Saddle-point Problems in Liquid Crystal Modelling

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With thanks to...

Chuck Gartland (Kent State University)
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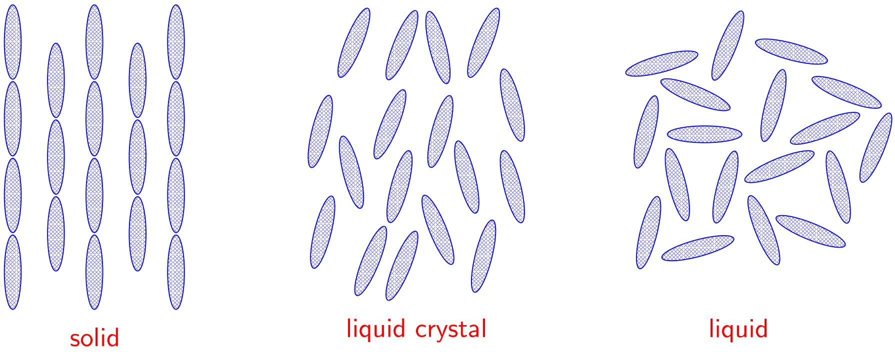
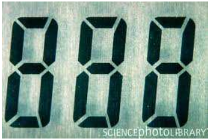
Liquid crystals



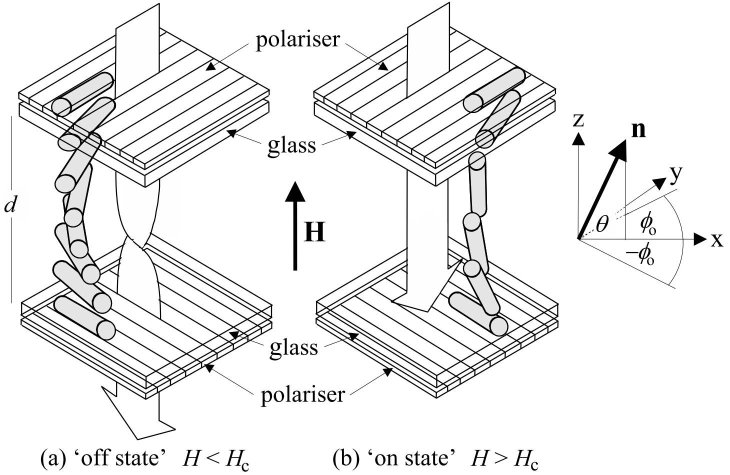
- occur between solid crystal and isotropic liquid states
- may have different equilibrium configurations
- naturally prefer states with minimum energy

Liquid Crystal Displays

- IDEA: force switching between stable states by altering applied voltage, magnetic field, boundary conditions, . . .
- used in a wide range of LCDs

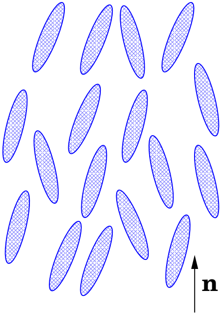


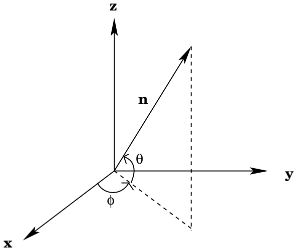
Twisted Nematic Device



(diagram taken from STEWART (2004)*)*

Director-based model





- 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

Finding equilibrium configurations

- minimise the free energy density

$$\mathcal{F} = \int_V F_{bulk}(\theta, \psi, \nabla\theta, \nabla\psi) + \int_{\mathcal{S}} F_{surface}(\theta, \phi)\, d\mathcal{S}$$

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

- if fixed boundary conditions are applied, surface energy term can be ignored
- solutions with least energy are physically relevant
- use calculus of variations: Euler-Lagrange equations

Elastic energy

- Frank-Oseen elastic energy with one-constant approximation

$$F_{elastic} = \frac{1}{2} K \|\nabla \mathbf{n}\|^2$$

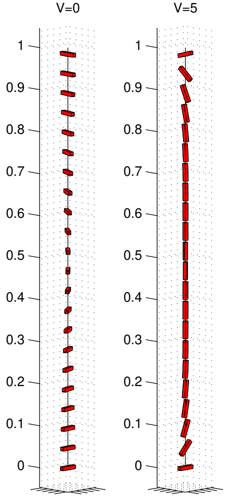
- electrostatic energy

$$F_{electrostatic} = -\frac{1}{2}\epsilon_0 \epsilon_\perp E^2 - \frac{1}{2}\epsilon_0 \epsilon_a (\mathbf{n} \cdot \mathbf{E})^2$$

  - applied electric field $\mathbf{E}$ of magnitude E
  - dielectric anisotropy $\epsilon_a = \epsilon_\| - \epsilon_\perp$
  - permittivity of free space ϵ_0

Twisted Nematic Device

- nematic liquid crystal sample between two parallel plates a distance d apart
- strong anchoring parallel to plate surfaces
- rotate one plate through $\pi/2$ radians
- electric field $\mathbf{E} = (0, 0, E(z))$, applied voltage V
- electric potential U with $E = \dfrac{dU}{dz}$



Problem 1: TND director model

- director $\mathbf{n} = (u, v, w)$, electric potential U with $E = \dfrac{dU}{dz}$
- equilibrium equations on $z \in [0, d]$

$$F = \frac{1}{2} \int_0^d \left\{ K \|\nabla \mathbf{n}\|^2 - \epsilon_0 \epsilon_\perp E^2 - \epsilon_0 \epsilon_a (\mathbf{n} \cdot \mathbf{E})^2 \right\} \, dz$$

- discretise with linear finite elements on a grid of $N + 1$ points z_k a distance Δz apart
- constraints $|\mathbf{n}| = 1$ applied pointwise using Lagrange multipliers λ
- $n = N - 1$ unknowns for each variable u, v, w, U, λ

Constrained minimisation

$$\mathbf{G} = \frac{\Delta z}{2}\left[f(u_1,\ldots,u_n,v_1,\ldots,v_n,w_1,\ldots,w_n,U_1,\ldots,U_n)\right.$$
$$\left. - \lambda_1(u_1^2+v_1^2+w_1^2-1) - \ldots \lambda_n(u_n^2+v_n^2+w_n^2-1)\right]$$

- solve $\nabla\mathbf{G}(\mathbf{x}) = \mathbf{0}$ for $\mathbf{x} = [\mathbf{u},\mathbf{v},\mathbf{w},\lambda,\mathbf{U}]$

  $N+1$ grid points $\Rightarrow n = N-1$ unknowns

- use Newton's method: linear system

$$\nabla^2\mathbf{G}(\mathbf{x}_j)\cdot\delta\mathbf{x}_j = -\nabla\mathbf{G}(\mathbf{x}_j)$$

- $5n \times 5n$ coefficient matrix is Hessian $\nabla^2\mathbf{G}(\mathbf{x})$

$$\nabla^2\mathbf{G} = \begin{bmatrix} \nabla^2_{\mathbf{nn}}\mathbf{G} & \nabla^2_{\mathbf{n}\lambda}\mathbf{G} & \nabla^2_{\mathbf{nU}}\mathbf{G} \\ \nabla^2_{\lambda\mathbf{n}}\mathbf{G} & \nabla^2_{\lambda\lambda}\mathbf{G} & \nabla^2_{\mathbf{U}\lambda}\mathbf{G} \\ \nabla^2_{\mathbf{Un}}\mathbf{G} & \nabla^2_{\lambda\mathbf{U}}\mathbf{G} & \nabla^2_{\mathbf{UU}}\mathbf{G} \end{bmatrix}$$

Full Hessian structure

$$\nabla^2 \mathbf{G} = \begin{bmatrix} \nabla^2_{\mathbf{nn}}\mathbf{G} & \nabla^2_{\mathbf{n}\lambda}\mathbf{G} & \nabla^2_{\mathbf{nU}}\mathbf{G} \\ \nabla^2_{\lambda\mathbf{n}}\mathbf{G} & \nabla^2_{\lambda\lambda}\mathbf{G} & \nabla^2_{\mathbf{U}\lambda}\mathbf{G} \\ \nabla^2_{\mathbf{Un}}\mathbf{G} & \nabla^2_{\lambda\mathbf{U}}\mathbf{G} & \nabla^2_{\mathbf{UU}}\mathbf{G} \end{bmatrix}$$

$$H = \begin{bmatrix} A & B & D \\ B^T & 0 & 0 \\ D^T & 0 & -C \end{bmatrix}$$

- H is a symmetric and indefinite double saddle-point matrix
  - A is positive definite iff $V < V_c$
  - B has full rank with $B^T B = \Delta z^2 I_n$
  - C is tridiagonal and positive definite
  - D has complex eigenvalues in conjugate pairs

Nullspace Method I

$$
\begin{aligned}
A\delta\mathbf{n} + B\delta\lambda + D\delta\mathbf{p} &= -\nabla_{\mathbf{n}} G \qquad (1) \\
B^T\delta\mathbf{n} &= -\nabla_{\lambda} G \qquad (2) \\
D^T\delta\mathbf{n} - C\delta\mathbf{p} &= -\nabla_{\mathbf{U}} G \qquad (3)
\end{aligned}
$$

- use $Z \in \mathbb{R}^{3n\times 2n}$ whose columns form a basis for the nullspace of B^T, i.e. $B^T Z = Z^T B = 0$
- write solution of (2) as $\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{x}$ where particular solution satisfies $B^T\widehat{\delta\mathbf{n}} = -\nabla_\lambda G$
- system size reduced from $5n \times 5n$ to $3n \times 3n$

Nullspace Method II

- reduced system $\mathcal{H}\hat{\mathbf{x}} = \hat{\mathbf{b}}$:

$$\begin{bmatrix} Z^T A Z & Z^T D \\ D^T Z & -C \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \delta \mathbf{U} \end{bmatrix} = \begin{bmatrix} -Z^T(\nabla_{\mathbf{n}} G + A\widehat{\delta \mathbf{n}}) \\ -\nabla_{\mathbf{U}} G - D^T \widehat{\delta \mathbf{n}} \end{bmatrix}$$

- recover full solution from

$$\begin{aligned} \widehat{\delta \mathbf{n}} &= -B(B^T B)^{-1} \nabla_\lambda G \\ \delta \mathbf{n} &= Z\mathbf{x} + \widehat{\delta \mathbf{n}} \\ \delta \lambda &= (B^T B)^{-1} B^T(-\nabla_{\mathbf{n}} G - A\delta \mathbf{n} - D\delta \mathbf{U}) \end{aligned}$$

- here $B^T B$ is diagonal so solve is cheap

Nullspace of B^T

$$B = -\Delta z \begin{bmatrix} \mathbf{n}_1 & & & \\ & \mathbf{n}_2 & & \\ & & \ddots & \\ & & & \mathbf{n}_n \end{bmatrix}, \quad \mathbf{n}_j = \begin{bmatrix} u_j \\ v_j \\ w_j \end{bmatrix}$$

- use eigenvectors of orthogonal projection $I - \mathbf{n}_j \otimes \mathbf{n}_j$, e.g.

$$\mathbf{l}_j = \begin{bmatrix} -\frac{v_j}{u_j} \\ 1 \\ 0 \end{bmatrix}, \qquad \mathbf{m}_j = \begin{bmatrix} -\frac{w_j}{u_j} \\ 0 \\ 1 \end{bmatrix} \qquad (u_j \neq 0)$$

$$Z = \begin{bmatrix} \mathbf{l}_1 & \mathbf{m}_1 & & & & & \\ & & \mathbf{l}_2 & \mathbf{m}_2 & & & \\ & & & & \ddots & & \\ & & & & & \mathbf{l}_n & \mathbf{m}_n \end{bmatrix}$$

Preconditioned Minres

- Solve reduced system using Minres iterative method.
- Instead of solving $\mathcal{H}\hat{\mathbf{x}} = \hat{\mathbf{b}}$, solve

$$\mathcal{P}^{-1/2}\mathcal{H}\mathcal{P}^{-1/2}(\mathcal{P}^{1/2}\hat{\mathbf{x}}) = \mathcal{P}^{-1/2}\hat{\mathbf{b}}$$

  for some preconditioner $\mathcal{P}$

- Choose $\mathcal{P}$ so that

  (i) eigenvalues of $\mathcal{P}^{-1/2}\mathcal{H}\mathcal{P}^{-1/2}$ are well clustered

  (ii) $\mathcal{P}\mathbf{u} = \mathbf{r}$ is easily solved

Ideal Block Preconditioner

- block preconditioner: $\mathcal{P} = \begin{bmatrix} Z^T A Z & 0 \\ 0 & C \end{bmatrix}$

- preconditioned matrix:

$$\tilde{\mathcal{H}} = \mathcal{P}^{-1/2} \mathcal{H} \mathcal{P}^{-1/2} = \begin{bmatrix} I & M^T \\ M & -I \end{bmatrix}$$

$$M = C^{-1/2} Z^T D (Z^T A Z)^{-1/2}$$

- $3n$ eigenvalues of $\tilde{\mathcal{H}}$ are

(i) 1 with multiplicity $n+1$

(ii) -1 with multiplicity 1

(iii) $\pm\sqrt{1+\sigma_k^2}$ for $k = 1, \dots, n-1$

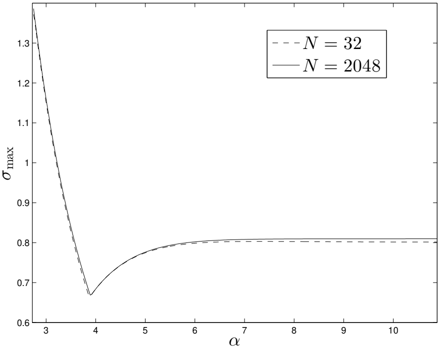
$\sigma_k \equiv$ singular value of M

Estimate of Minres convergence

- to achieve $\|\mathbf{r}_k\|_2 \leq \epsilon \|\mathbf{r}_0\|_2$ need

$$k \simeq \frac{1}{2}\sqrt{1+\sigma_{\max}^2}\,\ln\left(\frac{2}{\epsilon}\right)$$

- $\sigma_{\max}$ is essentially independent of N



Minres Iteration Counts

N	off state first step	off state last step	on state first step	on state last step
64	4	1	5	7
256	4	1	5	7
1,024	4	1	5	7
4,096	4	1	5	7
16,384	4	1	5	7
65,536	4	1	5	7

Practical preconditioners

- Block systems can also be solved iteratively.
- Example: use a fixed number of PCG iterations with AMG preconditioner (HSL_MI20).

	1 PCG/AMG iteration				3 PCG/AMG iterations			
	off state		on state		off state		on state	
N	first	last	first	last	first	last	first	last
32	6	5	7	9	4	1	5	7
128	7	6	7	9	4	1	5	7
512	7	6	8	9	4	1	5	7
2,048	7	6	8	9	4	2	5	7
8,192	7	6	8	9	4	2	5	7

Summary of Problem 1

Director modelling of TND device in 1D cell

- Obtain a double saddle-point system due to imposing the unit vector constraint $|\mathbf{n}| = 1$ and coupling with the electric (magnetic) field.
- Efficient preconditioned nullspace solver developed with potential for full 2D and 3D simulations.
- Issues remain re how to precondition $Z^T A Z$ for these more general cases.

Other difficulties with director modelling:

- dealing with multivalued angles
- modelling equivalence of $\mathbf{n}$ and $-\mathbf{n}$
- modelling defect cores (mathematical singularities)

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
- basis representation

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

- applied electric field **E**, electric potential U
- unknowns $q_1, q_2, q_3, q_4, q_5, U$

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

Elastic and thermotropic energies

- elastic energy: induced by distorting the **Q**-tensor in space

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

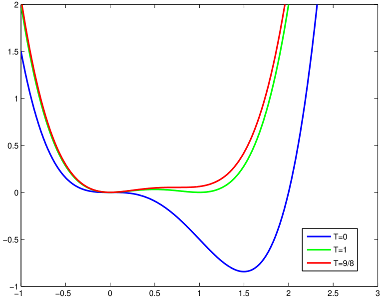
- thermotropic energy: potential function which dictates which state the liquid crystal would prefer to be in (uniaxial, biaxial or isotropic)

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

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



Electrostatic energy

- electrostatic energy: due to an applied electric field $\mathbf{E}$

$$F_{electrostatic} = -\frac{1}{2}\epsilon_0 \boldsymbol{E} \cdot \epsilon \boldsymbol{E} - \boldsymbol{P}_{fl} \cdot \boldsymbol{E}$$

- flexoelectric term (average permittivity $\bar{e}$):

$$\boldsymbol{P}_{fl} = \bar{e}\,\mathrm{div}\,\boldsymbol{Q}$$

- electric potential U with $\mathbf{E} = -\nabla U$

- electric displacement

$$\boldsymbol{D} = \epsilon_0(\bar{\epsilon}\boldsymbol{I} + \Delta\epsilon^* \boldsymbol{Q})\nabla U + \bar{e}\,\mathrm{div}\boldsymbol{Q}$$

Minimising the free energy

- solve Euler-Lagrange equations

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

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

- 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

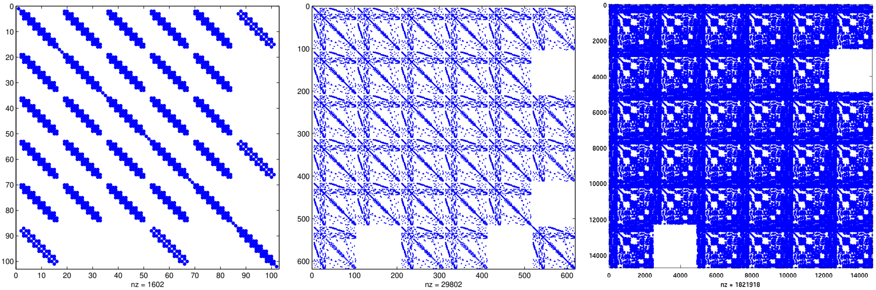
$$(\mathcal{K} + 2a\mathcal{M} + \mathcal{N}|_{\mathbf{u}_0})\delta\mathbf{u} = -(\mathcal{K} + 2a\mathcal{M})\mathbf{u}_0 - \mathcal{R}|_{\mathbf{u}_0}$$

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

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

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

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



1D 2D 3D

1D problem

- GMRES iterations with diagonal 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
- real eigenvalues for $V < V_c$
- complex eigenvalues for $V > V_c$

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

Block diagonal preconditioner

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

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

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

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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

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

Approximation for A

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

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

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

GMRES iteration counts

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

N_{el}	N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
16	198	79	78	93	107
32	390	99	97	117	132
64	774	112	117	125	139
128	1542	119	118	127	140
256	3078	121	120	126	140
512	6150	122	121	128	140

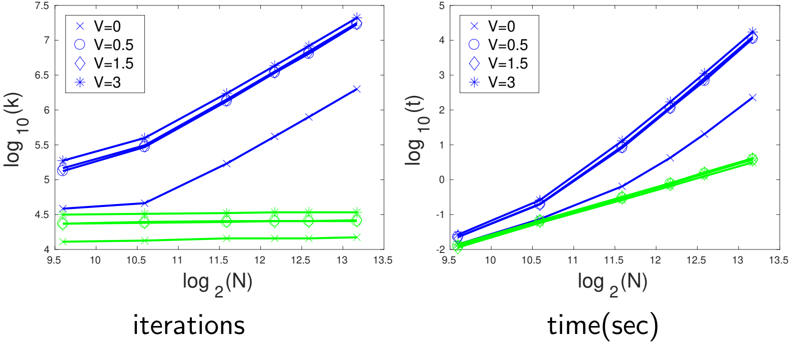
GMRES iteration counts

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

N_{el}	N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
16	198	79	78	93	107
32	390	99	97	117	132
64	774	112	117	125	139
128	1542	119	118	127	140
256	3078	121	120	126	140
512	6150	122	121	128	140

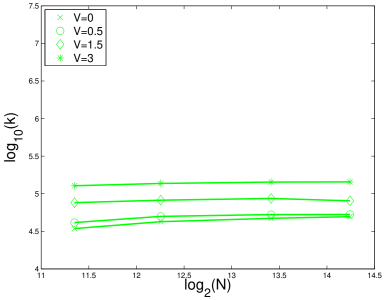
$\bar{A} = bl\_diag(K),\ \bar{S} = K$

N_{el}	N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
16	198	79	82	100	105
32	390	99	100	118	126
64	774	112	111	121	131
128	1542	118	118	121	132
256	3078	121	120	123	133
512	6150	122	121	123	132

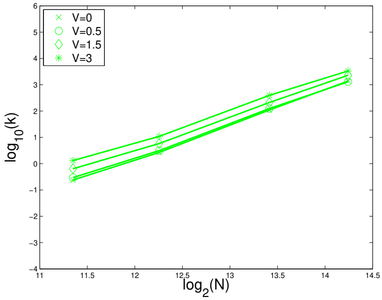


GMRES, preconditioned GMRES

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



iterations

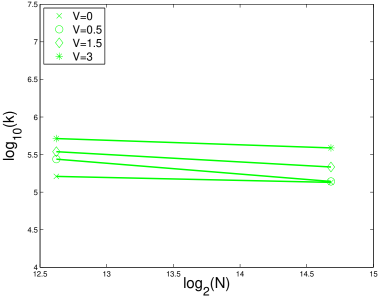


time(sec)

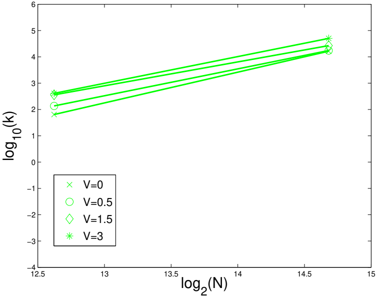
preconditioned GMRES

- hierarchic finite elements of degree two
- unstructured grids of triangles
- from 2610 to 19374 degrees of freedom

Three dimensions



iterations



time(sec)

preconditioned GMRES

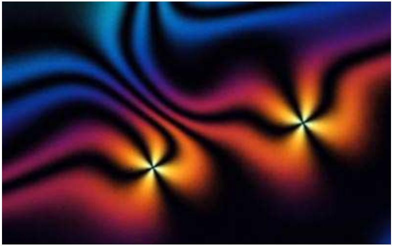
- unstructured grids of tetrahedra
- 6306 and 26274 degrees of freedom

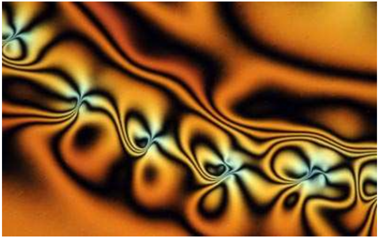
Summary of Problem 2

- **Q**-tensor models of liquid crystals lead to complicated algebraic equations.
- Nonlinearities involved make it difficult to identify dominant terms, with many conflicting issues involving 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.
- Would be nice to have some theory!

Coupled flow and orientation

- More and more applications in e-readers, moving colour displays, digital ink. . .
- Require numerical models linking molecular orientation and flow.





Photographs by Israel Lazo, Kent State University.

Q-tensor Model

- tensor order parameter (symmetric and traceless)

$$\mathbf{Q} := \langle \overbrace{\boldsymbol{u} \otimes \boldsymbol{u}} \rangle = \langle \boldsymbol{u} \otimes \boldsymbol{u} - \frac{1}{3}\mathbf{I} \rangle$$

- material and co-rotational time derivatives

$$\dot{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + (\nabla \mathbf{Q})\boldsymbol{v}, \qquad \mathring{\mathbf{Q}} = \dot{\mathbf{Q}} - 2\,\overbrace{\mathbf{WQ}}$$

- flow with velocity $\boldsymbol{v}$

- symmetric and skew parts of the velocity gradient

$$\mathbf{D} = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T), \qquad \mathbf{W} = \frac{1}{2}(\nabla \boldsymbol{v} - (\nabla \boldsymbol{v})^T)$$

Governing Equations

- dissipation $R = R(\mathring{\mathbf{Q}}, \mathbf{Q}, \mathbf{D})$
- stress tensor

$$\mathbf{T} = -p\,\mathbf{I} - \nabla\mathbf{Q} \odot \frac{\partial W}{\partial \nabla \mathbf{Q}} + \frac{\partial R}{\partial \mathbf{D}} + \mathbf{Q}\,\frac{\partial R}{\partial \mathring{\mathbf{Q}}} - \frac{\partial R}{\partial \mathring{\mathbf{Q}}}\,\mathbf{Q}$$

- coupled equations for alignment and flow:

$$\frac{\partial W}{\partial \mathbf{Q}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{Q}} + \frac{\partial R}{\partial \mathring{\mathbf{Q}}} = \mathbf{0}$$

$$\rho \dot{\boldsymbol{v}} = \operatorname{div} \mathbf{T}$$

Sonnet and Virga Dissipative Ordered Fluids: Theories for Liquid Crystals, Springer 2012

Special Case

- free energy based on Landau-deGennes potential

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

- coupled equations

$$\mathring{\mathbf{Q}} = \Delta\mathbf{Q} \quad - \quad \partial\phi/\partial\mathbf{Q} - \mathrm{Tu}\,\mathbf{D}$$

$$\nabla p \quad - \quad \Delta \boldsymbol{v} = \mathrm{div}\,\mathbf{F}$$

$$\mathbf{F} = \mathrm{Bf}\left\{\tfrac{1}{\mathrm{Tu}}\left[\mathbf{Q}(\Delta\mathbf{Q}) - (\Delta\mathbf{Q})\mathbf{Q} - \nabla\mathbf{Q}\odot\nabla\mathbf{Q}\right] + \Delta\mathbf{Q} - \partial\phi/\partial\mathbf{Q}\right\}$$

- the backflow parameter Bf measures the impact of the orientation on the flow;
- the tumbling parameter Tu measures the relative strength of problem viscosities.

Iterative Solution Strategy

- Decoupled solver:
  - For a given orientation field $\mathbf{Q}$, solve Stokes equation with $f = \operatorname{div} \mathbf{F}$ as a body force.
  - Use the obtained flow field to compute one time step in a discretised version of the orientation equation.
  - Repeat with the new orientation field.

- Solution strategy
  - Orientation equation: finite difference scheme with explicit Euler time discretisation
  - Stokes equation: IFISS Stokes solver with multigrid preconditioning

IFISS

Incompressible **F**low & **I**terative **S**olver **S**oftware

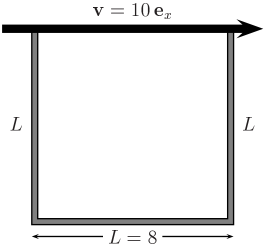
- open-source software package run under MATLAB or GNU OCTAVE written with Howard Elman (Maryland) and David Silvester (Manchester)

- download from

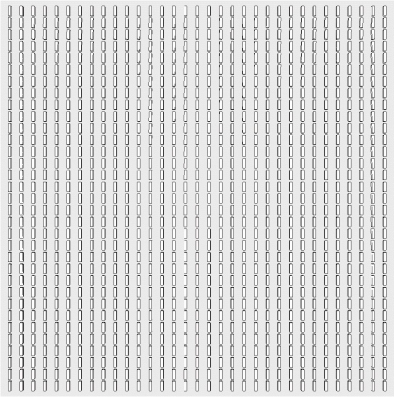
  `www.manchester.ac.uk/ifiss`

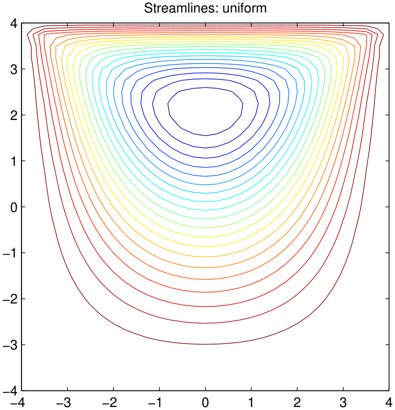
  `www.cs.umd.edu/∼elman/ifiss`

Lid Driven Cavity



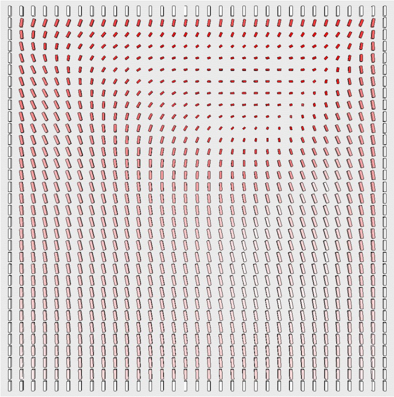
$$
\begin{aligned}
\mathrm{Re} &= \frac{VL\rho}{\zeta_4} = 8 \times 10^{-6} \\
\mathrm{De} &\approx \frac{V}{L} = 1.2 \\
\mathrm{Er} &\approx \frac{\zeta_1 VL}{L_1} = 80
\end{aligned}
$$

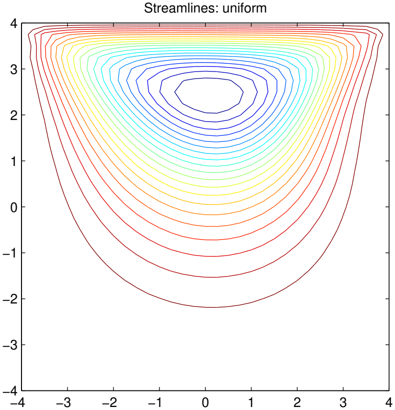




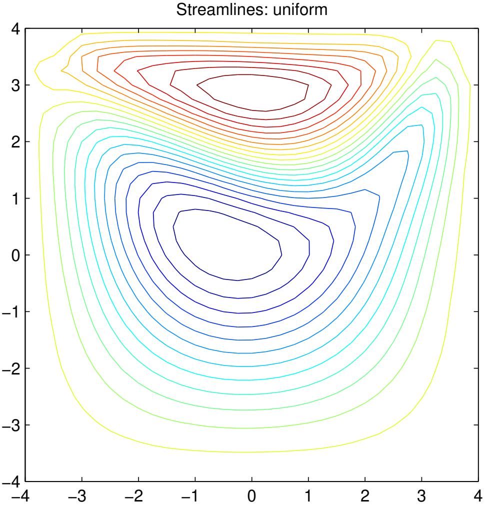
Streamlines: uniform
4
3
2
1
0
−1
−2
−3
−4
−4 −3 −2 −1 0 1 2 3 4

Later Orientation and Flow Field

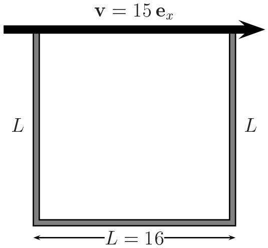




Flow Field Difference

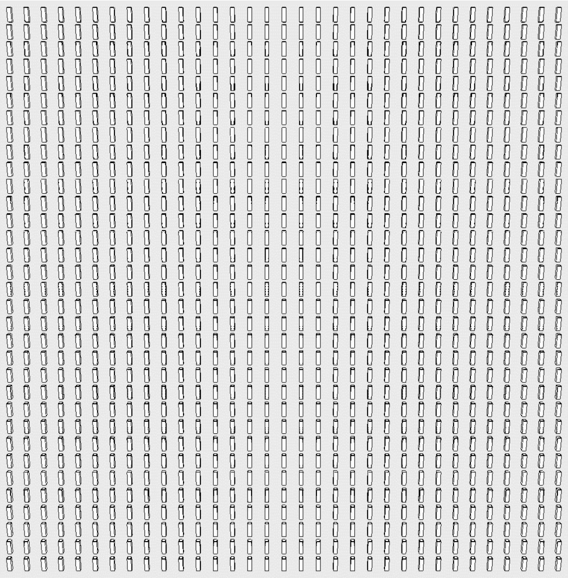


Out of Plane Orientation

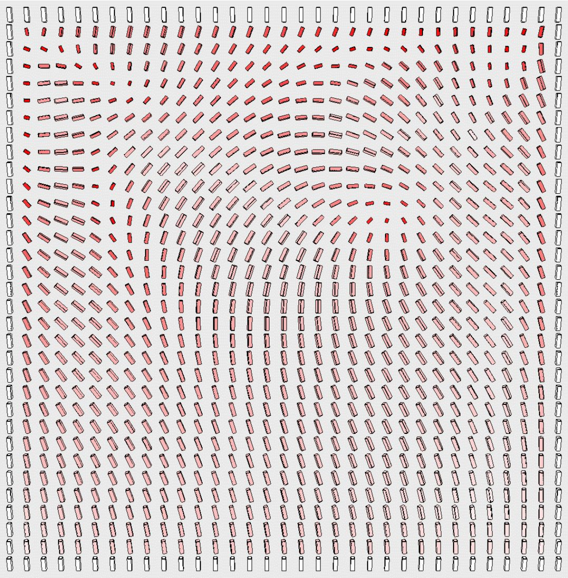


$$
\begin{aligned}
\mathrm{Re} &= \frac{VL\rho}{\zeta_4} = 2.4 \times 10^{-5} \\
\mathrm{De} &\approx \frac{V}{L} = 0.9 \\
\mathrm{Er} &\approx \frac{\zeta_1 VL}{L_1} = 240
\end{aligned}
$$

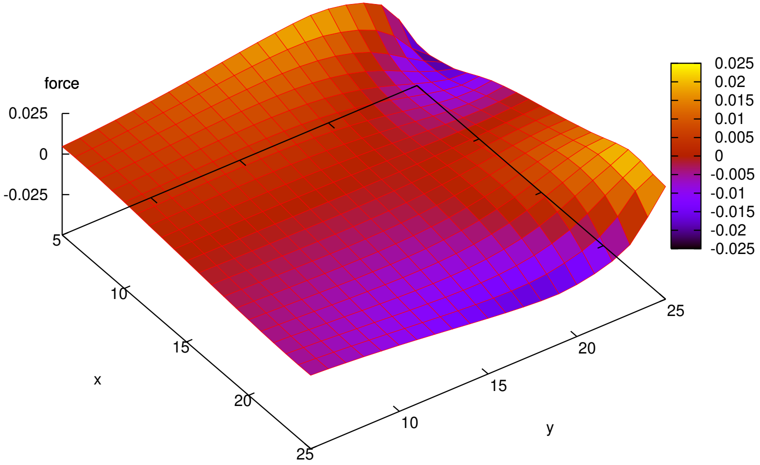
Initial Orientation



Later Orientation



Out of Plane Force



Summary

- Linear algebra subproblems often cause bottlenecks in computational models in terms of memory and CPU time.
- Spending some time and effort on developing efficient preconditioned iterative solvers can be beneficial.
- Three examples presented today:
  - For director models with unit vector constraints, systems can be solved efficiently using a preconditioned nullspace method (which should be efficient in 1D, 2D and 3D).
  - For **Q**-tensor models, a block preconditioner using the stiffness matrix shows promise: it is cheap to implement and may lead to convergence independent of meshsize.
  - For coupled flow-orientation models, important out-of-plane effects have been quantified and identified.
- Many interesting applications and challenges out there!