

Adaptive Grid Methods for Q-tensor Theory of Liquid Crystals

Alison Ramage
Dept of Mathematics
University of Strathclyde
Glasgow, Scotland



Christopher J. Newton
Hewlett-Packard plc
Bristol, England

This work was supported by an EPSRC Springboard Fellowship.

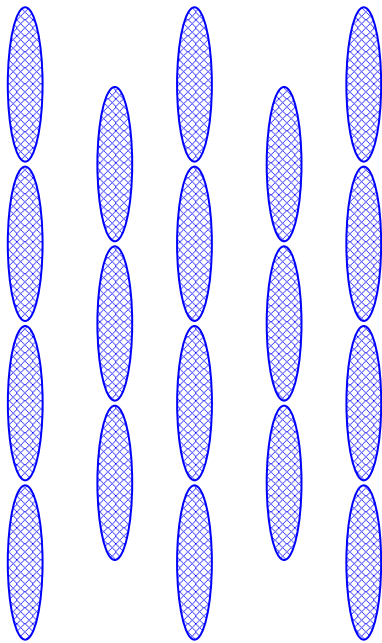
EPSRC Springboard Fellowship

- short-term support to enable researchers in the mathematical sciences to work
 - at the interface with another discipline;
 - with business or industry;
 - on a particularly innovative project or a short-term feasibility study.
- Fellowship acts as a **springboard** for future research
- funds awarded for one year of replacement teaching costs, October 2005 - September 2006

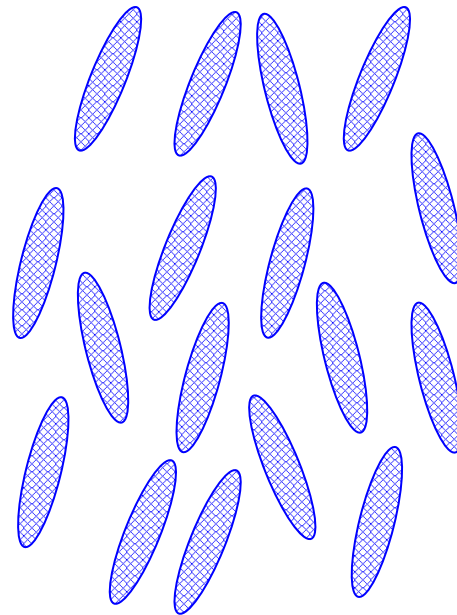
Adaptive Methods for Liquid Crystal Device Modelling

Liquid Crystals

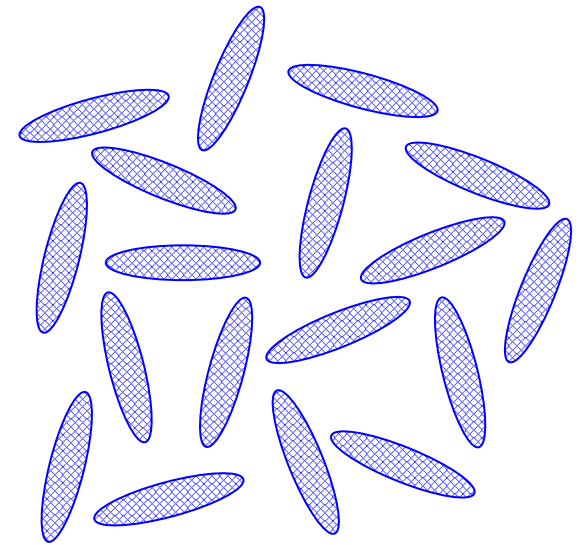
- occur between solid crystal and isotropic liquid states



solid



liquid crystal



liquid

- may have different **equilibrium** configurations
- **switch** between stable states by altering applied voltage, boundary conditions, . . .

Motivation from HP

- **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

Adaptive Grid Methods I

- local mesh refinement
 - extra nodes added locally in regions of high error
 - h refinement, p refinement
 - often requires complicated data structures which need updating frequently
- moving mesh methods
 - existing node points are moved to regions of high error
 - same grid connectivity maintained
 - r refinement
 - comparatively easy extension of existing software

Adaptive Grid Methods II

- velocity-based methods
 - mesh point velocities are calculated directly
 - moving finite element methods
 - geometric conservation laws
- location-based methods
 - mesh points are calculated directly
 - equidistribution methods
 - harmonic mapping
- adaptive grid on physical domain is image of uniform grid on computational domain under a suitable mapping

Equidistribution Principle I

- coordinates: physical $x \in [0, 1]$, computational $\xi \in [0, 1]$
- coordinate transformation:

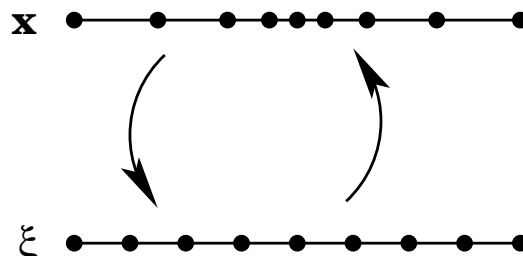
$$x = x(\xi, t), \quad \xi \in [0, 1], \quad x(0, t) = 0, \quad x(1, t) = 1$$

- uniform mesh on computational domain:

$$\xi_i = \frac{i}{N}, \quad i = 0, 1, \dots, N, \quad N \in \mathbb{Z}^+$$

- corresponding physical mesh:

$$0 = x_0 < x_1 < \dots < x_{N-1} < x_N = 1$$



Equidistribution Principle II

- choose (positive) **monitor function** $M(x, t)$
- equidistribution principle (EP):

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

- discrete forms:

$$\int_{x_i}^{x_{i+1}} M(s, t) ds = \int_{x_{i-1}}^{x_i} M(s, t) ds, \quad i = 1, \dots, N - 1$$

or

$$\int_{x_{i-1}}^{x_i} M(s, t) ds = \frac{1}{N} \int_0^1 M(s, t) ds, \quad i = 1, \dots, N$$

Monitor Functions

- (scaled) arc-length monitor function

$$M(u(x, t)) = \sqrt{\gamma + \left(\frac{\partial u(x, t)}{\partial x} \right)^2}$$

user-prescribed parameter $\gamma > 0$

- various other ideas e.g. Beckett and Mackenzie (2000)

$$M(u(x, t)) = \alpha + \left| \frac{\partial u(x, t)}{\partial x} \right|^{\frac{1}{m}}$$

α, m positive constants, $\alpha = \int_0^1 \left| \frac{\partial u(x, t)}{\partial x} \right|^{\frac{1}{m}} dx$

Aside on equidistribution

- **equidistribution principle**
differentiate EP twice with respect to ξ
- **variational principle**
find Euler-Lagrange equation associated with

$$I[x] = \frac{1}{2} \int_0^1 x_\xi^2(\xi) M^2(x(\xi)) d\xi$$

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

elliptic equidistribution generator

Adaptive Grid Methods III

- **dynamic** methods:
 - moving mesh partial differential equation (MMPDE)
 - mesh equation and underlying PDE solved together
- **static** methods: at a fixed time,
 - equation is discretised and solved on an initial mesh
 - adaptive mesh is constructed based on EP for monitor function
 - solution is interpolated onto new mesh
 - solution - mesh generation loop

Practical Algorithm

- Sanz-Serna and Christie, JCP 67, 1986
- 1D example:

$$u_t = F(u, u_x, u_{xx}, x, t)$$

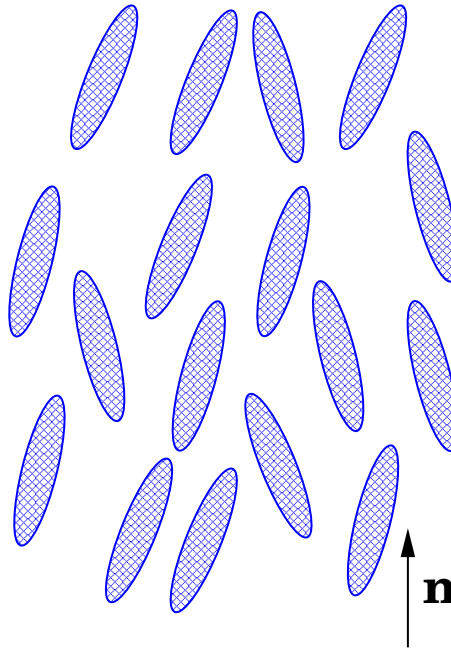
plus boundary and initial conditions

- time level t_n , grid x_j^n , approximation U_j^n to $u(x_j^n, t_n)$
- equidistribute solution **arc-length**:
 - (i) Use numerical scheme on grid x_j^n to find \bar{U}_j^{n+1} .
 - (ii) Join points (x_j^n, \bar{U}_j^{n+1}) by straight lines. Find the points on the polygon which divide its length into equal parts and project onto the x -axis. Compute U_j^{n+1} via interpolation.

Adaptive Grids and Liquid Crystals

- potential limitations of adaptive grids
 - theory of adaptive grids mostly in 1D
 - numerical simulations in 2D usually on model problems
 - nothing in 3D
- issues for this project
 - more than one physical PDE
 - choice of monitor function
 - complicated implementation/solution methods
- plan of work
 - initial feasibility study in 1D
 - focus on choice of monitor function in 2D

Liquid Crystal Modelling



- **director**: average direction of molecular alignment

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

- **order parameter**: measure of orientational order

$$S = \frac{1}{2} \langle 3 \cos^2 \theta_m - 1 \rangle$$

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

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

1D Model Problem (M1)

- 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 density

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

A_s, B_s, C_s, L_{1s} are positive constants

Euler-Lagrange Equation for M1

- ODE

$$S''' = \alpha S - \beta S^2 + \gamma S^3$$

$$\alpha = \frac{3A_s}{2L_{1s} + 1}, \quad \beta = \frac{3B_s}{2L_{1s} + 1}, \quad \gamma = \frac{3C_s}{2L_{1s} + 1}$$

- boundary conditions

$$S = 0 \text{ at } z = 0, \quad S = S_{eq} \text{ at } z = d$$

- at equilibrium:

$$S_{eq} = \frac{B_s + \sqrt{B_s^2 - 4A_sC_s}}{2C_s}$$

Euler-Lagrange Equation for M1

- integrate ODE twice to obtain

$$\int_0^{S(z)} \frac{ds}{\sqrt{G(S) - G(S_{eq})}} = z$$

$$G(S) = \alpha S^2 - \frac{2\beta}{3} S^3 + \frac{\gamma}{2} S^4$$

- no simple analytic solution: evaluate this numerically for specific values of S to obtain an approximate solution

A Second 1D Model Problem (M2)

- replace **quartic** thermotropic energy polynomial

$$F_t = \frac{1}{2}A_s S^2 - \frac{1}{3}B_s S^3 + \frac{1}{4}C_s S^4$$

by **quadratic** polynomial

$$F_q = \frac{F_{eq}}{S_{eq}} S \left(2 - \frac{1}{S_{eq}} S \right), \quad F_{eq} = F_t(S_{eq})$$

- both pass through $(0, 0)$ and have minimum at (S_{eq}, F_{eq})

Euler-Lagrange Equation for M2

- ODE

$$S'' = \hat{\alpha}(1 - \hat{\beta}S)$$

$$\hat{\alpha} = \frac{6F_{eq}}{S_{eq}(2L_{1s} + 1)}, \quad \hat{\beta} = \frac{1}{S_{eq}}$$

- boundary conditions

$$S = 0 \text{ at } z = 0, \quad S = S_{eq} \text{ at } z = d$$

- analytic solution

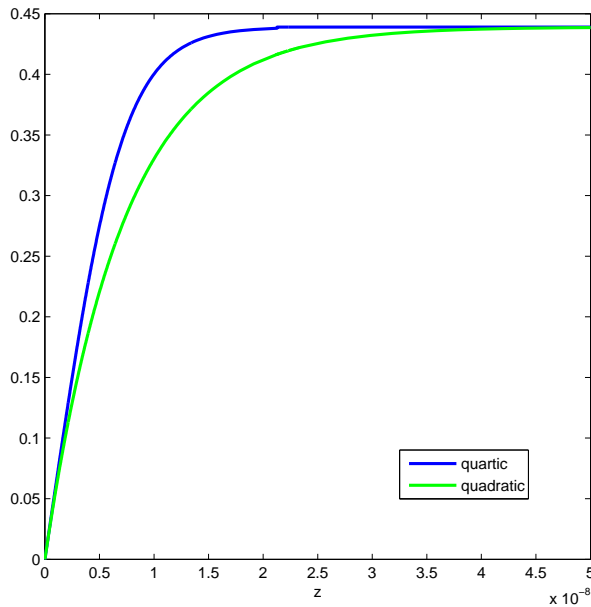
$$S(z) = S_{eq} \left(\frac{\sinh \rho z}{\tanh \rho d_s} - \cosh \rho z + 1 \right)$$

$$\rho = \sqrt{|\hat{\alpha}\hat{\beta}|}$$

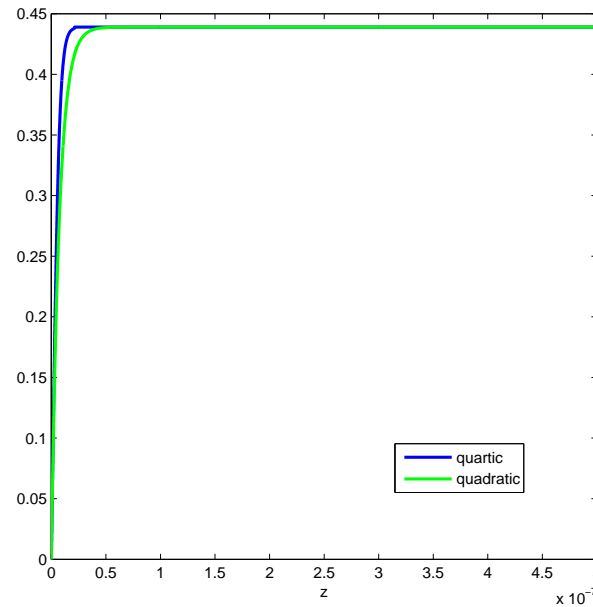
Analytic Solutions

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

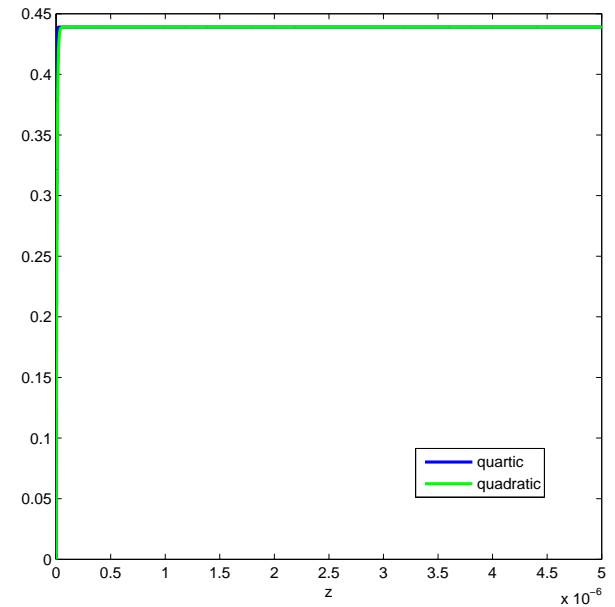
$$S(z) = S_{eq} \left(\frac{\sinh \rho z}{\tanh \rho d_s} - \cosh \rho z + 1 \right) \quad \rho = \sqrt{\left| \frac{6F_{eq}}{S_{eq}^2 (2L_{1s} + 1)} \right|}$$



$d = 0.1$ microns



$d = 1$ micron



$d = 10$ microns

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 both uniform and adaptive grids, it can be shown that

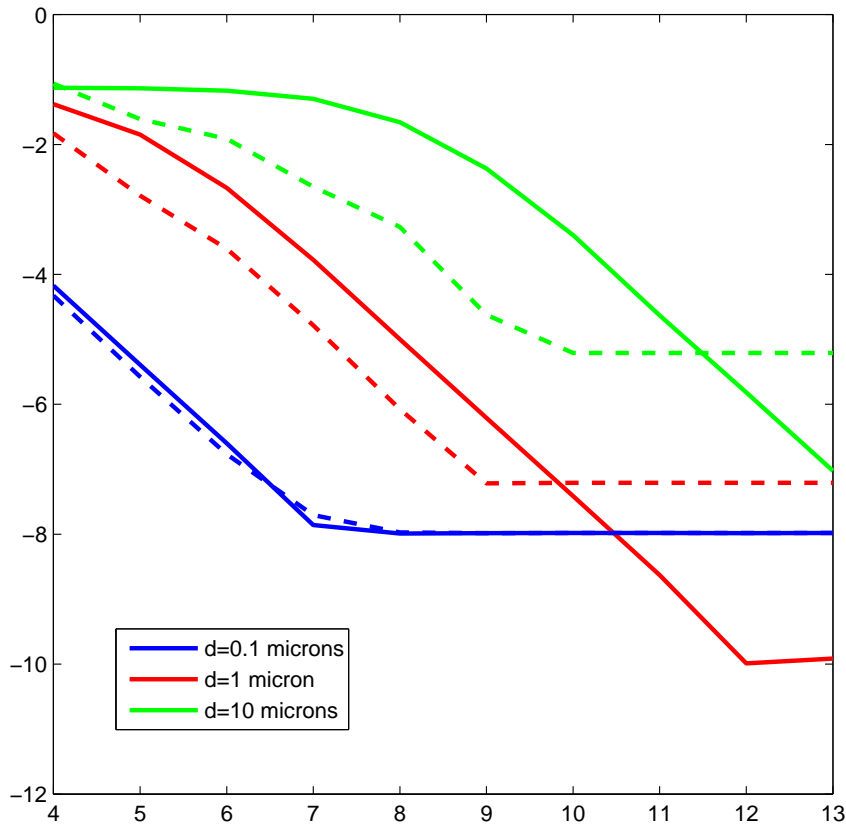
$$\|e\|_{L_\infty(0,d)} \leq \frac{C}{N^2}$$

- in practice use

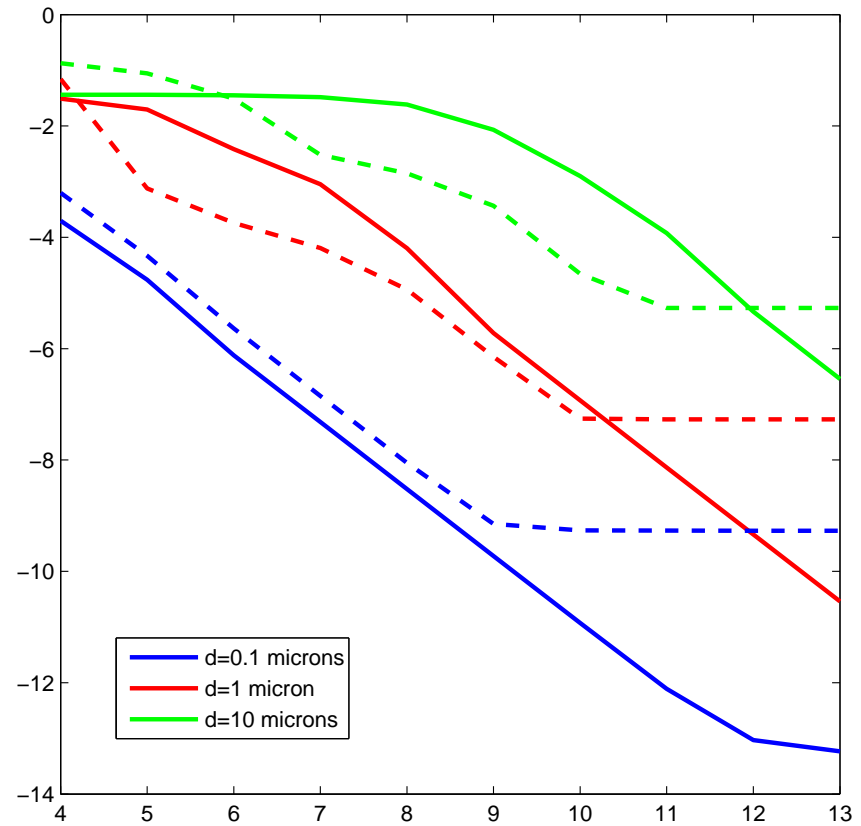
$$l_\infty = \max_{j=0,\dots,N/2} |S_f(z_j) - S_N(z_j)|$$

S_f on very fine uniform grid, S_N on grid with N points

Accuracy In Practice



Problem M2



Problem M1

- adaptive error contaminated by interpolation issues

Efficiency

- CPU times (in seconds) required to solve M2

	Adaptive Grid			
accuracy	N	solve	grid	total
1×10^{-4}	115	1.9491e-1	7.6075e-4	1.9590e-1
1×10^{-5}	258	2.2016e-1	9.7614e-4	2.2137e-1
1×10^{-6}	476	2.4822e-1	1.3882e-3	2.4344e-1
1×10^{-7}	817	2.7932e-1	1.9825e-3	2.8150e-1

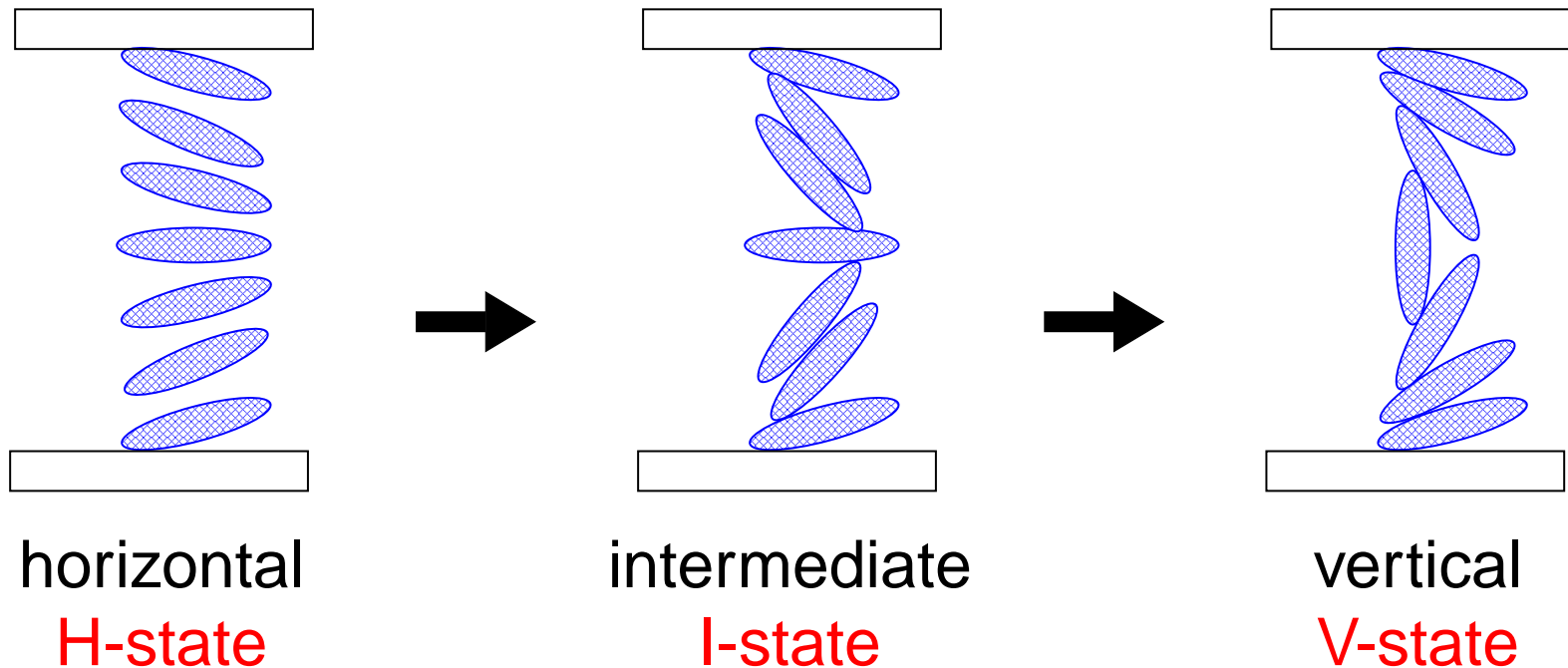
	Uniform Grid		
accuracy	N	total	% speedup
1×10^{-4}	174	1.9371e-1	-1.13
1×10^{-5}	338	2.3071e-1	4.05
1×10^{-6}	568	2.5882e-1	5.94
1×10^{-7}	1051	3.2753e-1	14.05

Order Reconstruction Problem I

- Barberi, Ciuchi, Durand, Iovane, Sikharulidze, Sonnet and Virga, Eur. J. Phys. E (2004)
- 1D domain $\Omega \equiv z \in [0, d]$
- cell surface treated at boundaries to induce alignments uniformly tilted by a specified **tilt angle** but oppositely directed
- **idea**: model order reconstruction which takes place when an electric field is applied

Order Reconstruction Problem II

- two topologically different equilibrium states: mostly **horizontal** alignment with a slight splay, mostly **vertical** alignment with a bend of almost π radians



- either state might have lower elastic energy, but energy barrier is always large enough to prevent spontaneous transition

Order Reconstruction Problem III

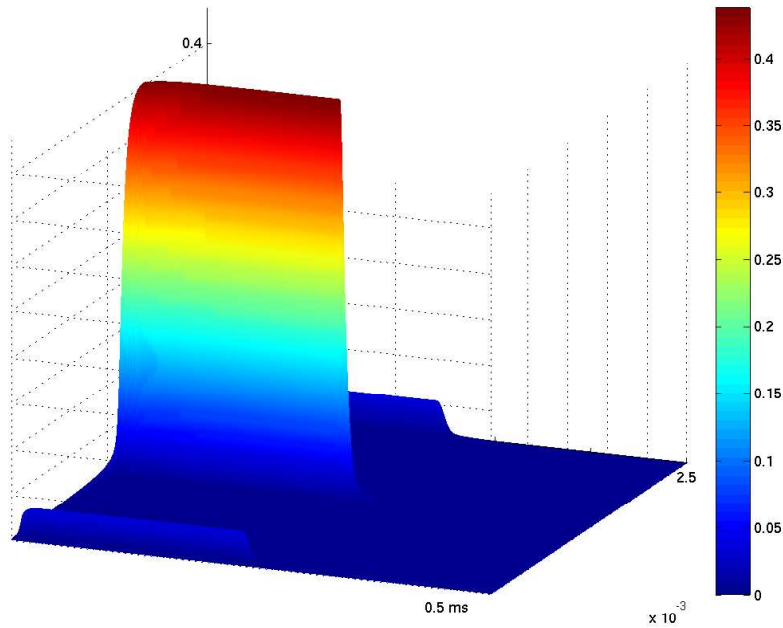
- no longer purely uniaxial: need full Q -tensor
- 5 coupled PDEs for q_i s, plus PDE for electric potential U
- monitor function based on $T(z) = \text{tr}(Q^2)$

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

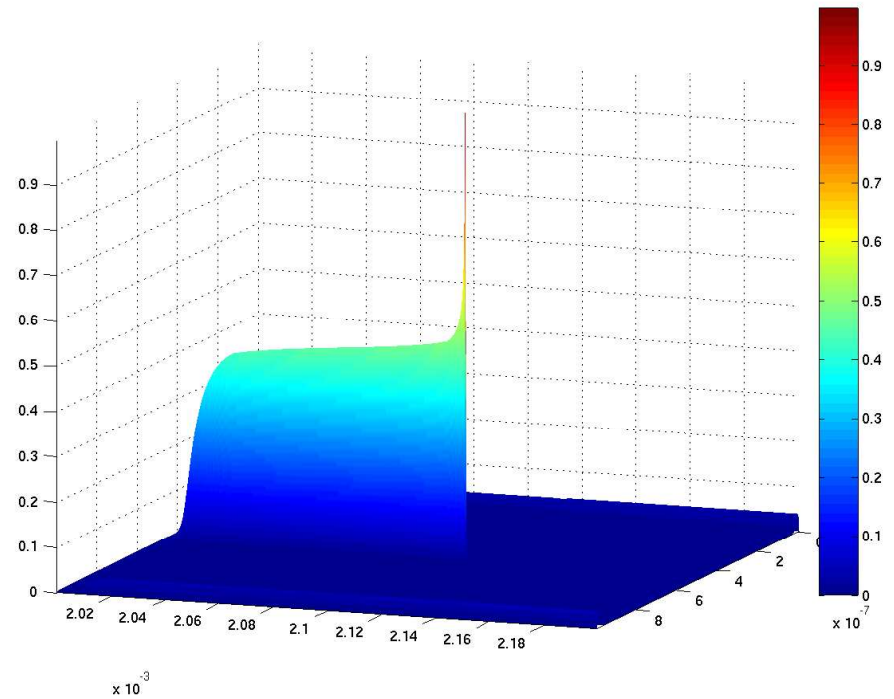
- quantify order reconstruction via measure of biaxiality

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

Numerical Results



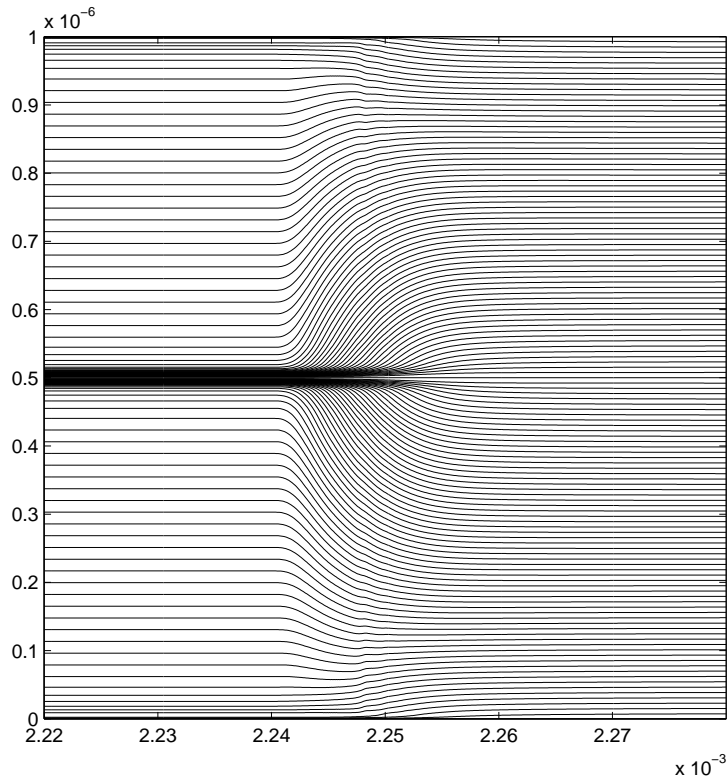
$$V = 11.3$$



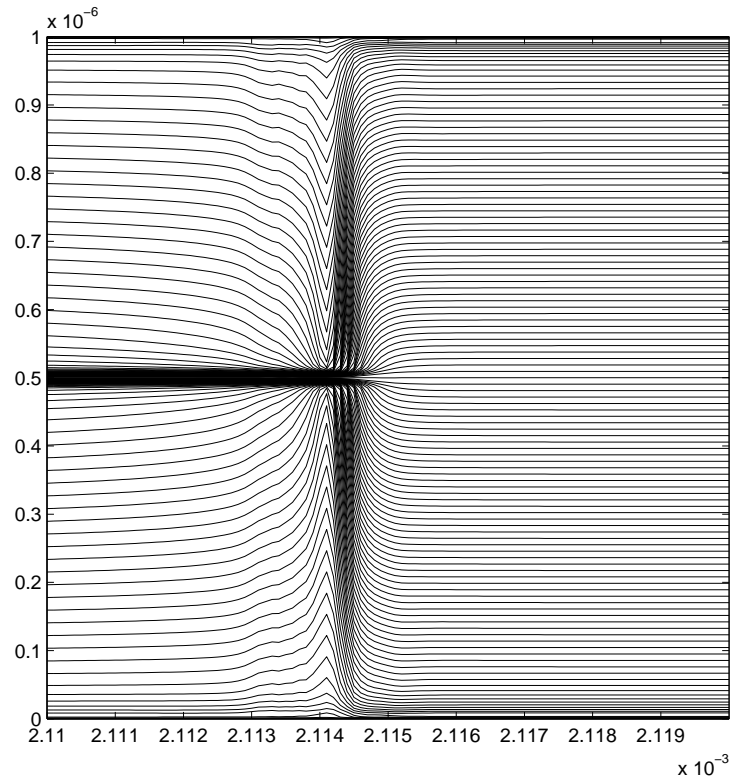
$$V = 11.32$$

- 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



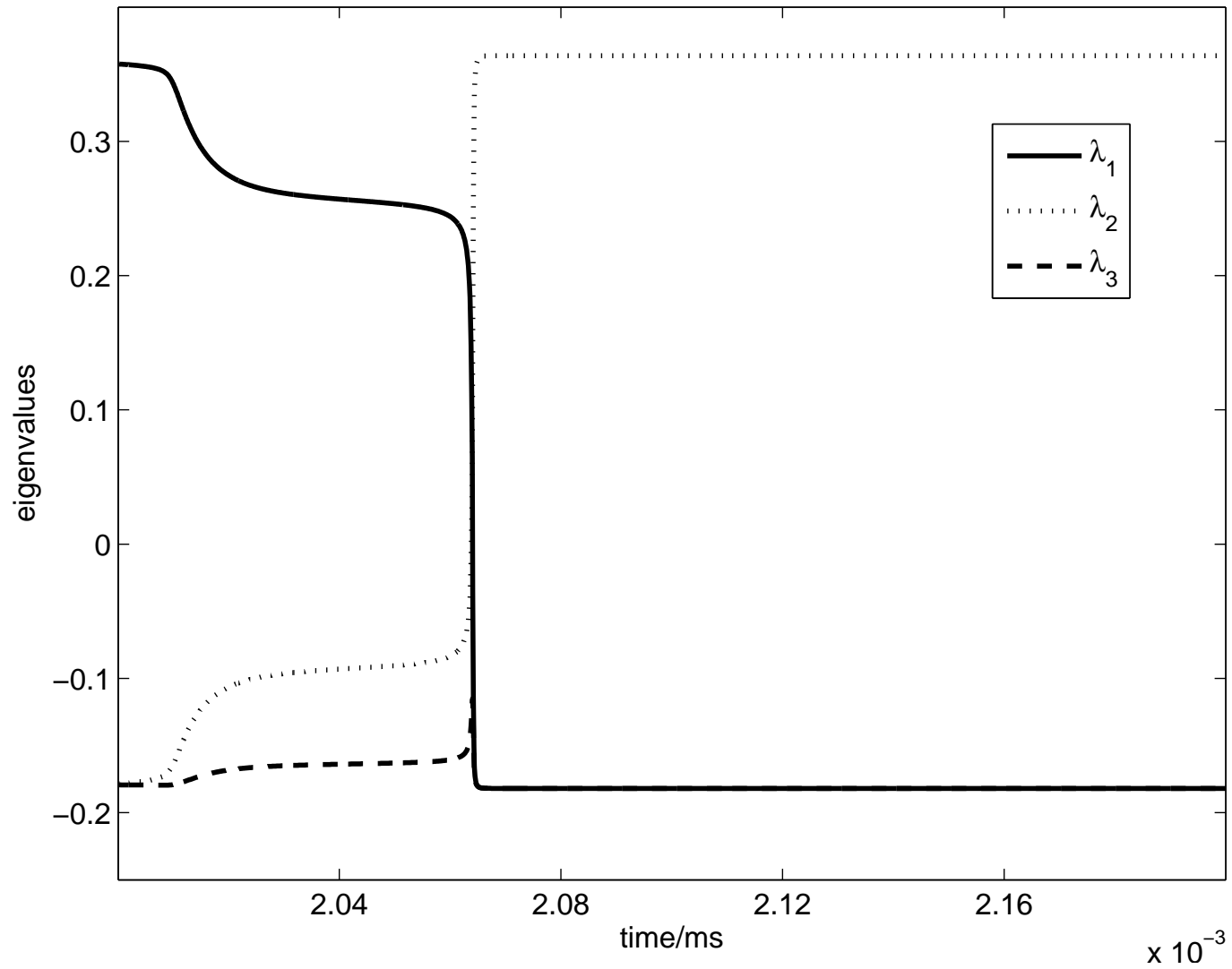
$$V = 11.3$$



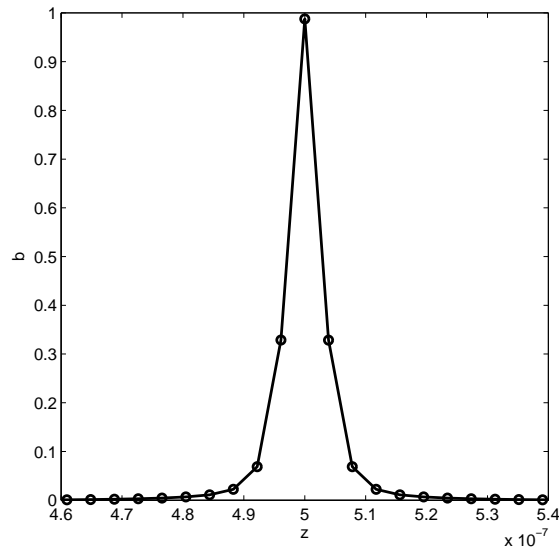
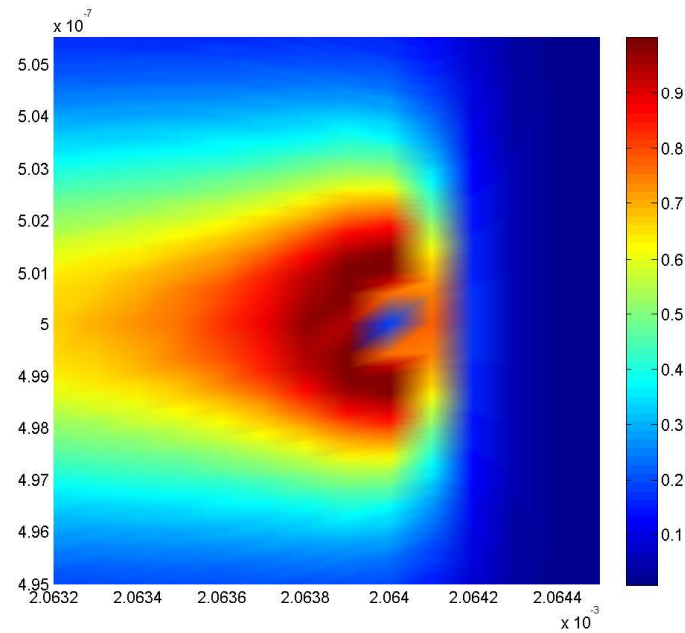
$$V = 11.32$$

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

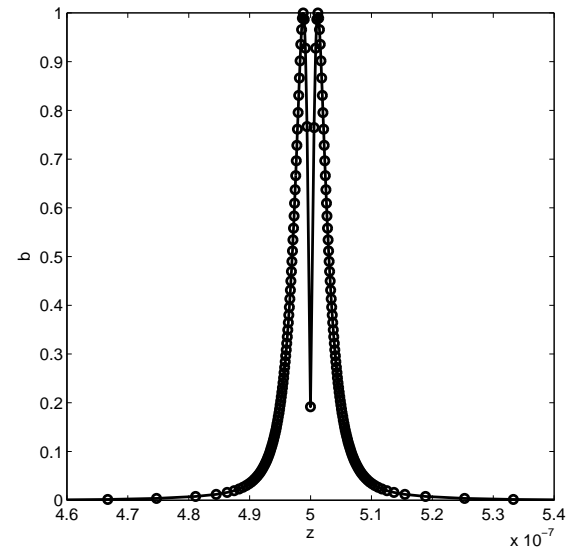
Exchange of Eigenvalues



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

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

spatial balance operator P
temporal smoothing parameter τ

Equidistribution in 2D

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

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

- MMPDE

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

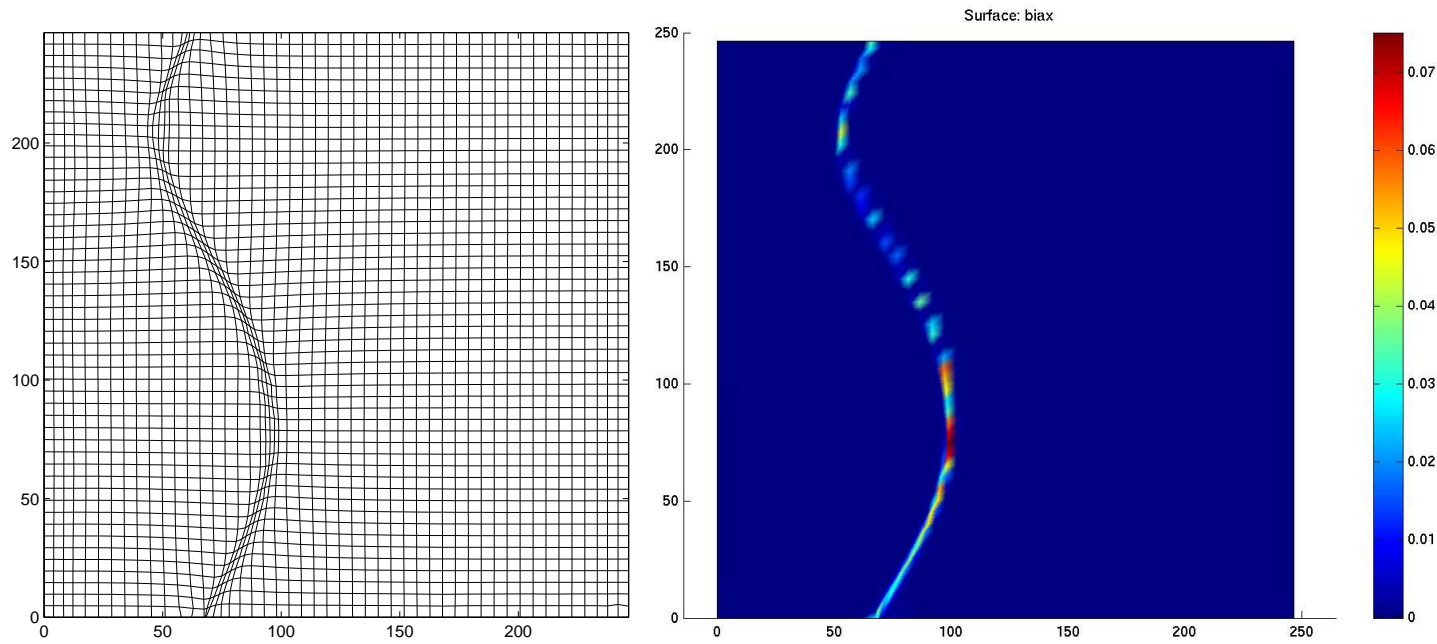
a, b, c, d, e depend on $\omega, x_{\xi}, x_{\eta}, y_{\xi}, y_{\eta}$

- 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 $x = d$
 - 1D MMPDE solved on $y = 0, y = d$



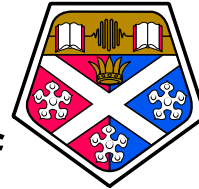
Summary

- 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 (to appear in *Molecular Crystals and Liquid Crystals*).
- *Adaptive Solution of a One-dimensional Order Reconstruction Problem in Q-Tensor Theory of Liquid Crystals*
Liquid Crystals, 34 (4), pp. 479 - 487, 2007.

23rd Biennial Conference on Numerical Analysis



University of
Strathclyde
Glasgow

June 23rd - 26th, 2009

`http://www.maths.strath.ac.uk/naconf`

`naconf@maths.strath.ac.uk`