Adaptive Grid Methods for Q-tensor Theory of Liquid Crystals

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EPSRC Springboard Fellowship

- short-term support to enable researchers in the mathematical sciences to work
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  - with business or industry;
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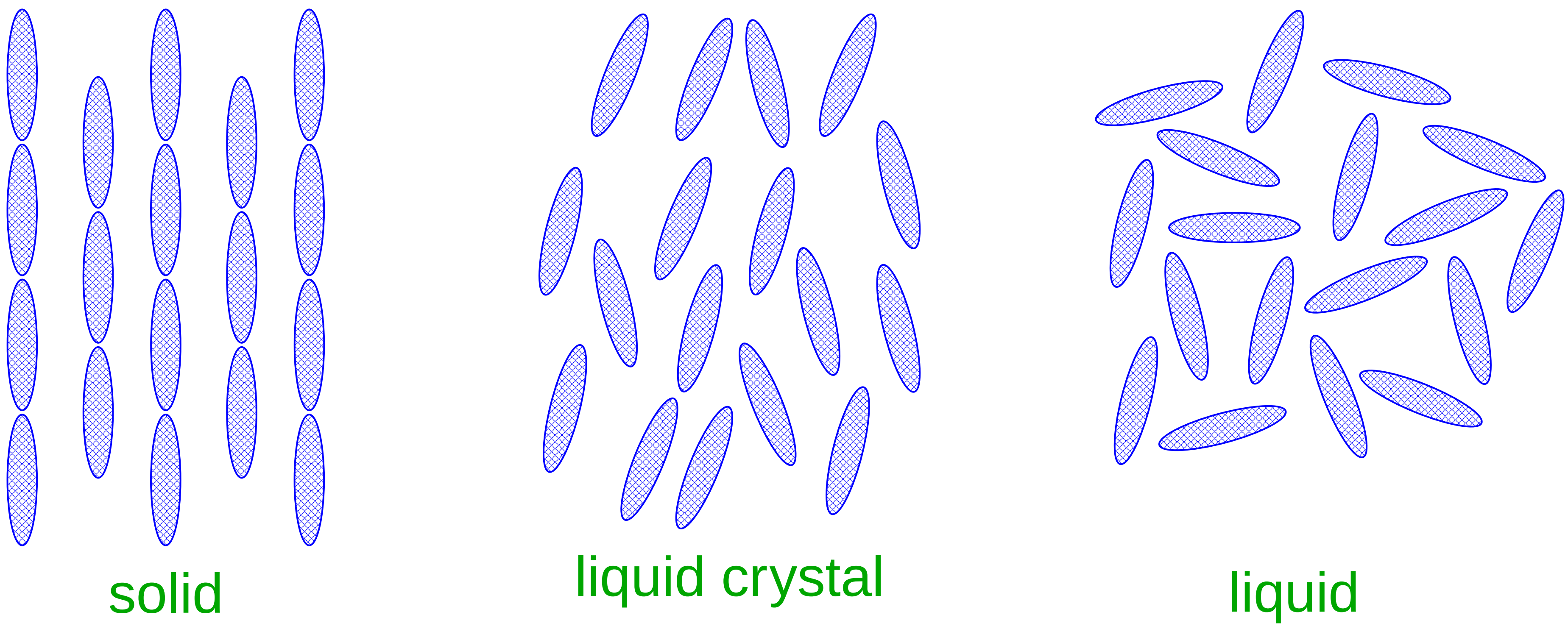
- Fellowship acts as a springboard for future research
- funds awarded for one year of replacement teaching costs

Adaptive Methods for Liquid Crystal Device Modelling

Liquid Crystals

- occur between solid crystal and isotropic liquid states



- 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:

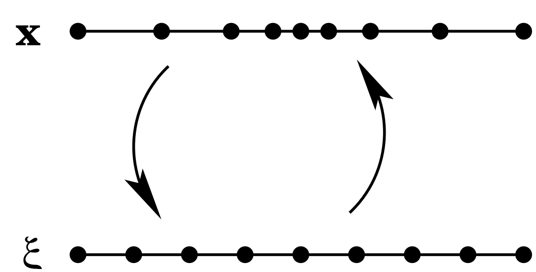
$$x = x(\xi, t),\ \xi \in [0,1], \qquad x(0,t) = 0,\ x(1,t) = 1$$

- uniform mesh on computational domain:

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

- corresponding physical mesh:

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



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:

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

or

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

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

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

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

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:

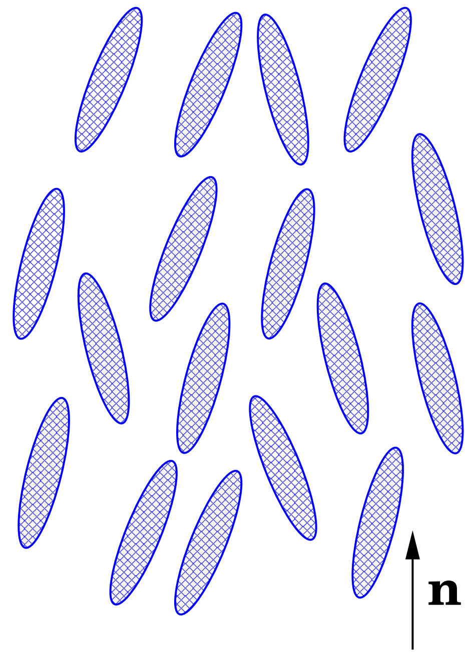
(i) Use numerical scheme on grid x_j^n to find $\bar{U}_j^{n+1}$.

(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
- results presented
  - initial feasibility study in 1D
  - realistic problem in 1D
  - extension to 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

$$S = \frac{1}{2} < 3\cos^2\theta_m - 1 >$$

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 (symmetric and traceless)

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

- express free energy density as

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

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

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

- 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

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

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

Euler-Lagrange Equation for M2

- ODE

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

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

- boundary conditions

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

- analytic solution

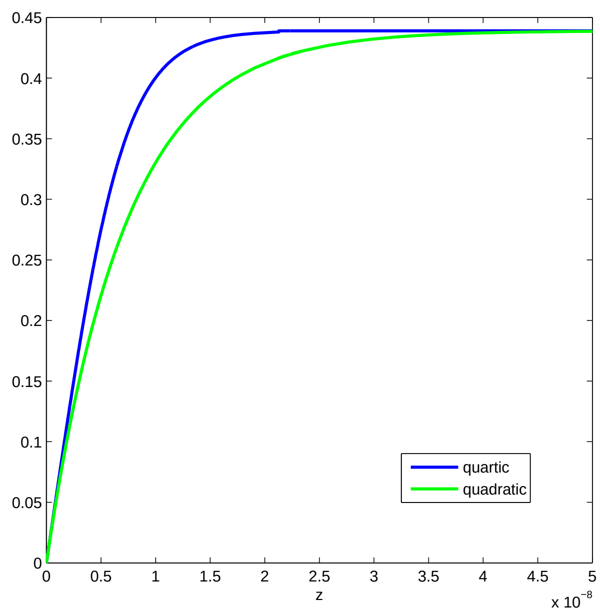
$$S(z) = S_{eq}\left(\frac{\sinh \rho z}{\tanh \rho d_s} - \cosh \rho z + 1\right)$$

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

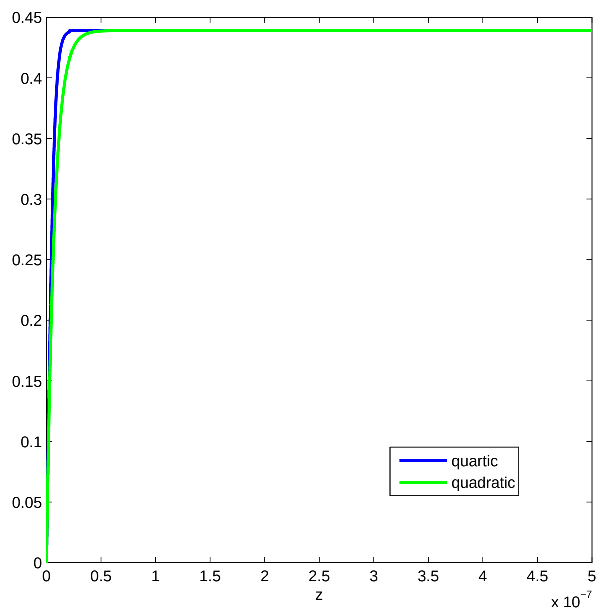
Analytic Solutions

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

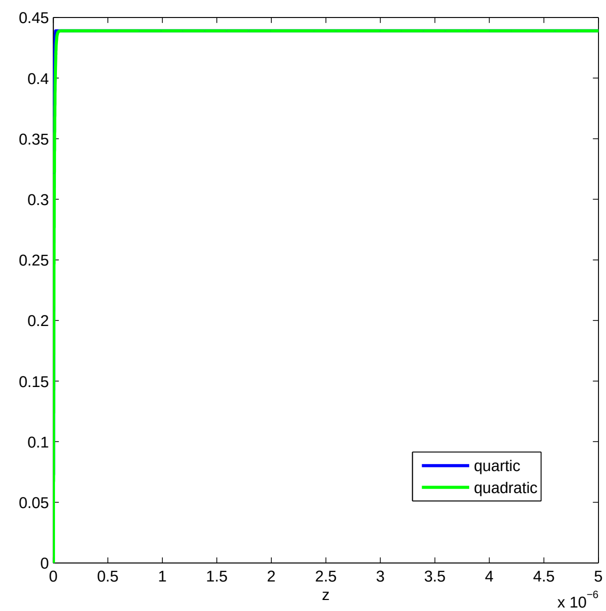
$$S(z) = S_{eq} \left(\frac{\sinh \rho z}{\tanh \rho d_s} - \cosh \rho z + 1 \right) \qquad \rho = \sqrt{\left| \frac{6 F_{eq}}{S_{eq}^2 (2L_{1s} + 1)} \right|}$$



$d = 0.1$ 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

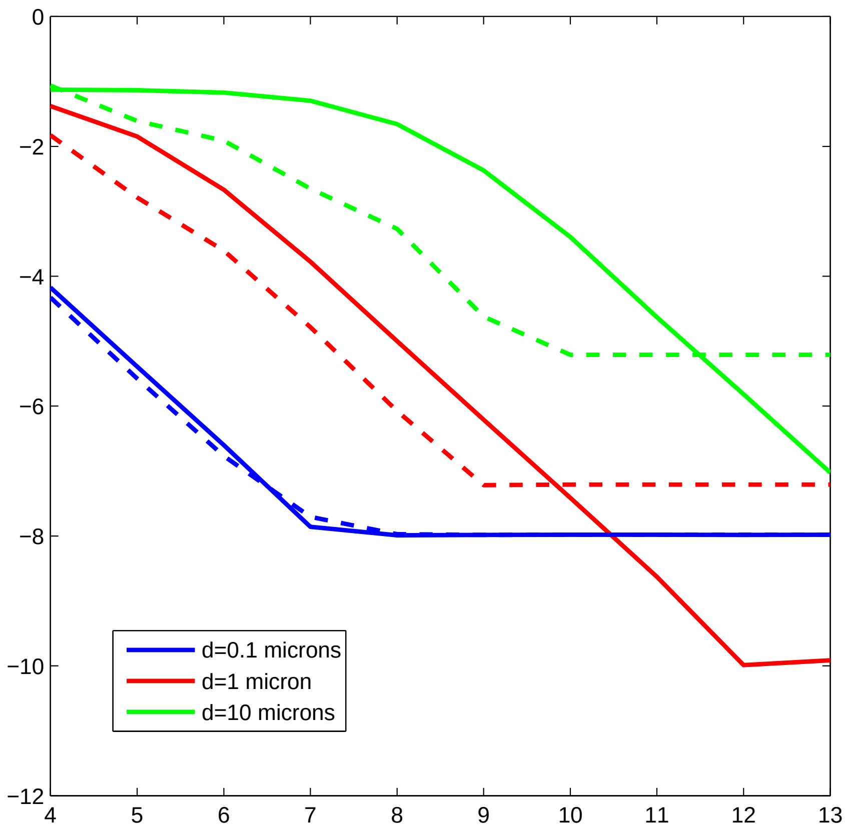
$$\|e\|_{L_\infty(0,d)} \leq \frac{C}{N^2}$$

- in practice use

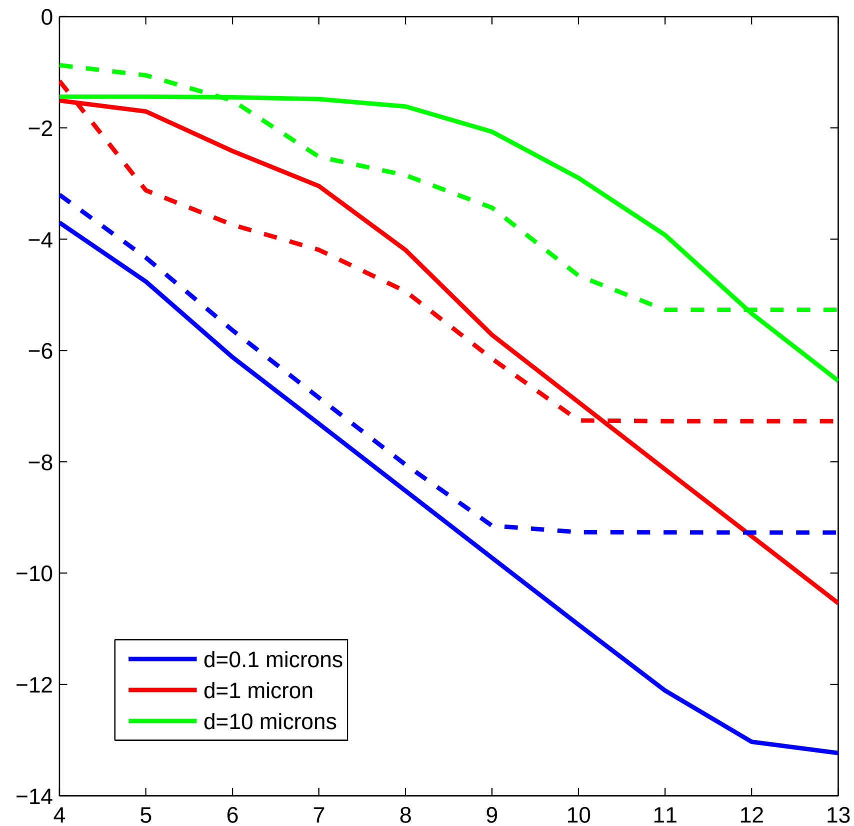
$$l_\infty = \max_{j=0,\ldots,N/2} |S_f(z_j) - S_N(z_j)|$$

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)

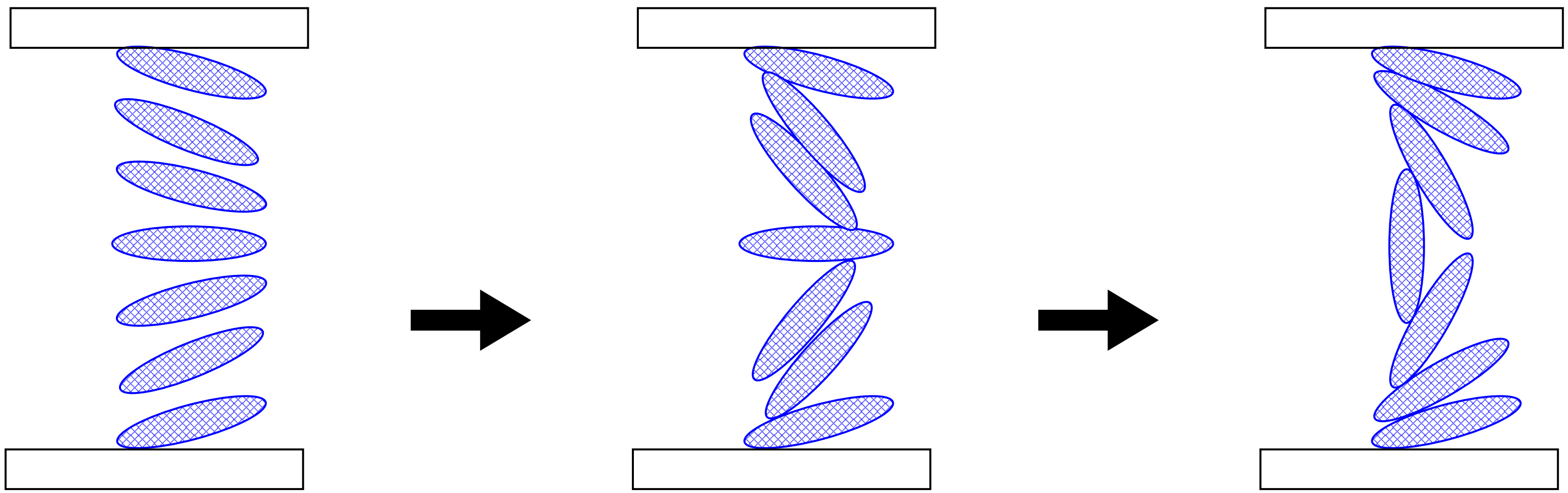
- 1D domain $\Omega \equiv z \in [0, d]$

- 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



horizontal | intermediate | vertical
H-state | I-state | V-state

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

Order Reconstruction Problem III

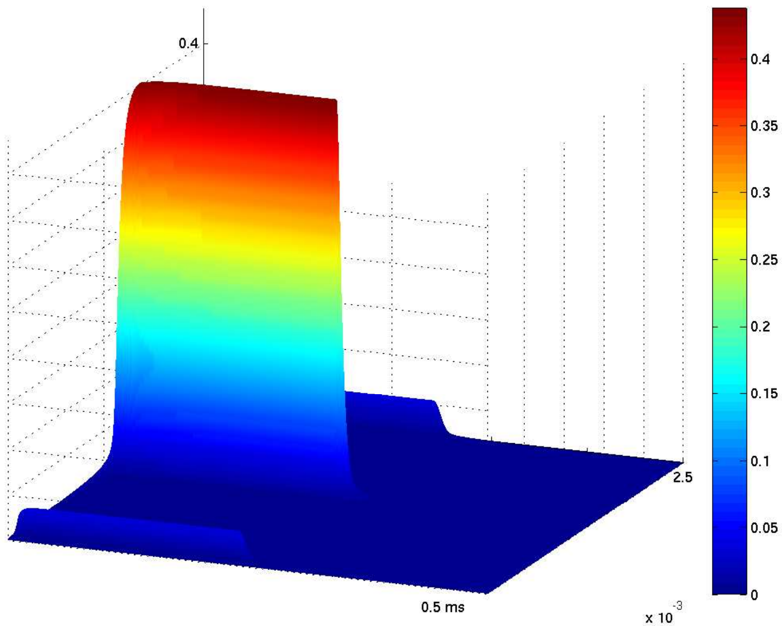
- no longer purely uniaxial: need full Q-tensor
- 5 coupled PDEs for q_is, plus PDE for electric potential U
- monitor function based on $T(z) = \mathrm{tr}(Q^2)$

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

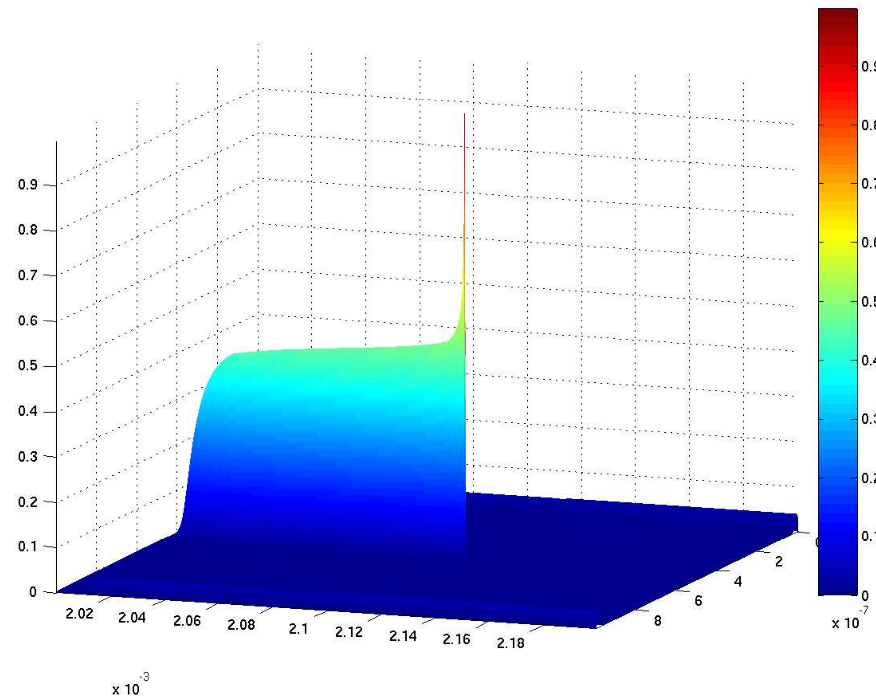
- quantify order reconstruction via measure of biaxiality

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

Numerical Results



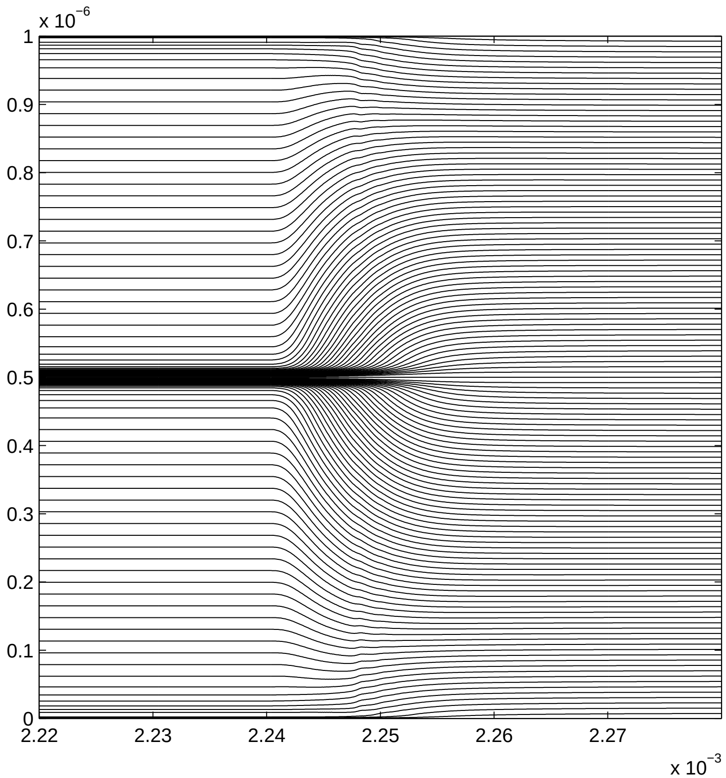
$V = 11.3$



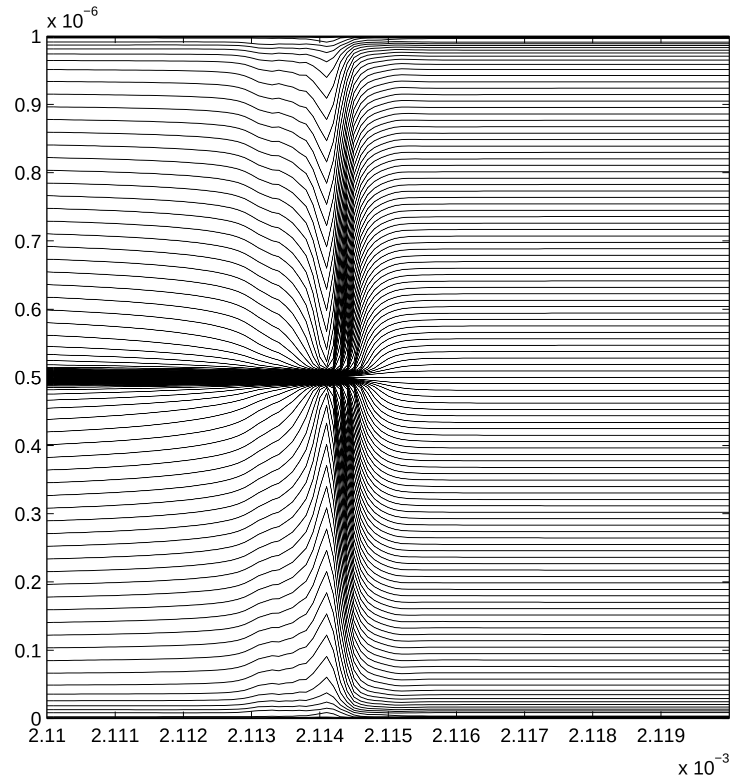
$V = 11.32$

- 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



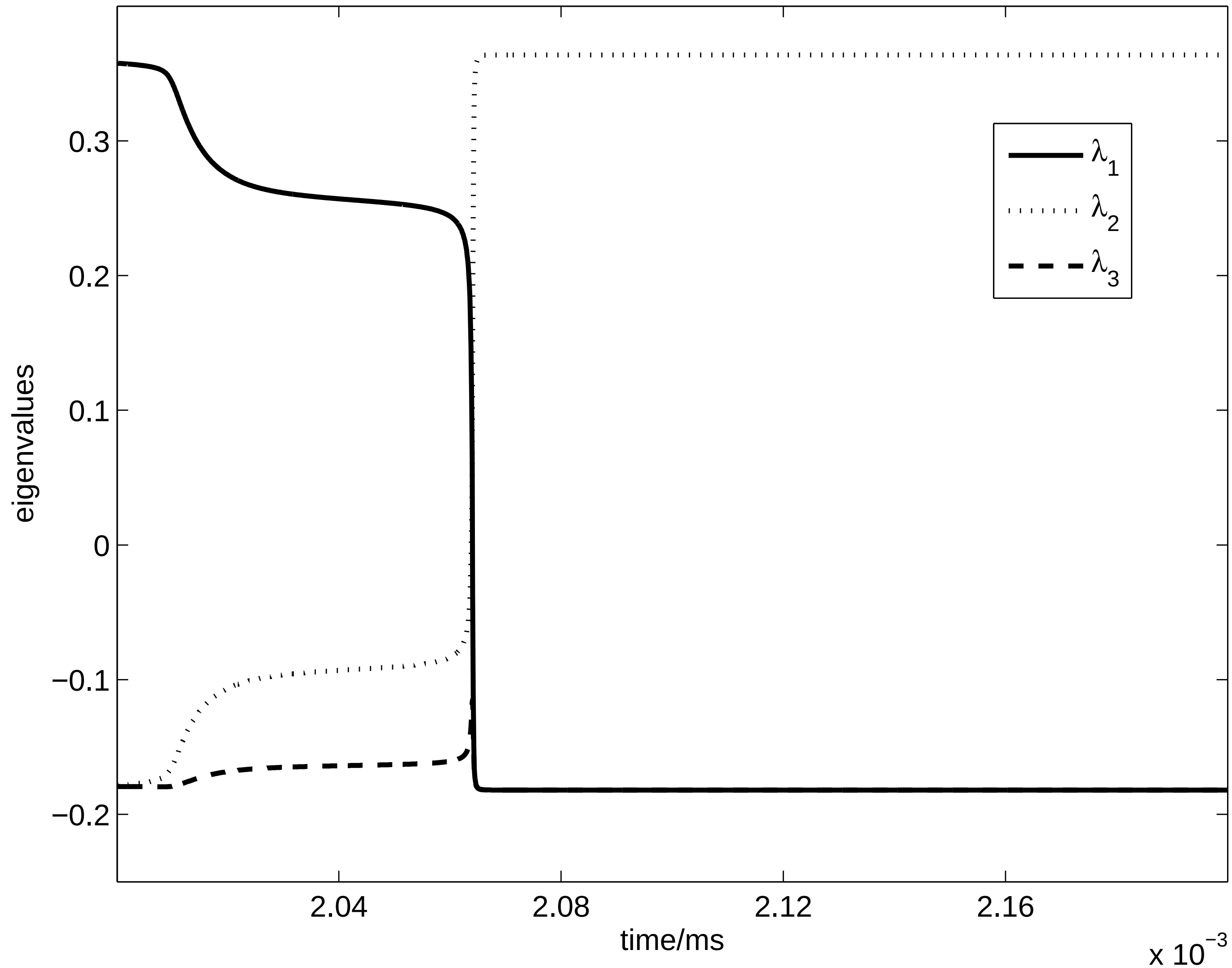
$V = 11.3$



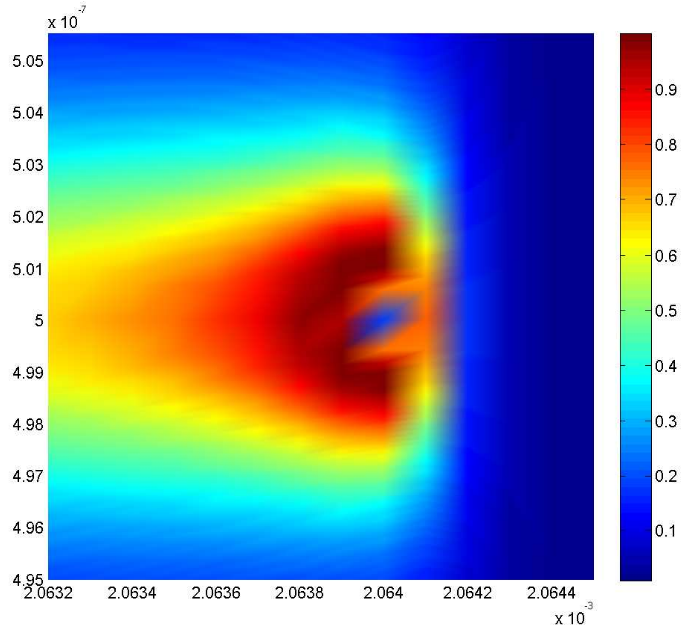
$V = 11.32$

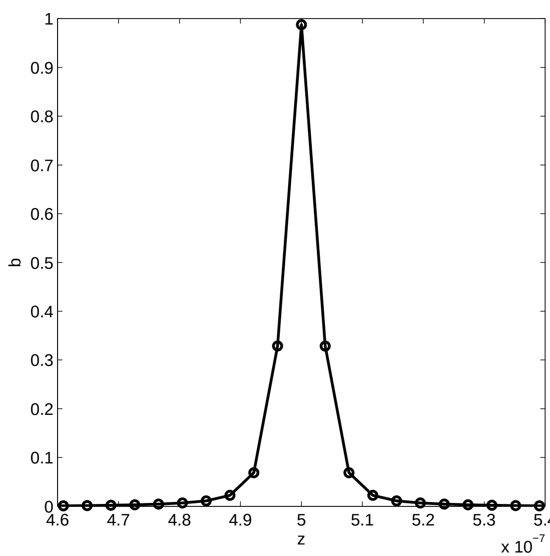
- approx. 25% fewer points (less CPU time) needed for adaptive grid

Exchange of Eigenvalues

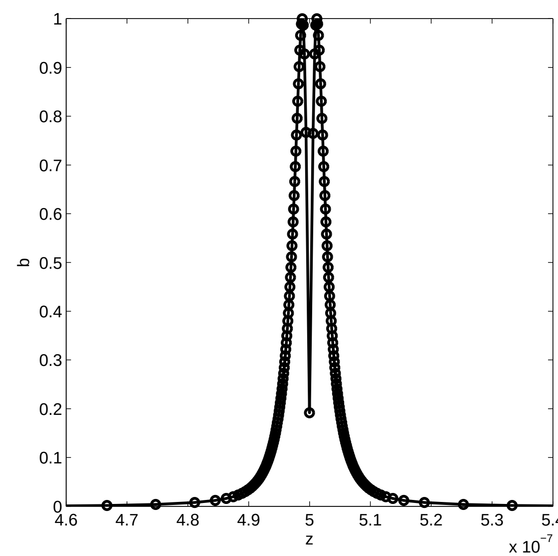


Detail of Biaxial Transition





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

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

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

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

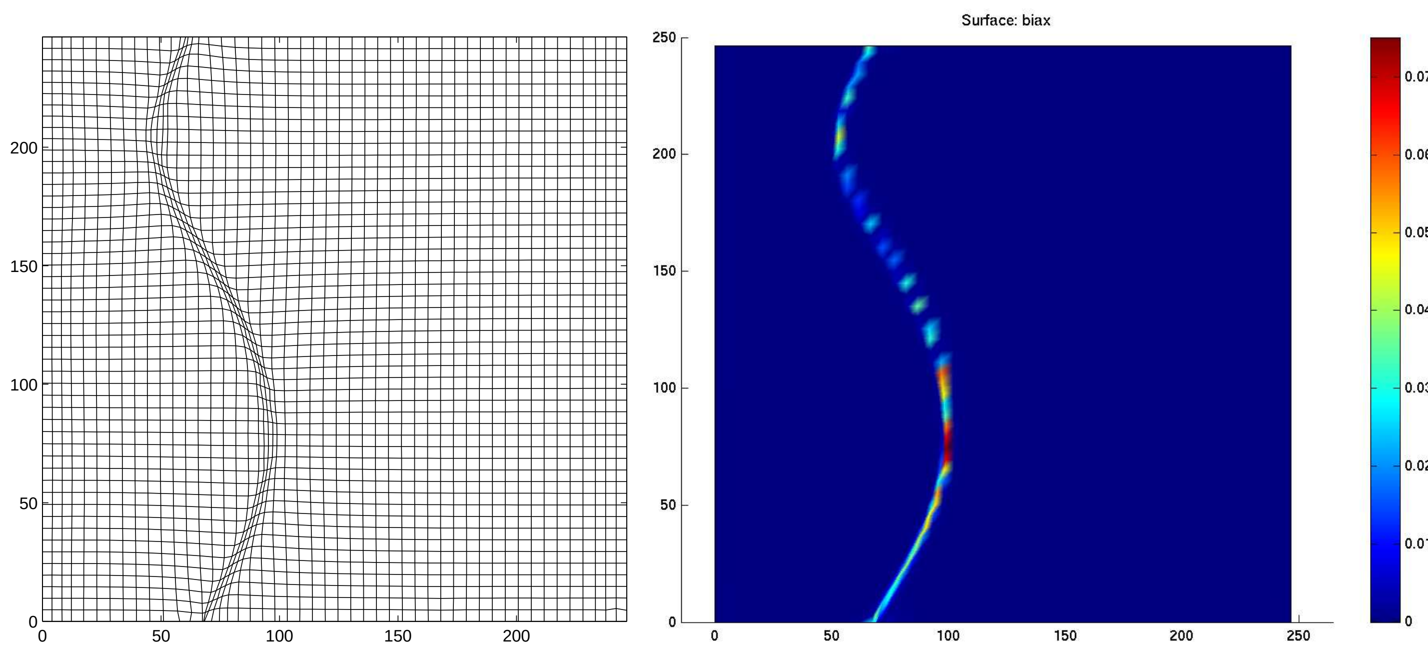
a, b, c, d, e depend on ω, x_ξ, x_η, y_ξ, y_η

- 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 $x = d$
  - 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*
  Molecular Crystals and Liquid Crystals, 480 (1), pp. 160 - 181, 2007.
- *Adaptive Solution of a One-dimensional Order Reconstruction Problem in Q-Tensor Theory of Liquid Crystals*
  Liquid Crystals, 34 (4), pp. 479 - 487, 2007.

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