Adaptive Grid Methods for Q-tensor Theory of Liquid Crystals

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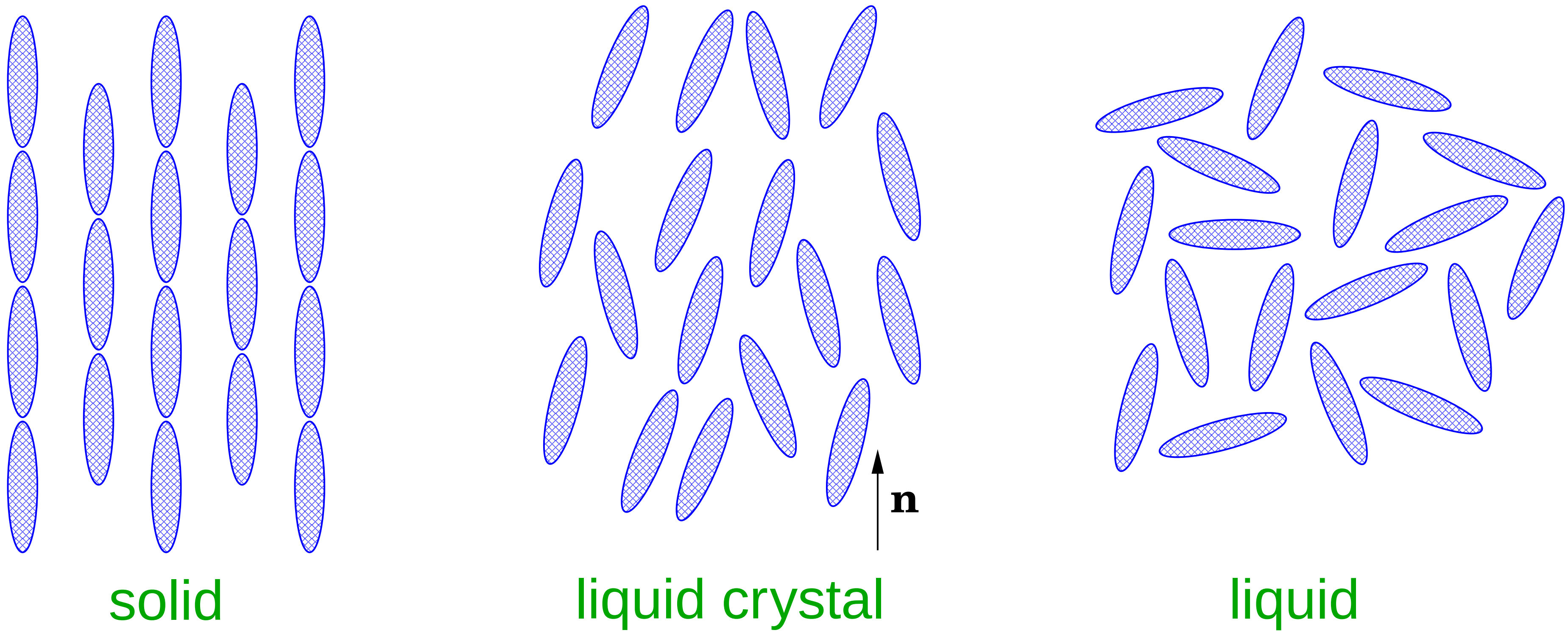
Liquid Crystals

- occur between solid crystal and isotropic liquid states



- director: average direction of molecular alignment

$$\mathbf{n} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$$

- order parameter: measure of orientational order

$\mathbb{Q}$-tensor Theory

- aim: minimise free energy density

$$\mathcal{F} = \int_V F(\theta, \phi, \nabla\theta, \nabla\phi)\, dV$$

- problems with multivalued angles/singularities
- tensor order parameter

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

- express free energy density as

$$\mathcal{F} = \int_V F(q_i, \nabla q_i)\, dV, \qquad i = 1, 2, 3, 4, 5$$

Motivation from Hewlett-Packard

- model: Q-tensor model of nematic liquid crystal cell
- aim: model dynamics of defect movement
- problem: characteristic lengths with large scale differences
- uniform grid: many grid points needed to capture defect behaviour
- idea: use adaptive grid methods to ensure there is no waste of computational effort

1D Model Problems

- homogeneous uniaxial alignment in $\Omega \equiv z \in [0, d]$
- z-axis aligned with $\mathbf{n}$

$$Q = \sqrt{\frac{3}{2}} S \begin{bmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{bmatrix}$$

Q depends only on scalar order parameter S

- bulk energy densities (A_s, B_s, C_s, L_{1s}, S_{eq}, F_{eq} +ve)

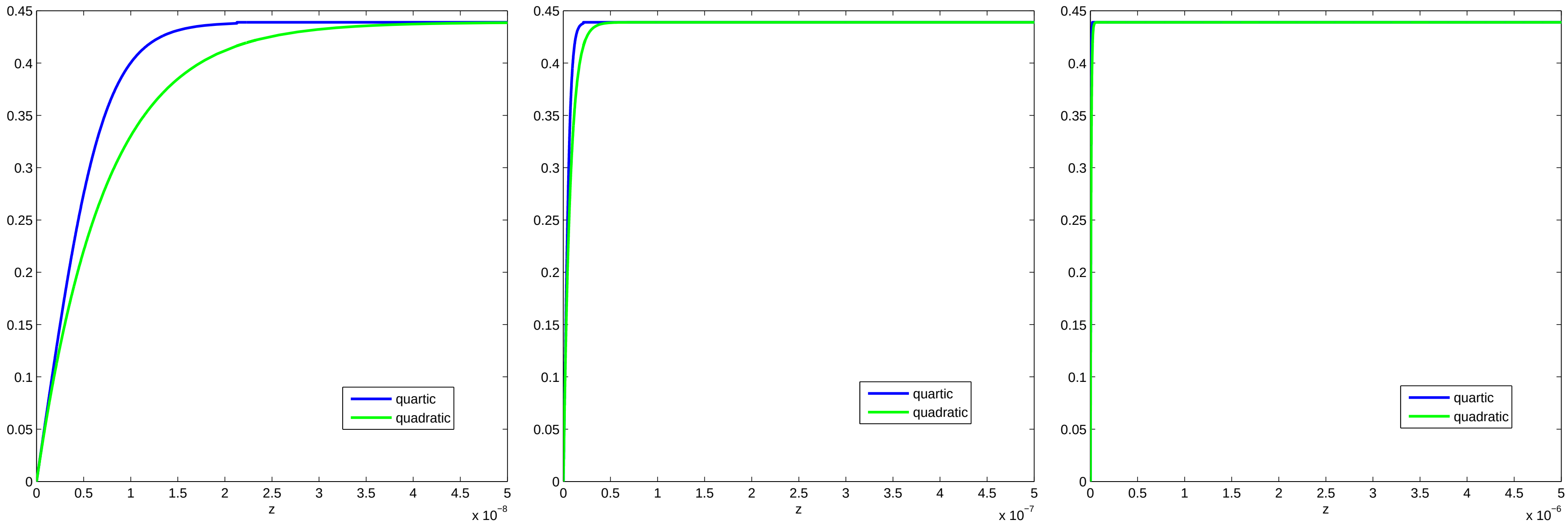
$$\frac{1}{2}A_s S^2 - \frac{1}{3}B_s S^3 + \frac{1}{4}C_s S^4 \quad + \quad \left(\frac{2L_{1s}+1}{6}\right)\left(\frac{\partial S}{\partial z}\right)^2 \quad (1)$$

$$\frac{F_{eq}}{S_{eq}} S \left(2 - \frac{1}{S_{eq}} S\right) \quad + \quad \left(\frac{2L_{1s}+1}{6}\right)\left(\frac{\partial S}{\partial z}\right)^2 \quad (2)$$

Analytic Solutions

$$\int_0^{S(z)} \frac{ds}{\sqrt{G(S) - G(S_{eq})}} = z \qquad G(S) = \alpha S^2 - \frac{2\beta}{3} S^3 + \frac{\gamma}{2} S^4$$

$$S(z) = S_{eq}\left(\frac{\sinh \rho z}{\tanh \rho d_s} - \cosh \rho z + 1\right) \qquad \rho = \sqrt{\left|\frac{6F_{eq}}{S_{eq}^2(2L_{1s}+1)}\right|}$$



$d = 0.1$ microns $\qquad$ $d = 1$ micron $\qquad$ $d = 10$ microns

Adaptive Grid Methods

- local mesh refinement: h refinement, p refinement
  - extra nodes added locally in regions of high error
  - often requires complicated data structures which need updating frequently

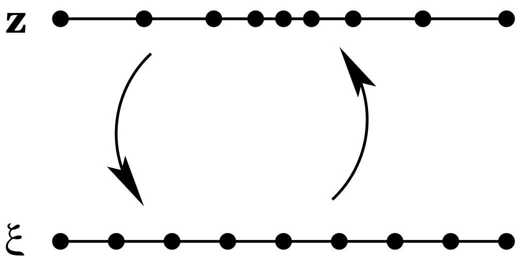
- moving mesh methods: r refinement
  - existing node points are moved to regions of high error
  - same grid connectivity maintained
  - comparatively easy extension of existing software

location-based method: adaptive grid on physical domain is image of uniform grid on computational domain under a suitable mapping

Equidistribution Principle in 1D

- coordinate transformation:

$$z = z(\xi, t),\ \xi \in [0,1]$$
$$z(0,t) = 0,\ z(1,t) = 1$$



- equidistribution principle (EP):

$$\int_0^{z(\xi,t)} M(s,t)\, ds = \xi \int_0^1 M(s,t)\, ds$$

- choose (positive) monitor function $M(z,t)$ e.g.

$$M(S(z,t)) = \sqrt{\hat{\alpha} + \left(\frac{\partial S}{\partial z}\right)^2}$$

Aside on MMPDEs

- equidistribution principle
  differentiate EP twice with respect to ξ

- variational principle
  find Euler-Lagrange equation associated with

$$I[z] = \frac{1}{2}\int_0^1 z_\xi^2(\xi)M^2(z(\xi))\,d\xi$$

$$z_{\xi\xi} + \frac{M_\xi}{M} z_\xi = 0$$

elliptic equidistribution generator

Theoretical Accuracy

- measure of error: using linear interpolant S_I

$$\|e\|_{L_\infty(0,d)} = \max_{z\in[0,d]} |S_{exact}(z) - S_I(z)|$$

- for green problem, it can be shown that

$$\|e\|_{L_\infty(0,d)} \leq \frac{C}{N^2}$$

  with both uniform and adaptive grids

- for red problem, using practical measure

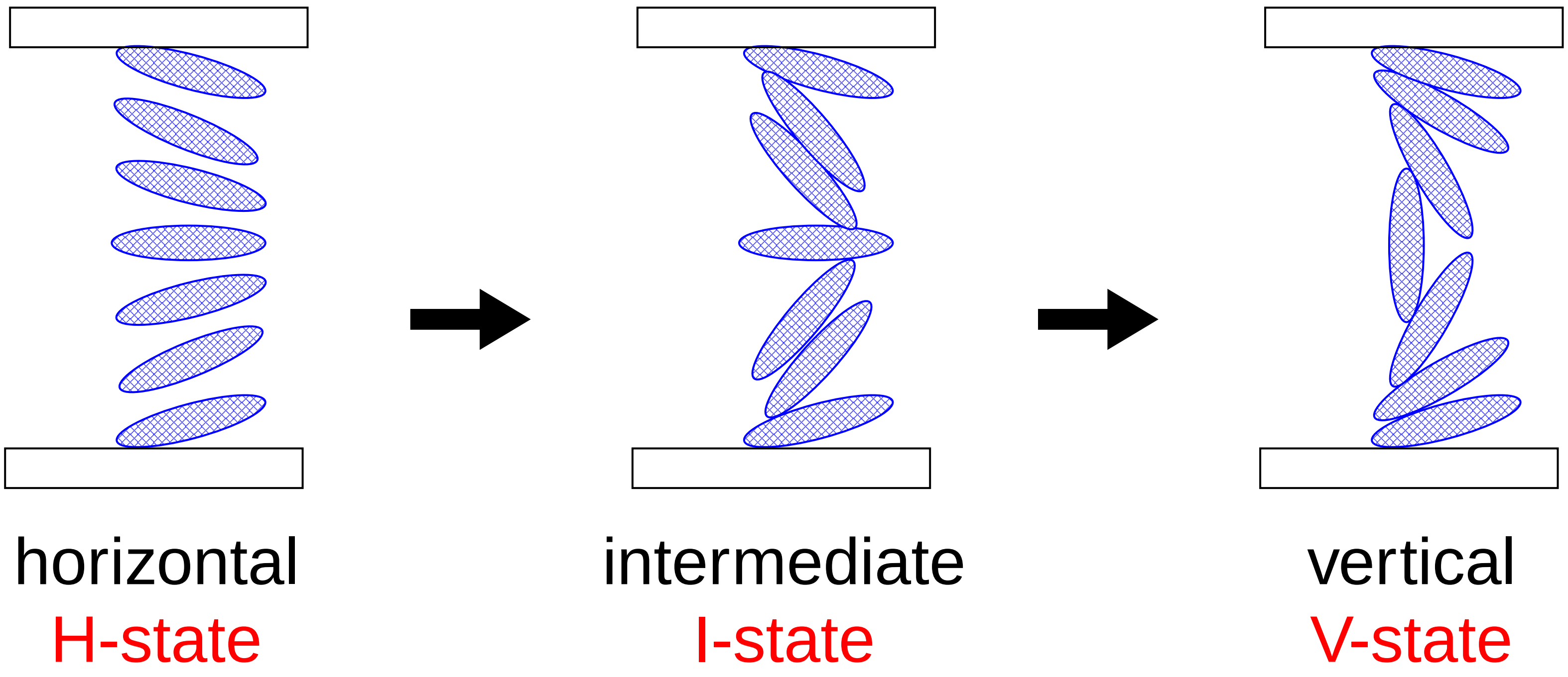
$$l_\infty = \max_{j=0,\dots,N/2} |S_f(z_j) - S_N(z_j)|$$

  adaptive grid error is $O(N^{-2})$

Order Reconstruction Problem I

Barberi et al., Eur. J. Phys. E (2004)

- cell surface treated at boundaries to induce alignments uniformly tilted by a specified tilt angle but oppositely directed
- two topologically different equilibrium states: mostly horizontal alignment with a slight splay, mostly vertical alignment with a bend of almost π radians



Order Reconstruction Problem II

- aim: model order reconstruction which takes place when an electric field is applied
- no longer purely uniaxial: need full Q-tensor
- 5 coupled PDEs for q_is, plus PDE for electric potential U
- 1D domain $z \in [0, d]$, monitor based on $T(z) = \mathrm{tr}(Q^2)$

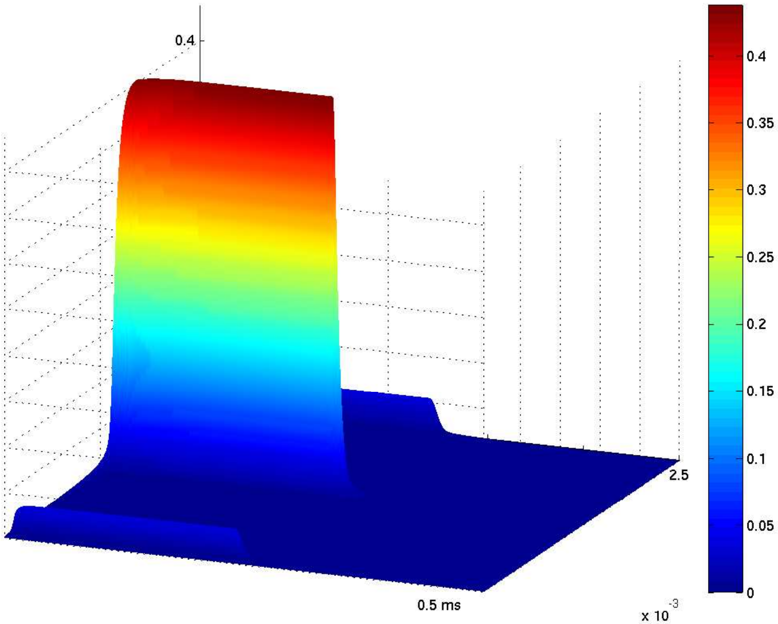
$$M(T(z)) = \sqrt{1 + \left(\frac{dT}{dz}\right)^2}$$

- quantify order reconstruction via measure of biaxiality

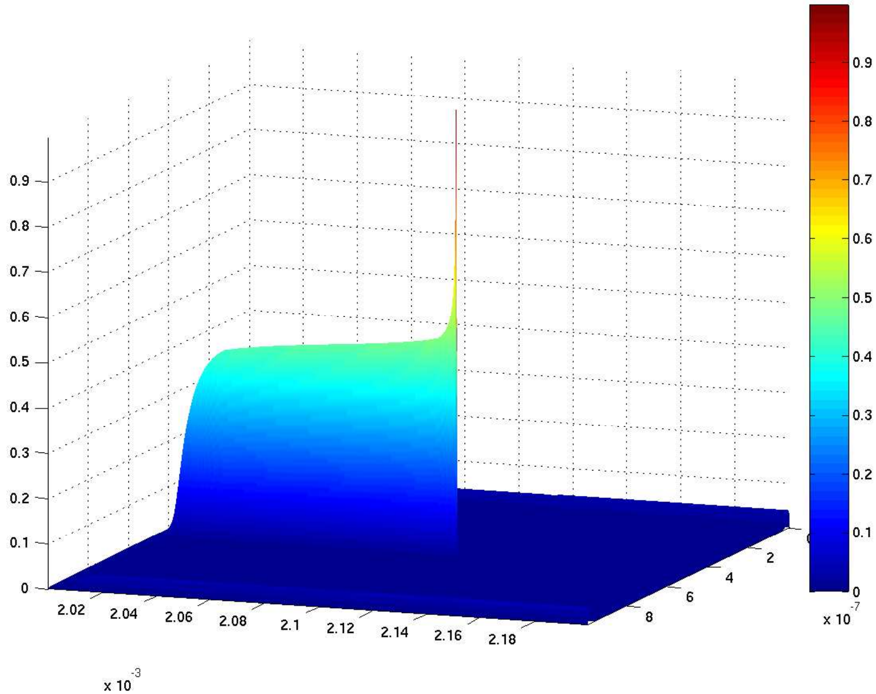
$$b = \sqrt{1 - \frac{6\,\mathrm{tr}(Q^3)^2}{\mathrm{tr}(Q^2)^3}}$$

- coded using COMSOL Multiphysics

Numerical Results



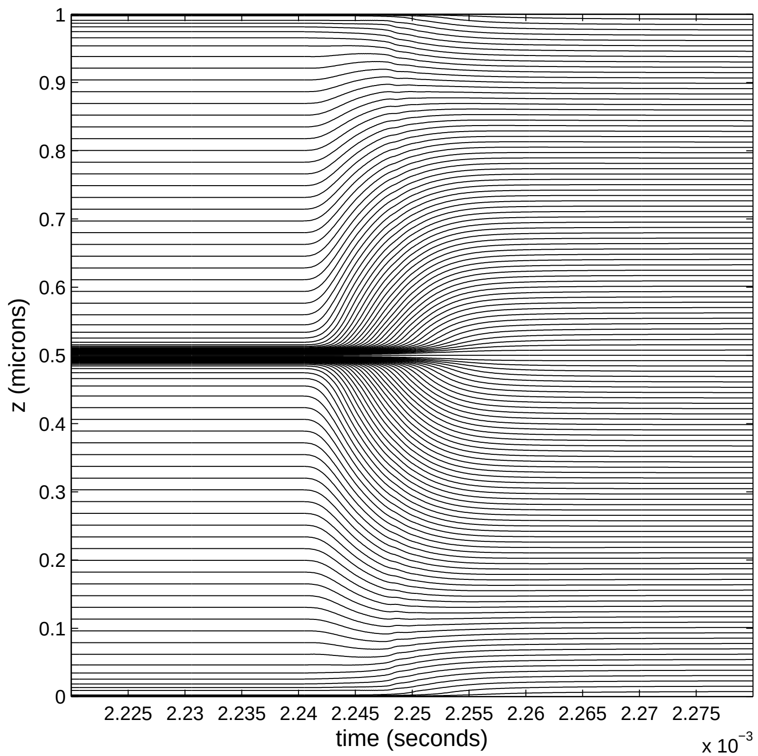
$V = 11.3$



$V = 11.32$

- solutions for electric field strength V just below and above the critical voltage at which switching occurs
- adaptive grid with 256 quadratic elements

Grid Trajectories



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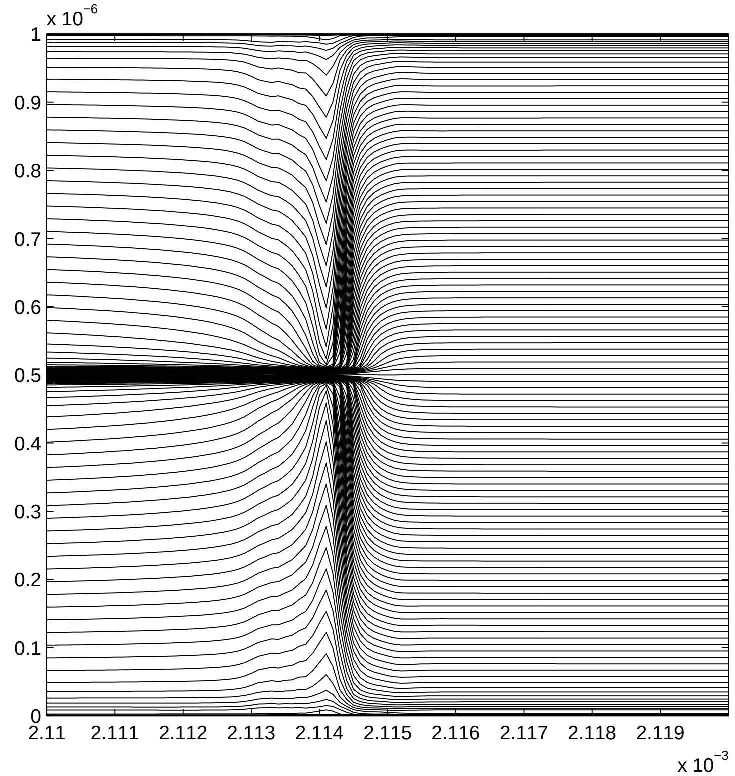
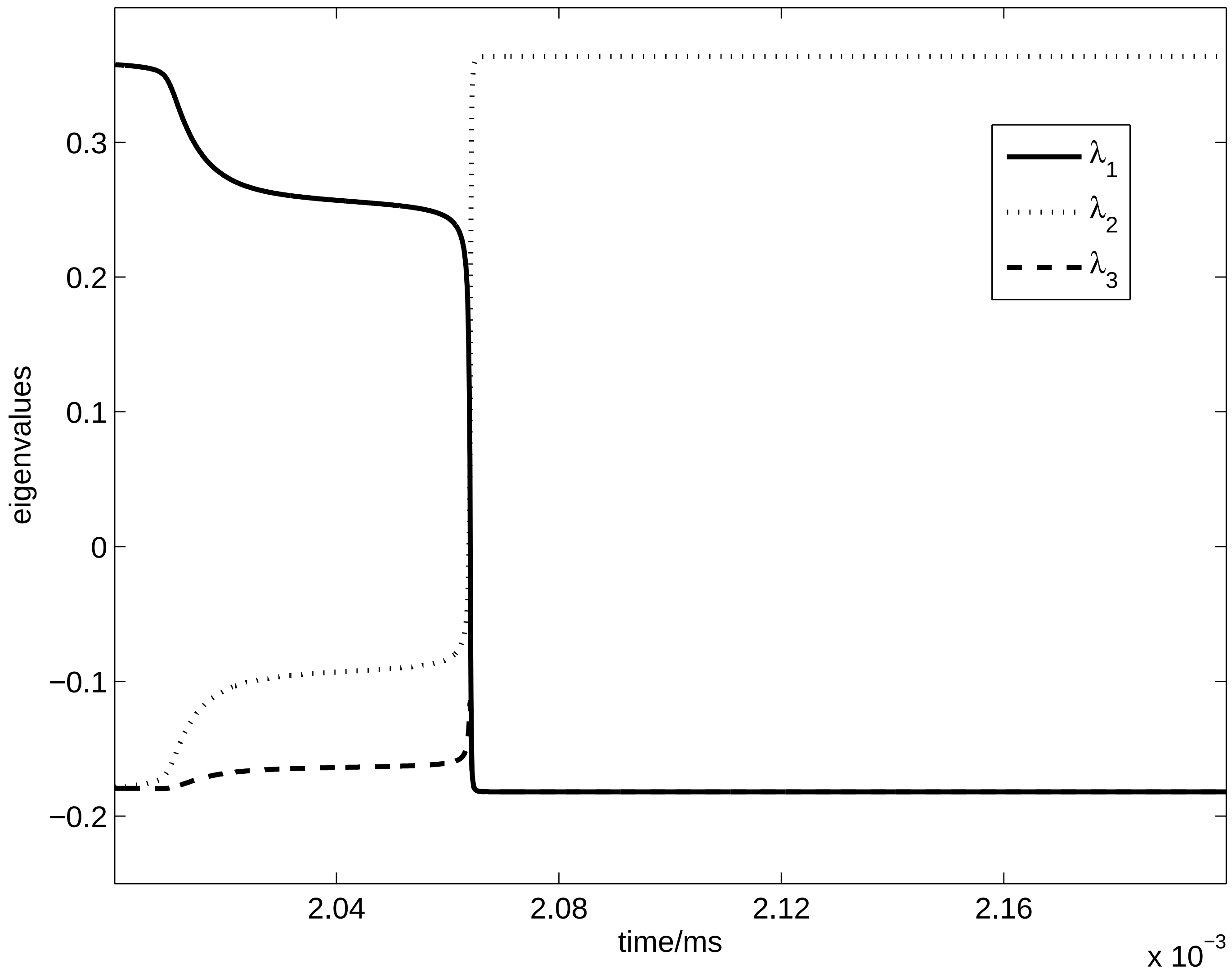


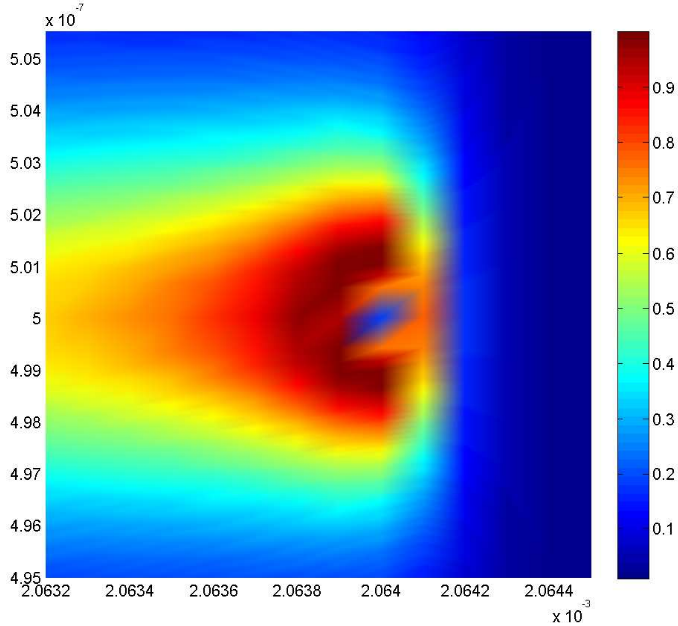
$V = 11.32$

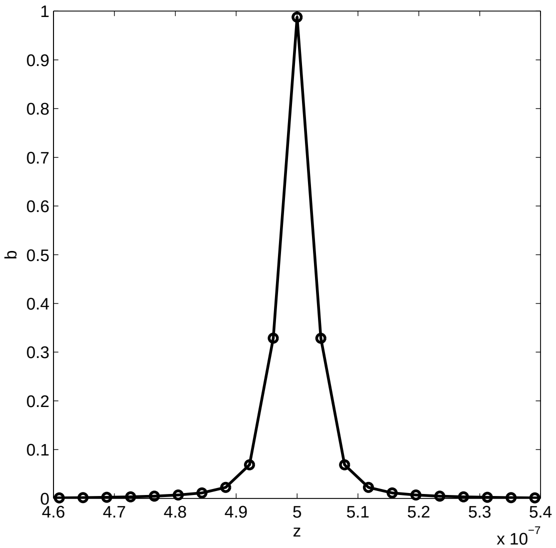
- approx. 25% fewer points (less CPU time) needed for adaptive grid

Exchange of Eigenvalues

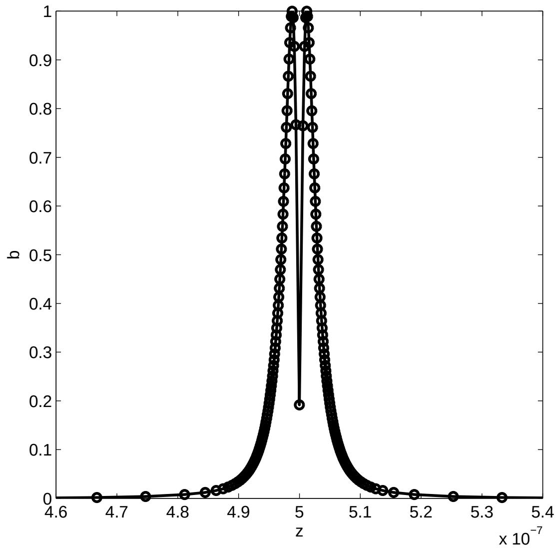


Detail of Biaxial Transition





uniform grid



adaptive grid

Equidistribution in 2D

- physical $\mathbf{x} = [x, y]^T$, computational $\xi = [\xi, \eta]^T$
- minimise

$$I[\xi] = \frac{1}{2} \int_D [(\nabla \xi)^T G_1^{-1} \nabla \xi + (\nabla \eta)^T G_2^{-1} \nabla \eta] \, d\mathbf{x}$$

G_1, G_2 symmetric positive definite monitor matrices

- Euler-Lagrange equations: modified gradient flow

$$\frac{\partial \xi}{\partial t} = \frac{P}{\tau} \nabla \cdot (G_1^{-1} \nabla \xi), \qquad \frac{\partial \eta}{\partial t} = \frac{P}{\tau} \nabla \cdot (G_2^{-1} \nabla \eta) = 0$$

spatial balance operator P
temporal smoothing parameter τ

Equidistribution in 2D

- interchange roles of dependent/independent variables
- Winslow-type monitor matrices

$$G_1 = G_2 = \begin{bmatrix} w & 0 \\ 0 & w \end{bmatrix}, \qquad w(\mathbf{x}, t) = \sqrt{\hat{\alpha} + |\nabla[\mathrm{tr}(Q^2)]|^2}$$

- MMPDE

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

a, b, c, d, e depend on ω, x_ξ, x_η, y_ξ, y_η

- coded using COMSOL Multiphysics

2D Test Problem

Zhang et al., Liquid Crystals (2004)

- 2D test problem
  - square cell $[0, d] \times [0, d]$
  - variable pretilt on $x = 0$, fixed pretilt on $x = d$
  - periodic boundary conditions on $y = 0$, $y = d$

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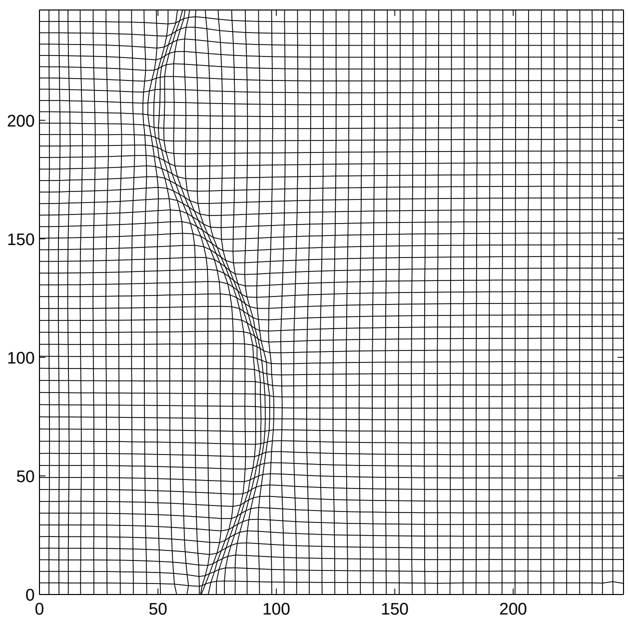

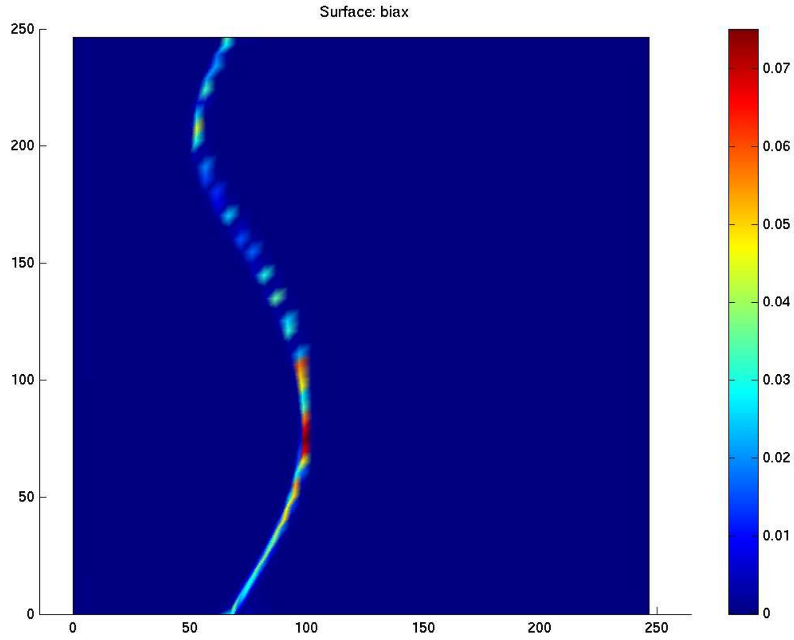

Summary

- model problem analysis shows
  - adaptive grid error is $O(N^{-2})$ for a simple model problem
  - adaptive grid error appears to be $O(N^{-2})$ for a more realistic model problem
- arc-length monitor function based on $tr(Q^2)$ works well
- to obtain a specified level of accuracy, adaptive grid requires fewer points: inaccurate solutions/switching times can be obtained if uniform grid is not fine enough
- 3-year EPSRC project (from June 1st 2007) with Ainsworth, Mottram (Strathclyde) and Newton (Hewlett-Packard)

  Adaptive Numerical Methods for Optoelectronic Devices

- *Adaptive Grid Methods for Q-Tensor Theory of Liquid Crystals: A One-Dimensional Feasibility Study*
  Strathclyde Mathematics Research Report No. 13, 2006.
- *Adaptive Solution of a One-dimensional Order Reconstruction Problem in Q-Tensor Theory of Liquid Crystals*
  Liquid Crystals, 34 (4), pp. 479 - 487, 2007.