Saddle-point Problems in Liquid Crystal Modelling

Alison Ramage
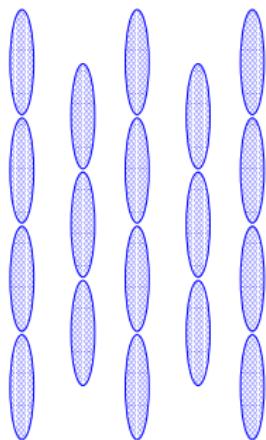
Department of Mathematics and Statistics, University of Strathclyde
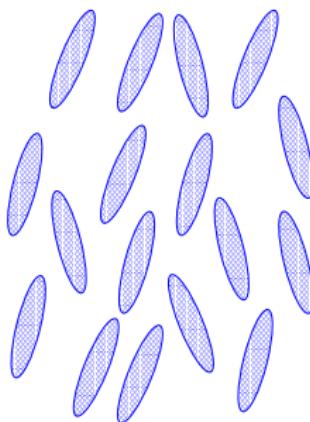
With thanks to. . .

University of
Strathclyde
Glasgow
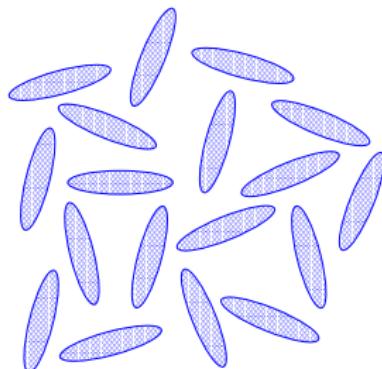
# Liquid crystals

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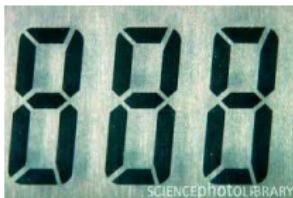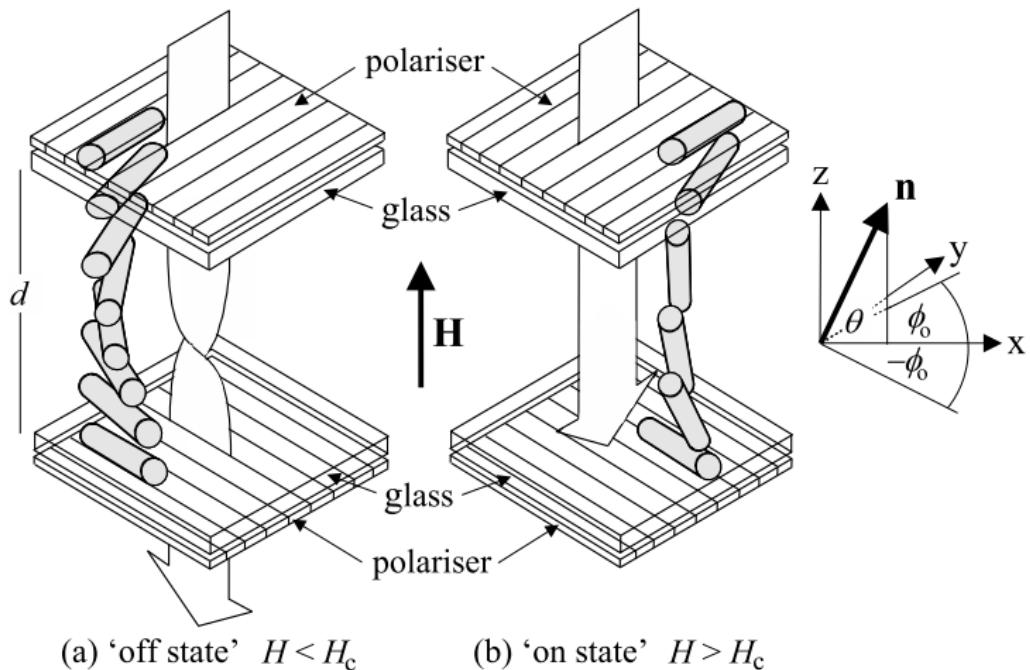
- occur between solid crystal and isotropic liquid states
- may have different equilibrium configurations
- naturally prefer states with minimum energy

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


(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$
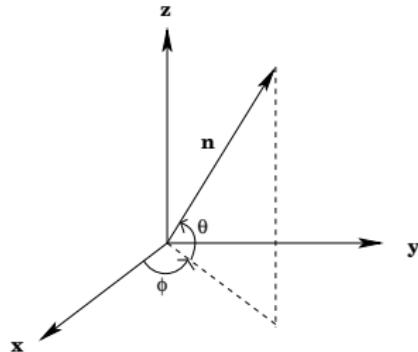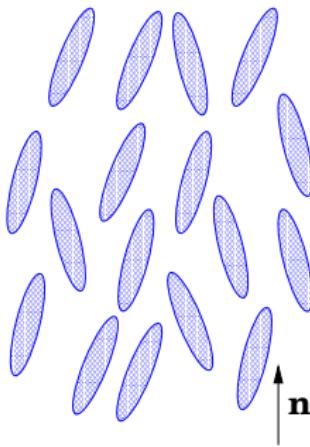
(diagram taken from STEWART (2004))

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

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

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

- with strong anchoring (Dirichlet boundary conditions), there is no contribution from surface energy

- solutions with least energy are physically relevant

- use calculus of variations: Euler-Lagrange equations

Energy contributions

- Frank-Oseen elastic energy with one-constant approximation

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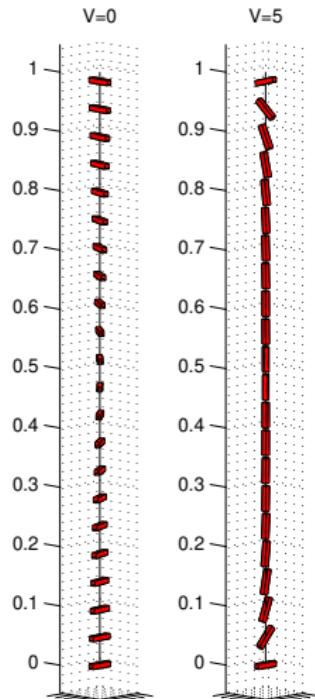
- electrostatic energy

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

- applied electric field $\mathbf{E}$ of magnitude E
- dielectric anisotropy $\quad \epsilon_a = \epsilon_\parallel - \epsilon_\perp$
- permittivity of free space $\quad \epsilon_0$

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 $E = \dfrac{dU}{dz}$

- director $\mathbf{n} = (u, v, w)$, electric potential U

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

- Newton's method: linear system $\quad \nabla^2\mathbf{G}(\mathbf{x}_j) \cdot \delta\mathbf{x}_j = -\nabla\mathbf{G}(\mathbf{x}_j)$

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

$$\nabla^2\mathbf{G} = \begin{bmatrix} \nabla^2_{\mathbf{nn}}\mathbf{G} & \nabla^2_{\mathbf{n}\lambda}\mathbf{G} & \nabla^2_{\mathbf{nU}}\mathbf{G} \\ \nabla^2_{\lambda\mathbf{n}}\mathbf{G} & \nabla^2_{\lambda\lambda}\mathbf{G} & \nabla^2_{\mathbf{U}\lambda}\mathbf{G} \\ \nabla^2_{\mathbf{Un}}\mathbf{G} & \nabla^2_{\lambda\mathbf{U}}\mathbf{G} & \nabla^2_{\mathbf{UU}}\mathbf{G} \end{bmatrix} = \begin{bmatrix} A & B & D \\ B^T & 0 & 0 \\ D^T & 0 & -C \end{bmatrix}$$

- H is a symmetric and indefinite double saddle-point matrix of dimension $5n \times 5n$

$$A\delta\mathbf{n} + B\delta\lambda + D\delta\mathbf{p} = -\nabla_{\mathbf{n}}G \tag{1}$$

$$B^T\delta\mathbf{n} = -\nabla_{\lambda}G \tag{2}$$

$$D^T\delta\mathbf{n} - C\delta\mathbf{p} = -\nabla_{\mathbf{U}}G \tag{3}$$

- 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

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

- here $B^TB = \Delta z^2 I_n$ 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 $I_3 - \mathbf{n}_j \otimes \mathbf{n}_j$, e.g.

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

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

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

- 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 $k = 1, \ldots, n-1$
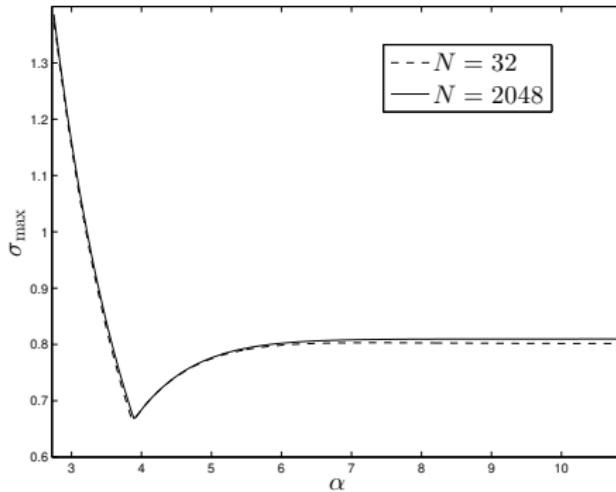
  $\qquad \sigma_k \equiv$ singular value of M

Estimate of Minres convergence

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

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

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

Minres Iteration Counts

N	off state		on state	
	first step	last step	first step	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)

Problem 2: TND **Q**-tensor model

- most common nematic LC consists of effectively uniaxial molecules: describe orientation of each molecule by a single vector **u** in direction of its main axis

- represent average orientation by symmetric and traceless order tensor

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

- (non-unique) five-dimensional basis representation, e.g.

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

- 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

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

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

- with strong anchoring (Dirichlet boundary conditions), there is no contribution from surface energy

- we can derive expressions for individual energy contributions in terms of $\mathbf{Q}$, $\nabla\mathbf{Q}$

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

Bulk 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 preferred state (uniaxial, biaxial or isotropic)

$$F_{thermotropic} = \frac{1}{2}A(T - T^*)\,\mathrm{tr}\ \mathbf{Q}^2 - \frac{\sqrt{6}}{3}B\,\mathrm{tr}\ \mathbf{Q}^3 + \frac{1}{4}C(\mathrm{tr}\ \mathbf{Q}^2)^2$$
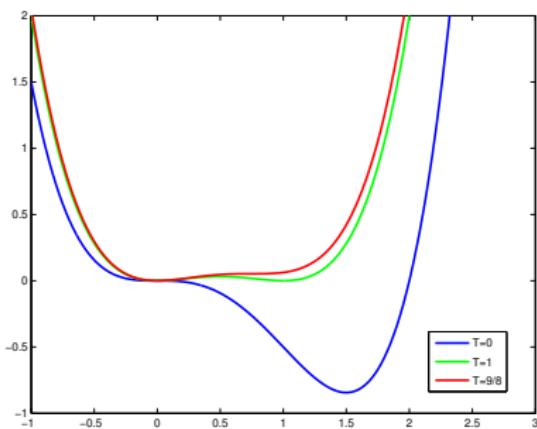
- electrostatic energy: due to an applied electric field **E** (electric potential U with $\mathbf{E} = -\nabla U$)

$$F_{electrostatic} = -\frac{1}{2}\epsilon_0\mathbf{E}\cdot\boldsymbol{\epsilon}\mathbf{E} - (\bar{e}\,\mathrm{div}\ \mathbf{Q})\cdot\mathbf{E}$$

Thermotropic energy

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

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

- assuming no free charges, solve the Maxwell equation

$$\nabla \cdot \mathbf{D} = 0, \qquad \text{electric displacement } \mathbf{D}$$

SUMMARY

- six coupled PDEs in 6 unknowns $\quad (q_1, q_2, q_3, q_4, q_5, U)$

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

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

- finite element approximation, quadratic elements: linearise about $\mathbf{u}_0$ and iterate

Linear system at each step

$$(\mathcal{K} + 2a\mathcal{M} + \mathcal{N}|_{\mathbf{u}_0})\delta\mathbf{u} = -(\mathcal{K} + 2a\mathcal{M})\mathbf{u}_0 - \mathcal{R}|_{\mathbf{u}_0}$$
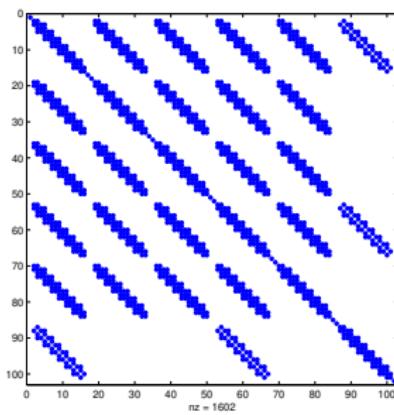
$$\mathcal{K} = \begin{bmatrix} K & & & & & \\ & K & & & & \\ & & K & & & \\ & & & K & & \\ & & & & K & \\ & & & & & \epsilon_0\bar{\epsilon}K \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M & & & & & \\ & M & & & & \\ & & M & & & \\ & & & M & & \\ & & & & M & \\ & & & & & 0 \end{bmatrix}$$

$$\mathcal{N}|_{\mathbf{u}_0} = \begin{bmatrix} N_{q_1}^1 & N_{q_2}^1 & N_{q_3}^1 & N_{q_4}^1 & N_{q_5}^1 & E_U^1 \\ N_{q_1}^2 & N_{q_2}^2 & N_{q_3}^2 & N_{q_4}^2 & N_{q_5}^2 & E_U^2 \\ N_{q_1}^3 & N_{q_2}^3 & N_{q_3}^3 & N_{q_4}^3 & N_{q_5}^3 & E_U^3 \\ N_{q_1}^4 & N_{q_2}^4 & N_{q_3}^4 & N_{q_4}^4 & N_{q_5}^4 & E_U^4 \\ N_{q_1}^5 & N_{q_2}^5 & N_{q_3}^5 & N_{q_4}^5 & N_{q_5}^5 & E_U^5 \\ D_{q_1} & D_{q_2} & D_{q_3} & D_{q_4} & D_{q_5} & D_U \end{bmatrix}$$
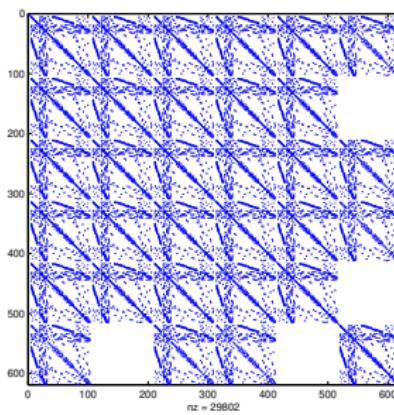
Saddle-point problem

$$\mathcal{A} = \begin{bmatrix} A & B_1 \\ B_2 & C \end{bmatrix}$$
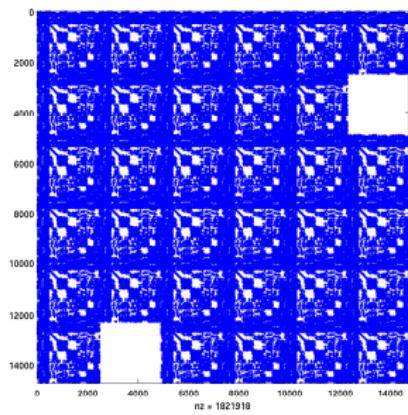
- A is $5n \times 5n$, B_1 is $5n \times n$, B_2 is $n \times 5n$
- nonsymmetric: A can be indefinite, C is positive definite

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

$$\mathcal{A} = \left[\begin{array}{cc} A & B_1 \\ B_2 & C \end{array} \right], \qquad \mathcal{P} = \left[\begin{array}{cc} \bar{A} & 0 \\ 0 & -\bar{S} \end{array} \right]$$

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

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

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

$$\mathcal{A} = \left[\begin{array}{cc} A & B_1 \\ B_2 & C \end{array} \right], \qquad \mathcal{P} = \left[\begin{array}{cc} \bar{A} & 0 \\ 0 & -\bar{S} \end{array} \right]$$

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

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

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

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

Approximation for A

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

$$\hat{N}_{q_i}^i = K + 2aM + N_{q_i}^i$$

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

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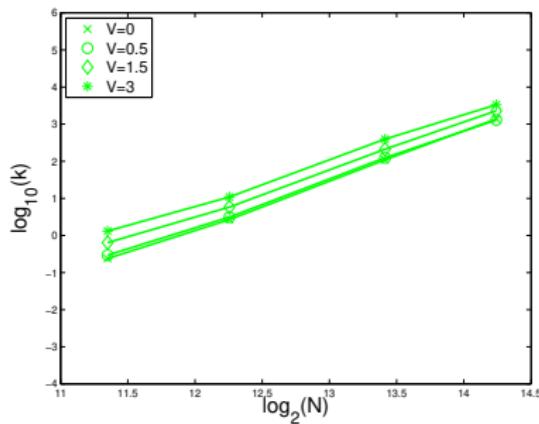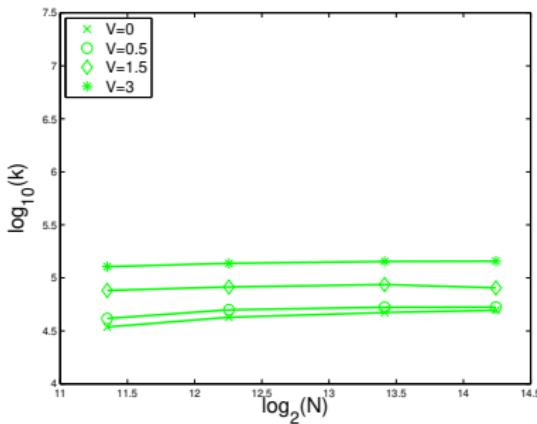
$\bar{A} = bl\_diag(K)$, $\bar{S} = C$

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

Two dimensions
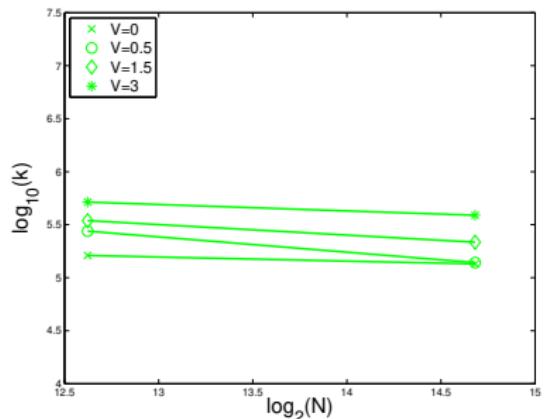
iterations   time(sec)
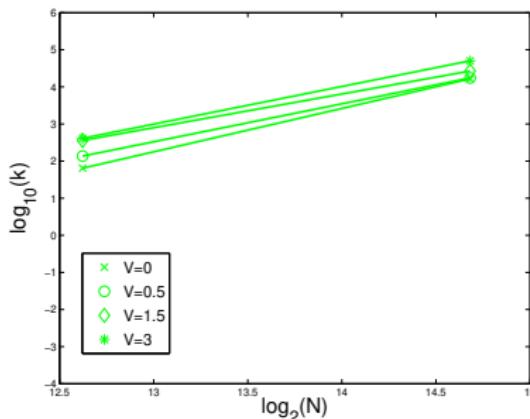
preconditioned GMRES

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

iterations   time(sec)

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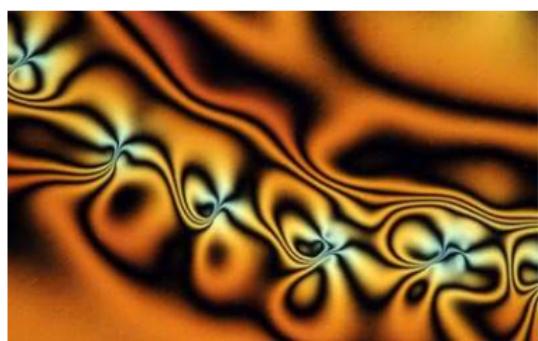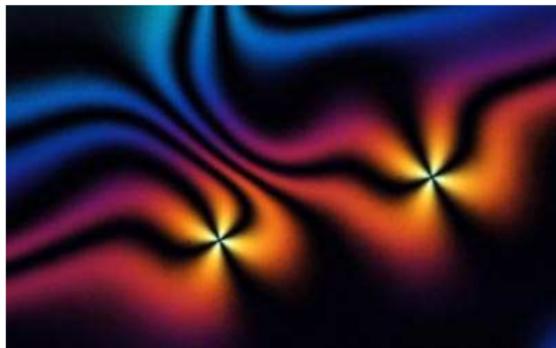
- unstructured grids of tetrahedra
- 6306 and 26274 degrees of freedom

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.

- Producing theoretical results is challenging.

- 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

- symmetric and traceless order tensor

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

- flow with velocity $\boldsymbol{v}$

- symmetric and skew parts of the velocity gradient

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

- material and co-rotational time derivatives

$$\dot{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + (\nabla \mathbf{Q})\boldsymbol{v}, \qquad \overset{\circ}{\mathbf{Q}} = \dot{\mathbf{Q}} - 2\overline{\mathbf{W}\mathbf{Q}}$$

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

- 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

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

- coupled equations
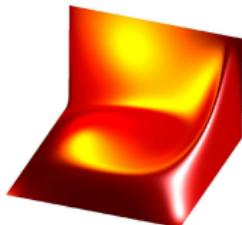
$$\mathring{\mathbf{Q}} = \Delta\mathbf{Q} \quad - \quad \partial\phi/\partial\mathbf{Q} - \operatorname{Tu}\mathbf{D}$$

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

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

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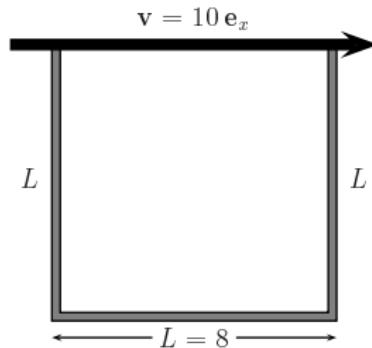
Incompressible **F**low & **I**terative **S**olver **S**oftware

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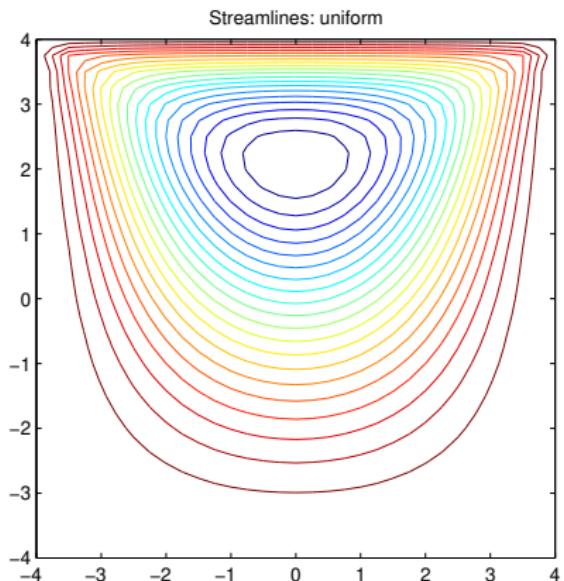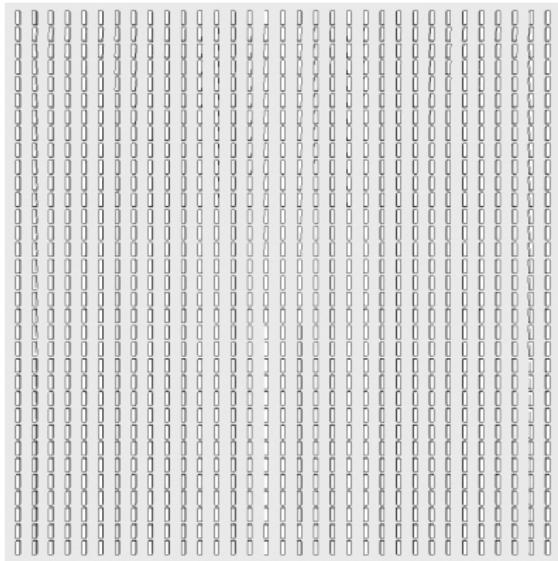
$$
\begin{aligned}
\text{Re} &= \frac{VL\rho}{\zeta_4} = 8 \times 10^{-6} \\
\text{De} &\approx \frac{V}{L} = 1.2 \\
\text{Er} &\approx \frac{\zeta_1 VL}{L_1} = 80
\end{aligned}
$$

Streamlines: uniform
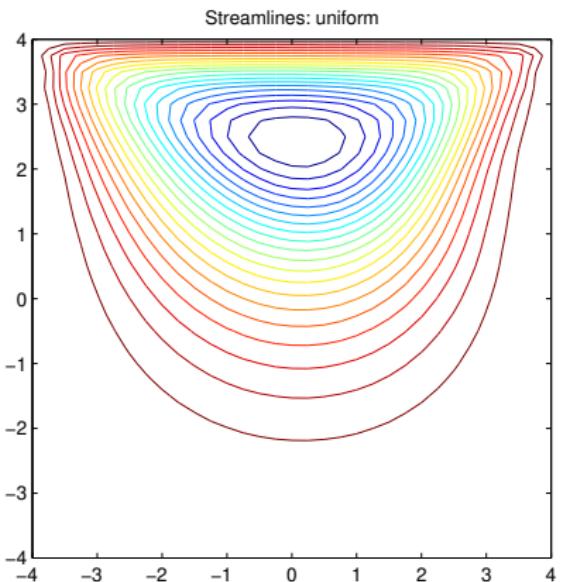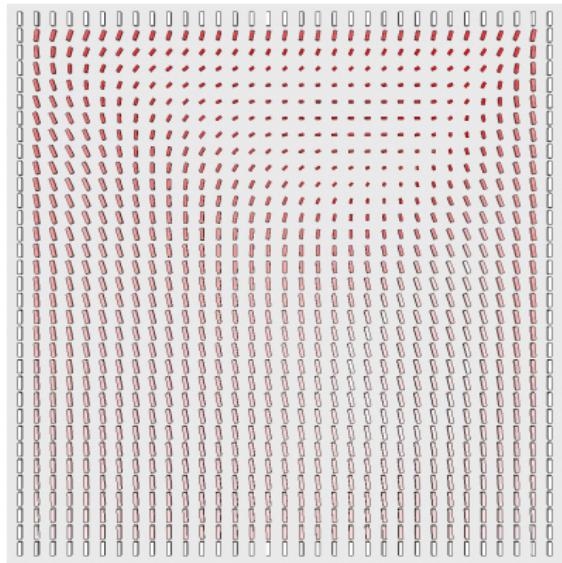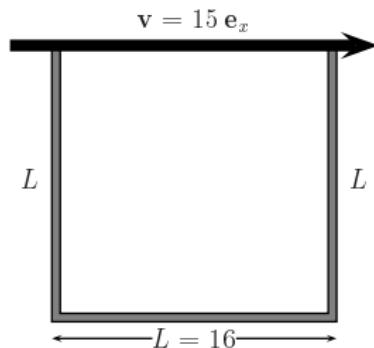
Later Orientation and Flow Field

Streamlines: uniform

Out of Plane Orientation
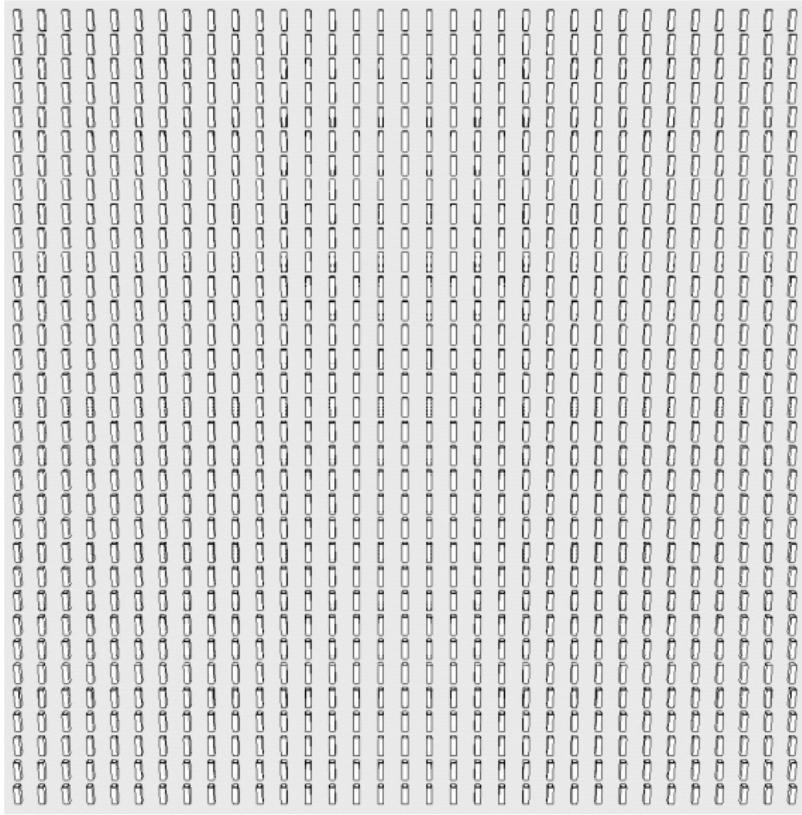
$$\mathrm{Re} \;=\; \frac{VL\rho}{\zeta_4} = 2.4 \times 10^{-5}$$
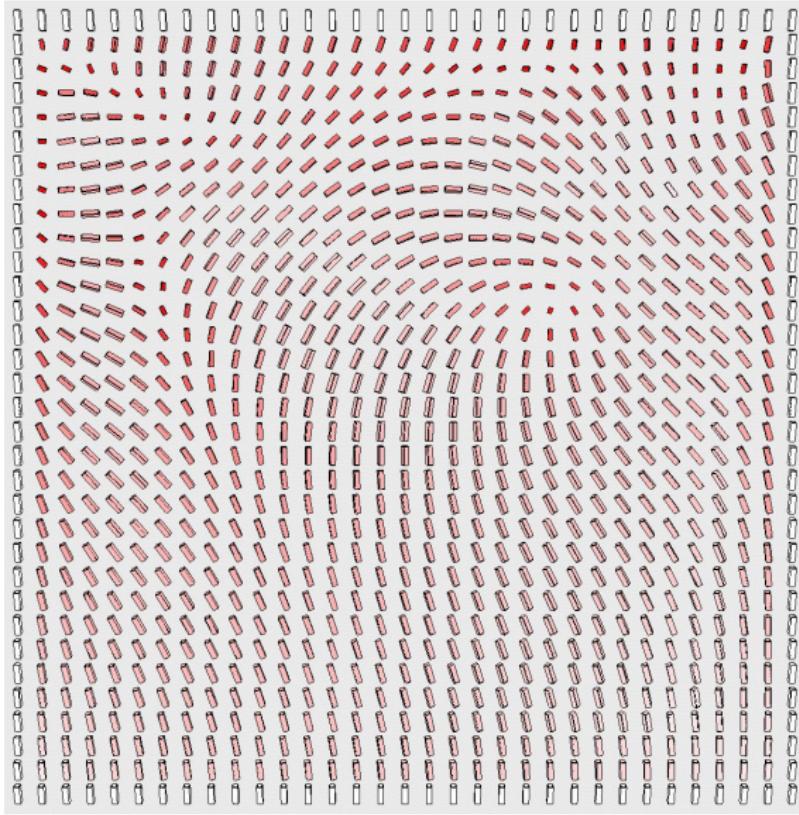
$$\mathrm{De} \;\approx\; \frac{V}{L} = 0.9$$

$$\mathrm{Er} \;\approx\; \frac{\zeta_1 VL}{L_1} = 240$$
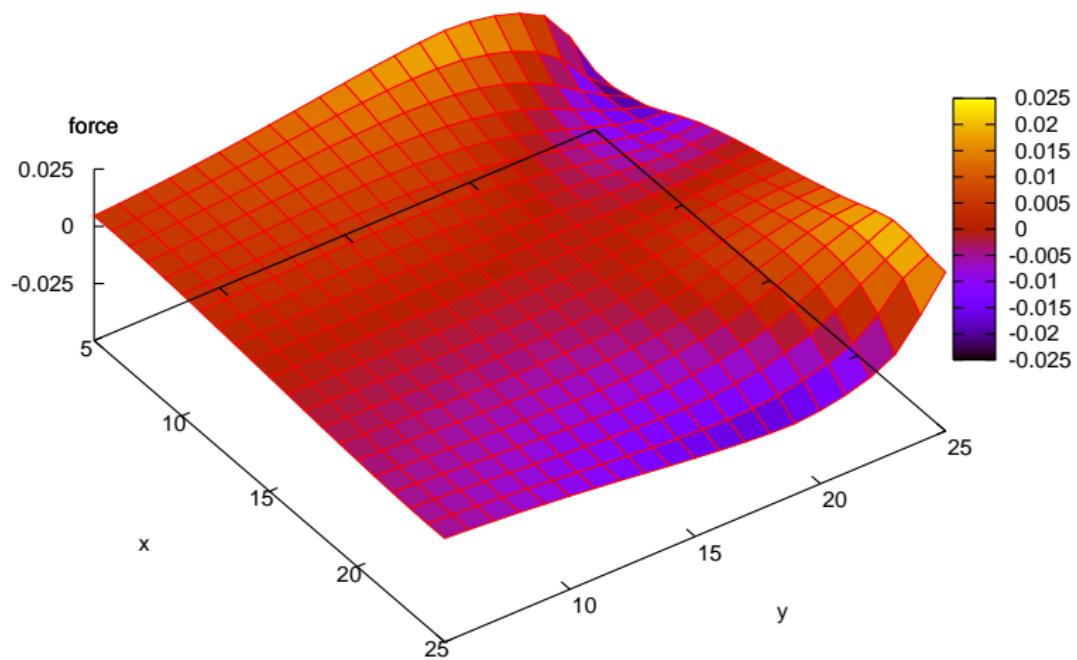
Later Orientation

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 $\mathbf{Q}$-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!

References

- A. RAMAGE AND E.C. GARTLAND, JNR
  A preconditioned nullspace method for liquid crystal director modeling, SIAM Journal on Scientific Computing 35(1), 2013.

- E.C. GARTLAND, JNR AND A. RAMAGE
  A renormalized Newton Method for liquid crystal director modeling, SIAM Journal on Numerical Analysis 53(1), 2015.

- A. RAMAGE AND A.M. SONNET
  Computational Fluid Dynamics for Nematic Liquid Crystals, BIT Numerical Mathematics 56(2), 573-586, 2016.

- A. RAMAGE AND A.M. SONNET
  Iterative solvers for Q-tensor models of nematic liquid crystals, in preparation.