Preconditioners in Liquid Crystal Modelling

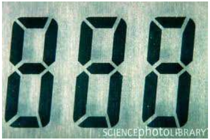
Alison Ramage*, Chris Newton†

∗ Department of Mathematics and Statistics, University of Strathclyde

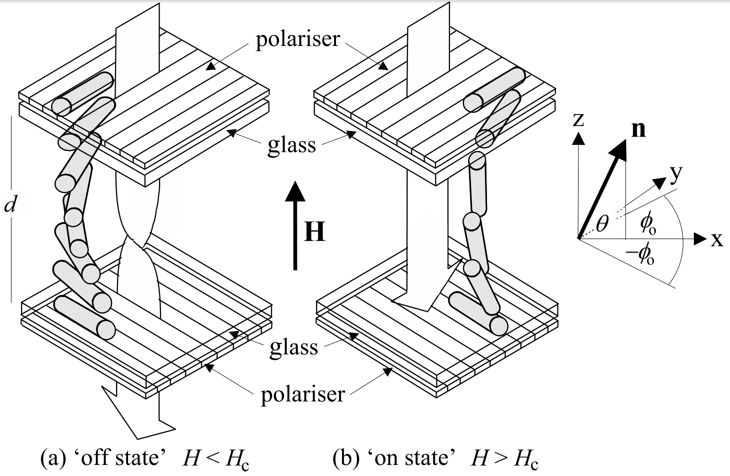
† Hewlett-Packard plc

Liquid Crystals

- occur between solid crystal and isotropic liquid states
- may have different equilibrium configurations
- switch between stable states by altering applied voltage, magnetic field, boundary conditions, . . .
- used in a wide range of LCDs



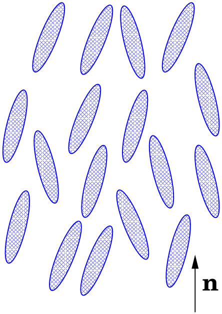
Liquid Crystal Displays

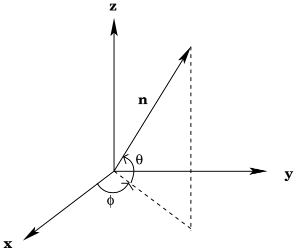


Twisted Nematic Device

(diagram taken from Stewart (2004))

Modelling: Director-based Models



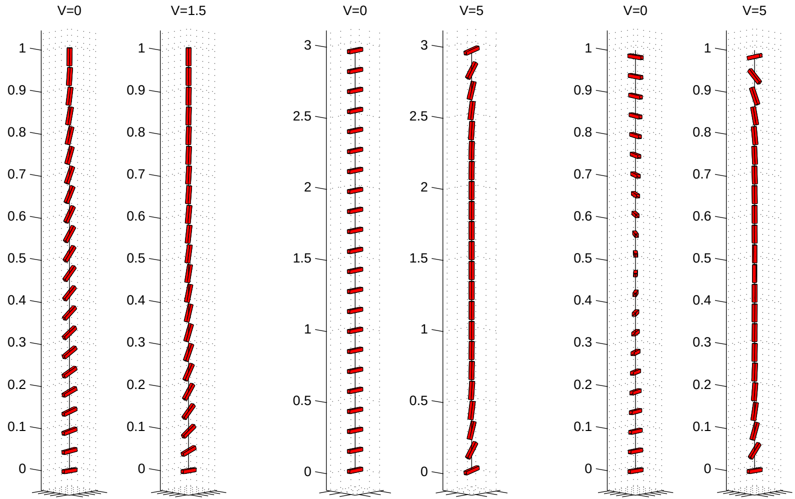


- director: average direction of molecular alignment

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

- Leslie-Ericksen dynamic theory for nematics

Sample configurations



HAN cell

Pi cell

TND cell

Some Issues with Director Modelling

- problems with numerical modelling can include
  - dealing with multivalued angles
  - modelling equivalence of $\mathbf{n}$ and $-\mathbf{n}$
  - modelling defect cores (mathematical singularities)
- problems with linear algebra can include
  - imposing the unit vector constraint $|\mathbf{n}| = 1$
  - double saddle-point system when electric field is introduced
- efficient preconditioned nullspace method has been developed in previous work
  RAMAGE AND GARTLAND JR, SISC 2013

Model: **Q**-tensor Theory

- symmetric traceless tensor

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

- local ensemble average over unit vectors **u** along molecular axes
- five degrees of freedom: two specifying the degree of order, three specifying the angles of the principal directions
- basis representation

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

- five unknowns $\quad q_1, \; q_2, \; q_3, \; q_4, \; q_5$

Finding Equilibrium Configurations

- minimise the free energy

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

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

- if fixed boundary conditions are applied, surface energy term can be ignored

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

Free energy density

- elastic energy: induced by distorting the $\mathbf{Q}$-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 state the liquid crystal would prefer to be in (uniaxial, biaxial or isotropic)

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

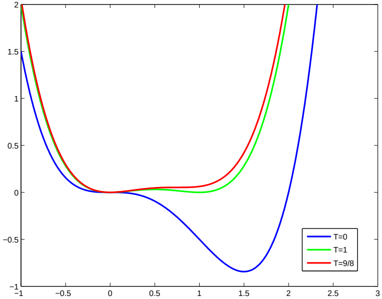
- electrostatic energy: due to an applied electric field $\mathbf{E}$ (electric potential U with $\mathbf{E} = -\nabla U$)

$$F_{electrostatic} = -\frac{1}{2}\left(\epsilon_0(\bar{\epsilon}\mathbf{I} + \epsilon_a\mathbf{Q})\nabla U\right) \cdot \mathbf{E}$$

Thermotropic Energy

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

- uniaxial case: $\frac{1}{2}A(T - T^*)\ S^2 - \frac{1}{3}B\ S^3 + \frac{1}{4}C\ S^4$



Coupled Equations

- solve Euler-Lagrange equations to minimise free energy

$$\begin{aligned} \nabla \cdot \boldsymbol{\Gamma}^i &= f^i, \qquad i = 1, \ldots, 5 \\ \nabla \cdot \mathbf{D} &= 0 \end{aligned}$$

$$\Gamma^i_j = \frac{\partial F_{bulk}}{\partial q_{i,j}}, \quad f^i = \frac{\partial F_{bulk}}{\partial q_i}, \quad q_{i,j} = \frac{\partial q_i}{\partial x_j}$$

- solution vector $\mathbf{u} = [\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4, \mathbf{q}_5, \mathbf{U}]^T$
- finite element approximation, quadratic elements
- linearise about $\mathbf{u}_0$ and iterate

Linear System At Each Step

$$(\mathcal{K} + 2a\mathcal{M} + \mathcal{N}|_{\mathbf{u}_0})\delta\mathbf{u} = -(\mathcal{K} + 2a\mathcal{M})\mathbf{u}_0 - \mathcal{R}|_{\mathbf{u}_0}$$

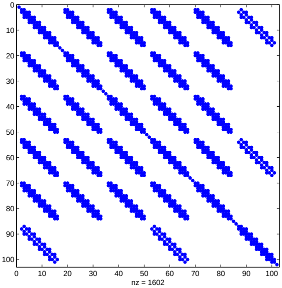
$$\mathcal{K} = \begin{bmatrix} K &&&&& \\ & K &&&& \\ && K &&& \\ &&& K && \\ &&&& K & \\ &&&&& \epsilon_0\bar{\epsilon}K \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M &&&&& \\ & M &&&& \\ && M &&& \\ &&& M && \\ &&&& M & \\ &&&&& 0 \end{bmatrix}$$

$$\mathcal{N}|_{\mathbf{u}_0} = \begin{bmatrix} N^1_{q_1} & N^1_{q_2} & N^1_{q_3} & N^1_{q_4} & N^1_{q_5} & E^1_U \\ N^2_{q_1} & N^2_{q_2} & N^2_{q_3} & N^2_{q_4} & N^2_{q_5} & E^2_U \\ N^3_{q_1} & N^3_{q_2} & N^3_{q_3} & N^3_{q_4} & N^3_{q_5} & E^3_U \\ N^4_{q_1} & N^4_{q_2} & N^4_{q_3} & N^4_{q_4} & N^4_{q_5} & E^4_U \\ N^5_{q_1} & N^5_{q_2} & N^5_{q_3} & N^5_{q_4} & N^5_{q_5} & E^5_U \\ D_{q_1} & D_{q_2} & D_{q_3} & D_{q_4} & D_{q_5} & D_U \end{bmatrix}$$

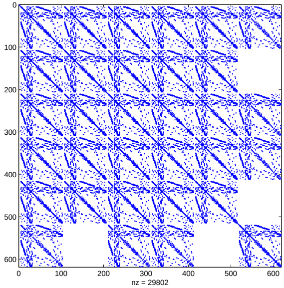
Saddle-point problem

$$\mathcal{A} = \begin{bmatrix} A & B_1 \\ B_2 & C \end{bmatrix}$$

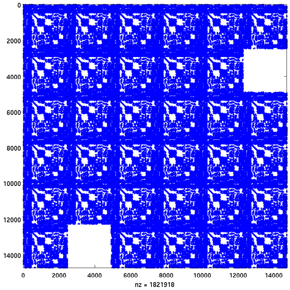
- A is $5n \times 5n$, B_1 is $5n \times n$, B_2 is $n \times 5n$
- A can be indefinite, C is positive definite



1D



2D



3D

GMRES Iterations

- 1D model with right preconditioning
- convergence tolerance 1e-8

N_{el}	N_{dof}	$V = 0$	$V = 0.5$	$V = 1.5$	$V = 5$
16	198	129	151	141	141
32	390	245	298	270	228
64	774	327	430	349	274
128	1542	372	546	441	395
256	3078	594	985	800	720
512	6150	1108	1821	1557	1408

- many (almost) multiple eigenvalues

Block Diagonal Preconditioner

$$\mathcal{A} = \begin{bmatrix} A & B_1 \\ B_2 & C \end{bmatrix}, \qquad \mathcal{P} = \begin{bmatrix} \bar{A} & 0 \\ 0 & -\bar{S} \end{bmatrix}$$

$$\bar{A} \approx A, \qquad \bar{S} \approx S = C - B_2 A^{-1} B_1$$

- $\bar{A} = A$, $\bar{S} = S$

N_{el}	N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
16	198	1	3	7	9
32	390	1	3	7	9
64	774	1	3	8	10
128	1542	1	3	7	10
256	3078	1	3	8	10
512	6150	1	3	7	10

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512	6150	1	3	7	10

- $\bar{A} = A,\ \bar{S} = C$: results exactly the same

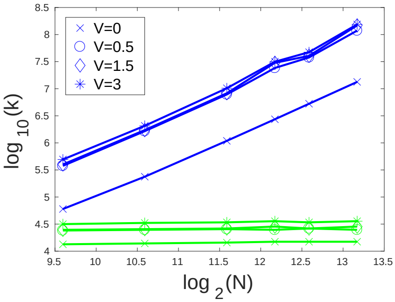
Approximation for A

$$A = \begin{bmatrix} \hat{N}^1_{q_1} & N^1_{q_2} & N^1_{q_3} & N^1_{q_4} & N^1_{q_5} \\ N^2_{q_1} & \hat{N}^2_{q_2} & N^2_{q_3} & N^2_{q_4} & N^2_{q_5} \\ N^3_{q_1} & N^3_{q_2} & \hat{N}^3_{q_3} & N^3_{q_4} & N^3_{q_5} \\ N^4_{q_1} & N^4_{q_2} & N^4_{q_3} & \hat{N}^4_{q_4} & N^4_{q_5} \\ N^5_{q_1} & N^5_{q_2} & N^5_{q_3} & N^5_{q_4} & \hat{N}^5_{q_5} \end{bmatrix}$$

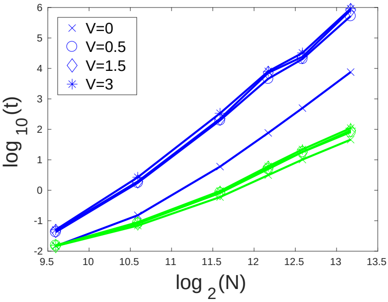
$$\hat{N}^i_{q_i} = K + 2aM + N^i_{q_i}$$

$$\bar{A} = bl\_diag(K)$$

One dimension



iterations

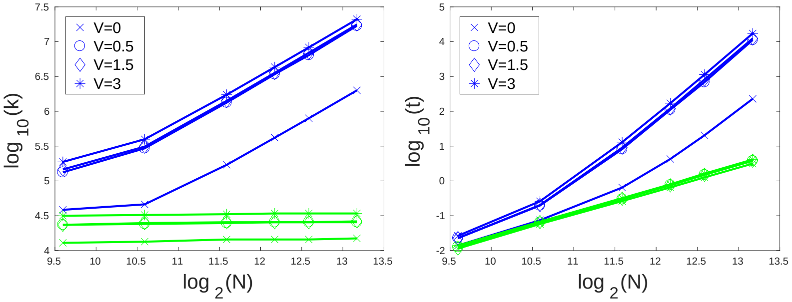


time(sec)

GMRES, preconditioned GMRES

- uniform nodal finite element grid
- from 774 to 9222 degrees of freedom

One dimension

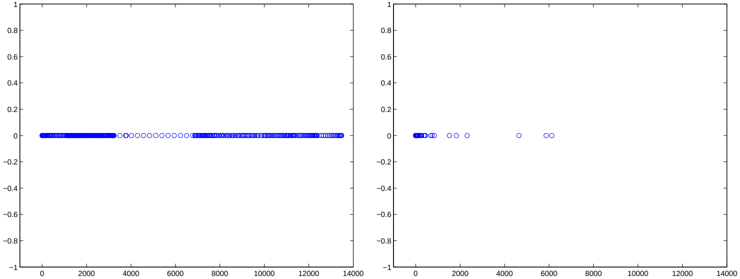


iterations time(sec)

GMRES, preconditioned GMRES

- uniform hierarchical finite element grid
- from 774 to 9222 degrees of freedom

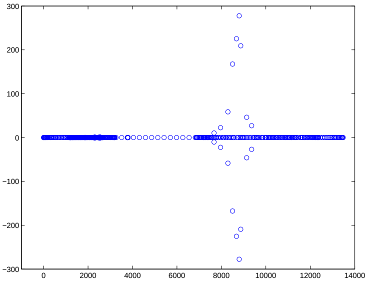
voltage $V = 0$



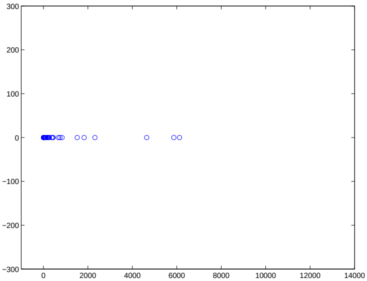
unpreconditioned preconditioned

1D Eigenvalues

voltage $V = 3$

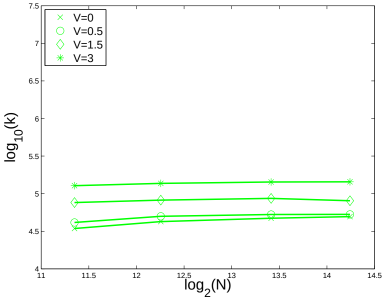


unpreconditioned

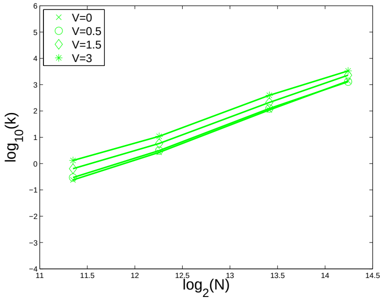


preconditioned

Two dimensions



iterations

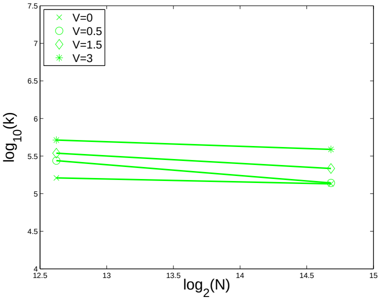


time(sec)

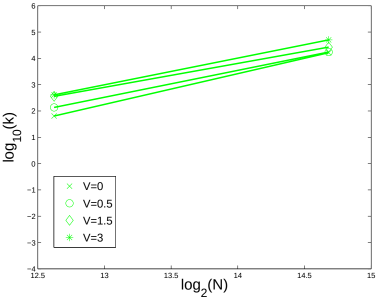
preconditioned GMRES

- unstructured grids of triangles
- from 2610 to 19374 degrees of freedom

Three dimensions



iterations



time(sec)

preconditioned GMRES

- unstructured grids of tetrahedra
- 6306 and 26274 degrees of freedom

Observations

- **Q**-tensor models of liquid crystals lead to complicated algebraic equations.
- Nonlinearities involved make it difficult to identify dominant terms, with many conflicting issues.
- Issues of singularity, indefiniteness, lack of symmetry.
- Block preconditioner using the stiffness matrix performs well on uniform nodal and hierarchical meshes.
  - Convergence independent of the mesh parameter.
  - Cheap to implement using factorisation.
- Further tests required on more complicated problems involving non-standard geometries and defects.
- Adaptive meshes may be required.

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University of Strathclyde, Glasgow, Scotland
June 27th-30th 2017

http://numericalanalysisconference.org.uk/

Elastic Energy

- energy induced by distorting the $\mathbf{Q}$-tensor in space
- energetically favourable for $\mathbf{Q}$ to be constant
- gradients in $\mathbf{Q}$ lead to an increase in energy

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

- parameters L_1 and L_2 related to the Frank elastic constants

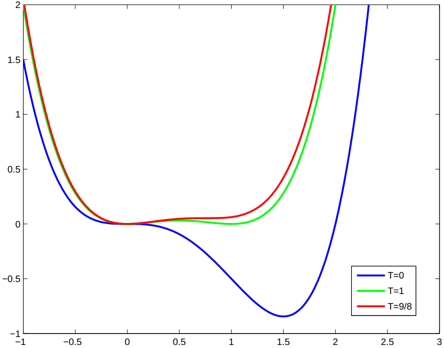
K_1	splay
K_2	twist
K_3	bend
$K_2 + K_4$	saddle-splay

Thermotropic Energy

- potential function which dictates which state the liquid crystal would prefer to be in: uniaxial, biaxial or isotropic

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

- uniaxial case: $\frac{1}{2}A(T - T^*)\ S^2 - \frac{1}{3}B\ S^3 + \frac{1}{4}C\ S^4$



Electrostatic energy

- applied electric field $\mathbf{E}$, electric potential U

$$\mathbf{E} = -\nabla U$$

- electric displacement

$$\mathbf{D} = -\epsilon_0(\bar{\epsilon}\mathbf{I} + \Delta\epsilon^*\mathbf{Q})\nabla U$$

average permittivity $\bar{\epsilon}$, dielectric anisotropy $\Delta\epsilon^*$

$$F_{electrostatic} = -\frac{1}{2}\mathbf{D}\cdot\mathbf{E}$$