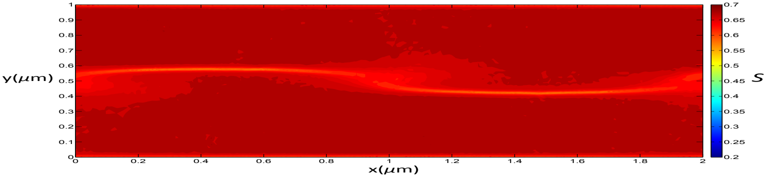
Test problem 2: 2D Pi-cell

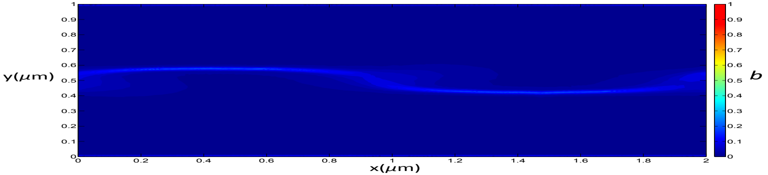
- two-dimensional Pi-cell geometry
  Zhang, Chung, Wang and Bos, *Liquid Crystals* 34(2), 2007
- electric field applied parallel to the cell thickness at time $t = 0$
- inhomogeneous transition mediated by the nucleation of defect pairs moving and annihilating each other
- initial director angle across 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

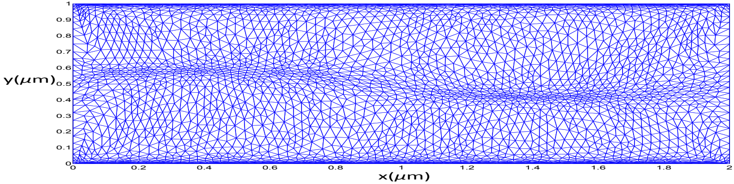
- pre-tilt angle $\theta = \pm 6^\circ$ at boundaries
- electric field strength $18 V \mu\mathrm{m}^{-1}$



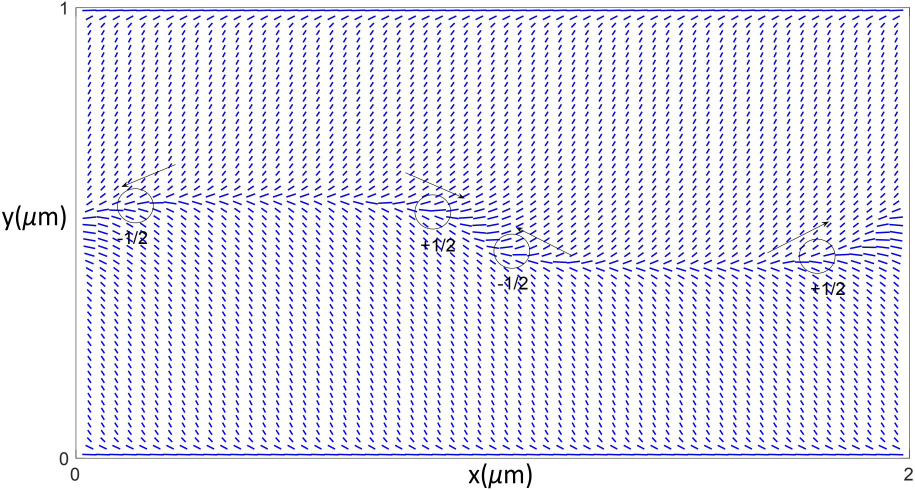
S, biaxiality and mesh after 12μs



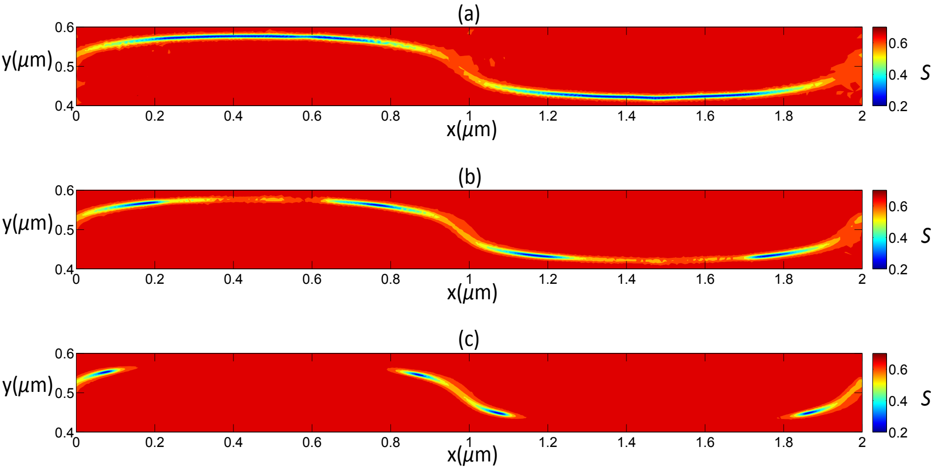




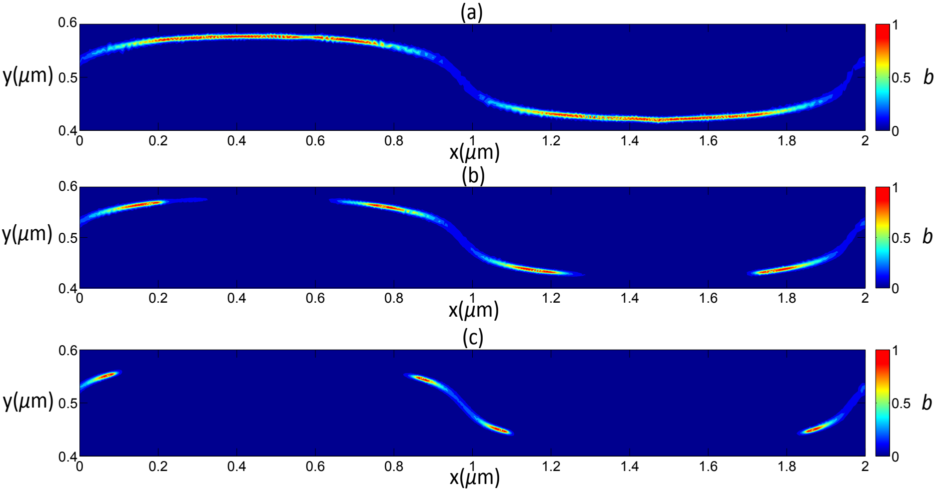
Director field after 15.5μs



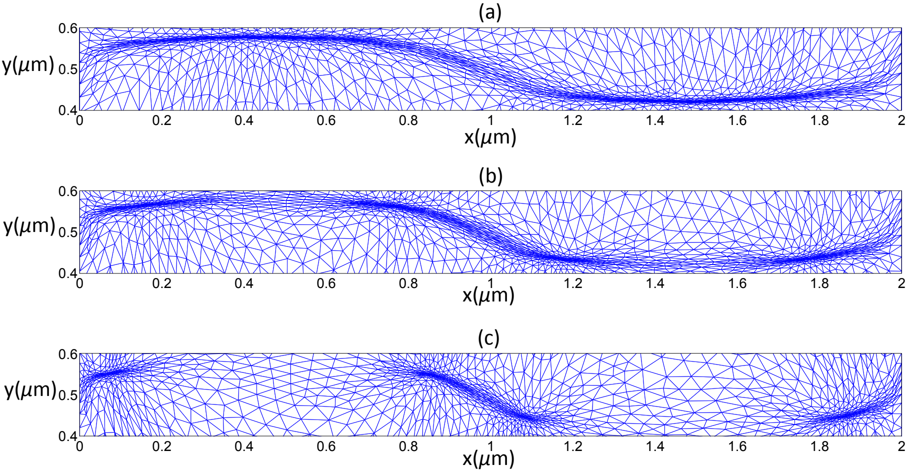
Order parameter S after (a) 15.5μs (b) 16μs and (c) 17μs



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

- We have developed a new efficient moving mesh method for $\mathbf{Q}$-tensor models of liquid crystal cells.
- We have shown that biaxiality is a good choice for the monitor input function.
- We demonstrated optimal spatial convergence for a model of a static $+1/2$ defect.
- We resolved the movement and core details of defects in a time-dependent Pi-cell problem.
- Modelling the creation and annihilation of moving singularities on very small length and time scales is a real challenge for numerical methods.
- Future challenges involve the extension to three dimensions and more irregular geometries (e.g. the ZBD).