Iterative Solution of Linear Systems in Liquid Crystal Modelling

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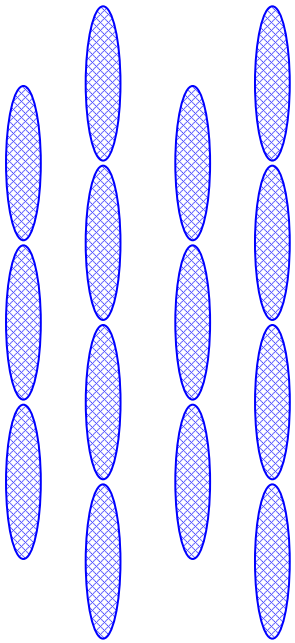
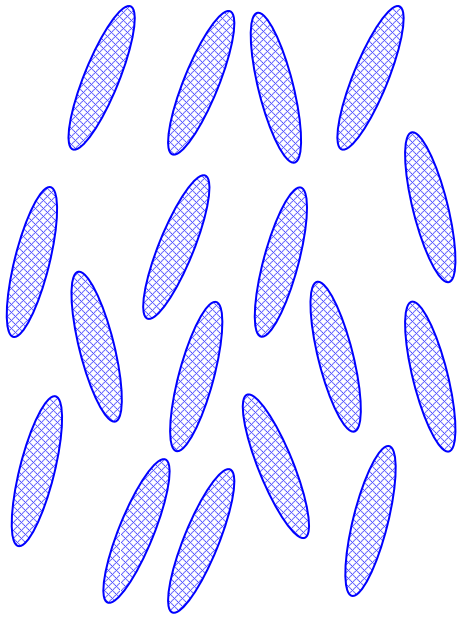
Liquid Crystals

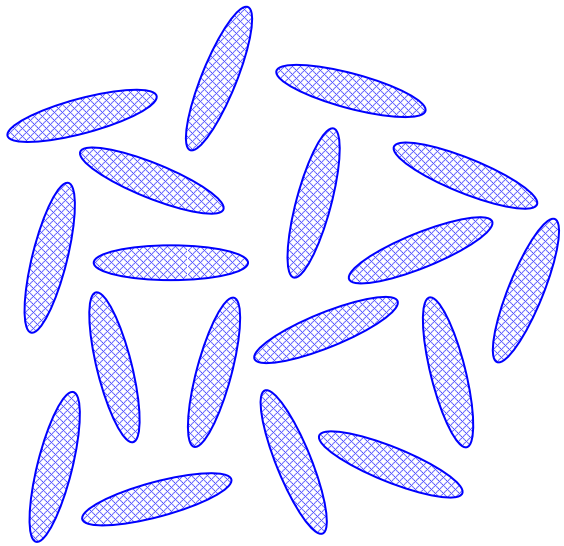
- occur between solid crystal and isotropic liquid states



solid



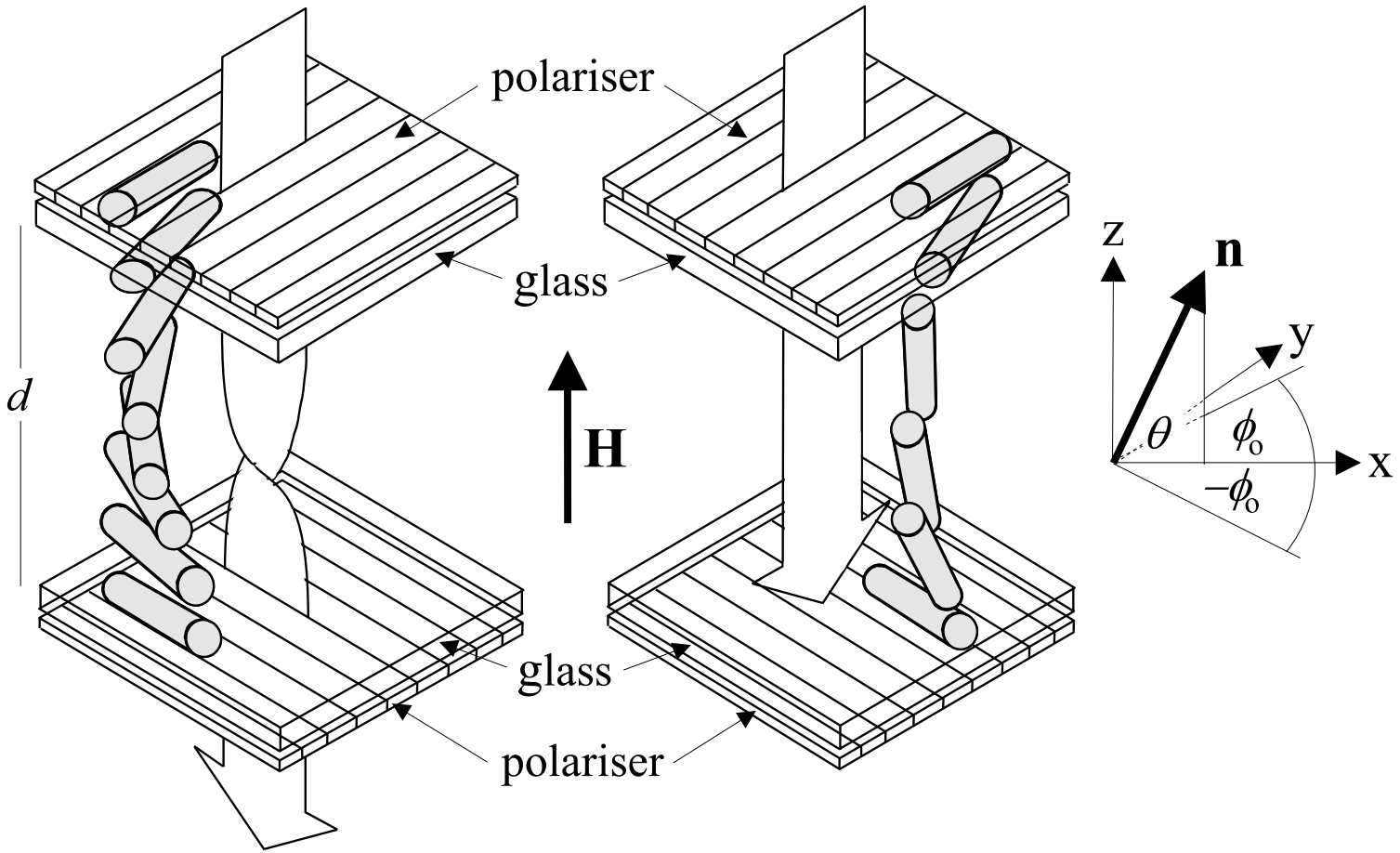
liquid crystal



liquid

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

Liquid Crystal Displays

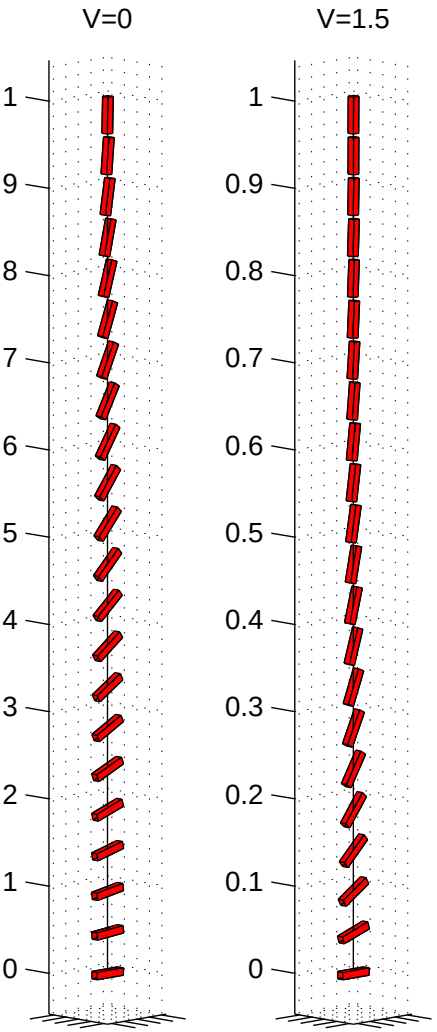


(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$

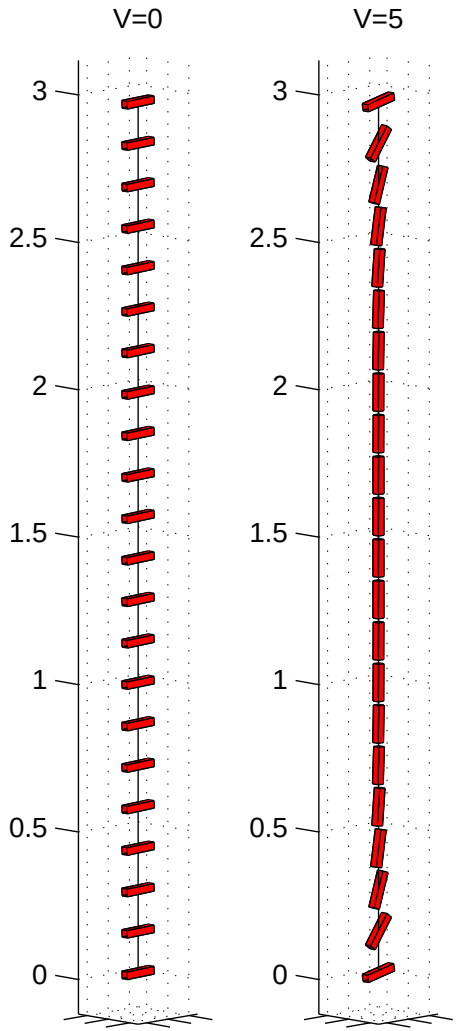
Twisted Nematic Device

(diagram taken from Stewart (2004))

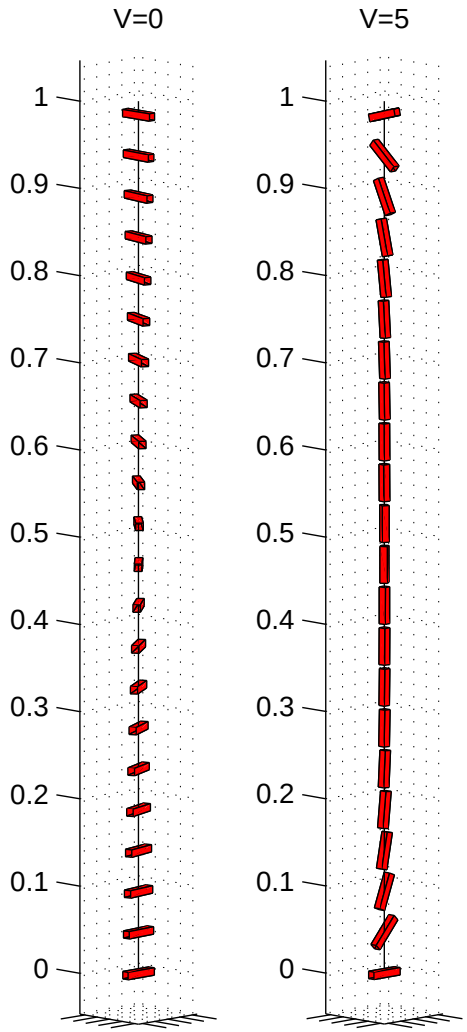
Sample configurations



HAN cell

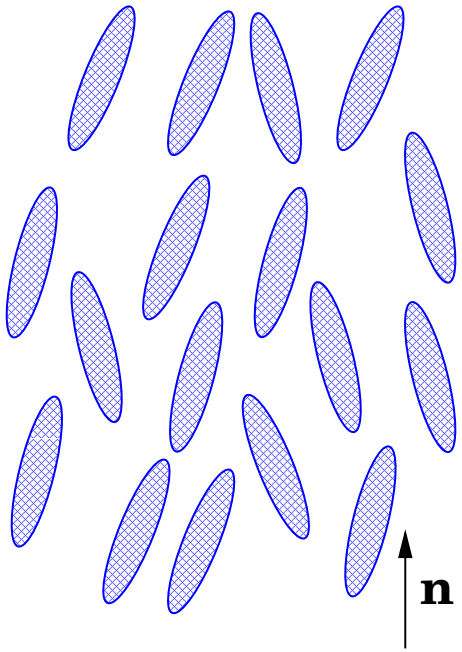


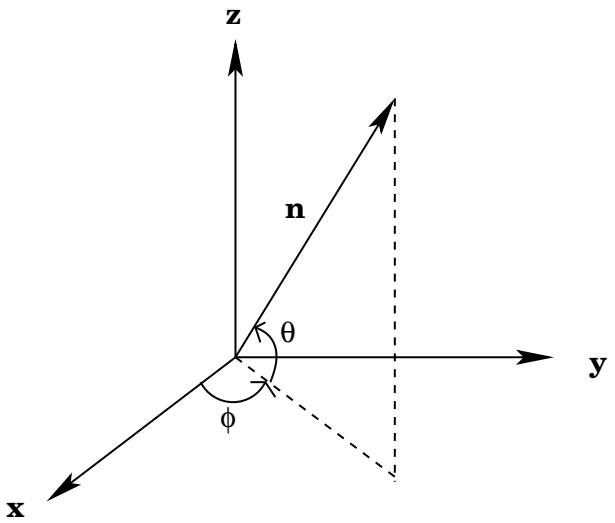
Pi cell



TND cell

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

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 (joint work with Chuck Gartland, Kent State University)

Alternative Model: $\mathbf{Q}$-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 $\mathbf{u}$ along molecular axes
- five degrees of freedom: two specifying the degree of order, three specifying the angles of the principal directions
- basis representation

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

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

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

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

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

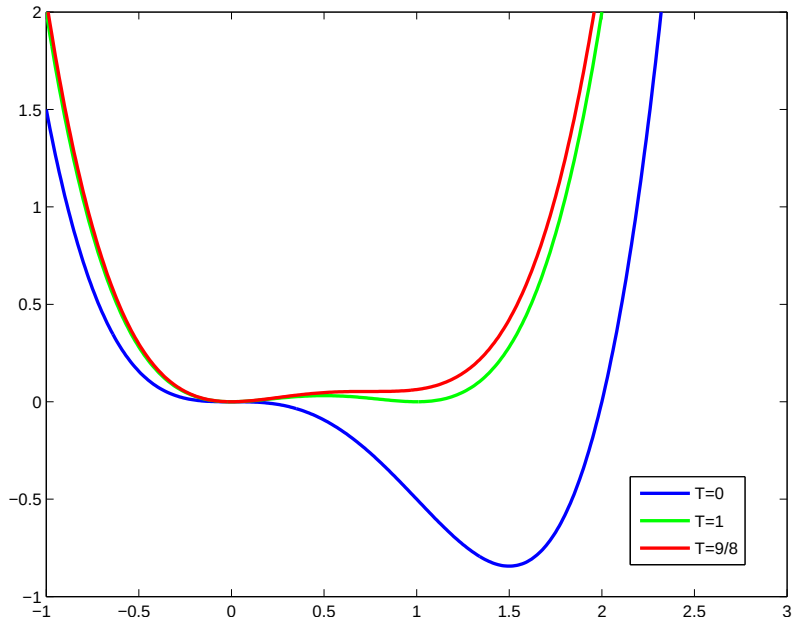
- electrostatic energy: due to an applied electric field $\mathbf{E}$ (electric potential U with $\mathbf{E} = -\nabla U$)

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

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



- see John Mackenzie's talk, Thursday 16:45, K3.25

Coupled Equations

- solve Euler-Lagrange equations to minimise free energy

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

$$\Gamma^i_j = \frac{\partial F_b}{\partial q_{i,j}}, \quad f^i = \frac{\partial F_b}{\partial q_i}, \quad q_{i,j} = \frac{\partial q_i}{\partial z_j}$$

- 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 nodal elements
- linearise about $\mathbf{u}_0$ and iterate

Linear System At Each Step

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

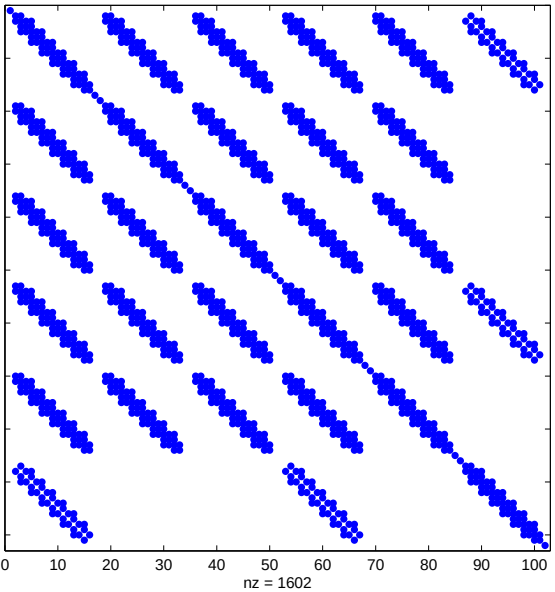
$$\mathcal{K} = \begin{bmatrix} K & & & & & \\ & K & & & & \\ & & K & & & \\ & & & K & & \\ & & & & K & \\ & & & & & \epsilon_0\bar{\epsilon}K \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M & & & & & \\ & M & & & & \\ & & M & & & \\ & & & M & & \\ & & & & M & \\ & & & & & 0 \end{bmatrix}$$

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

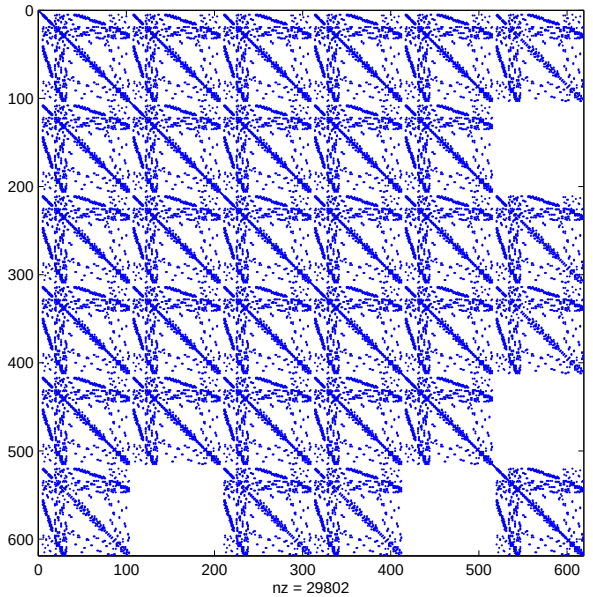
Saddle-point problem

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

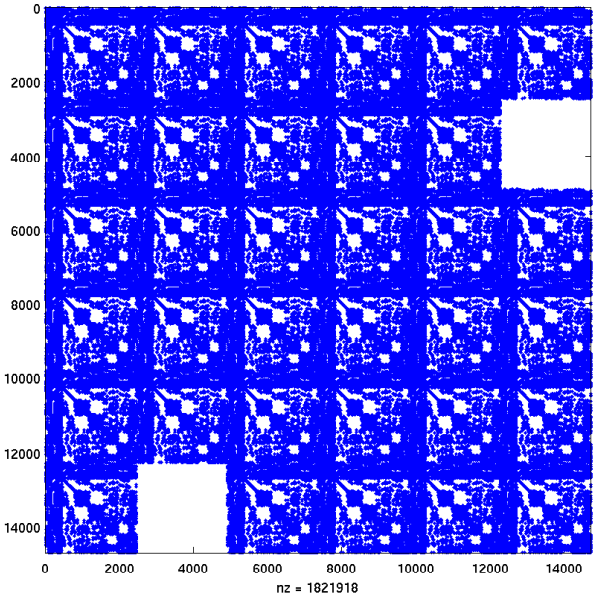
- A is $5n \times 5n$, B_1 is $5n \times n$, B_2 is $n \times 5n$
- A can be indefinite, C is positive definite



1D



2D



3D

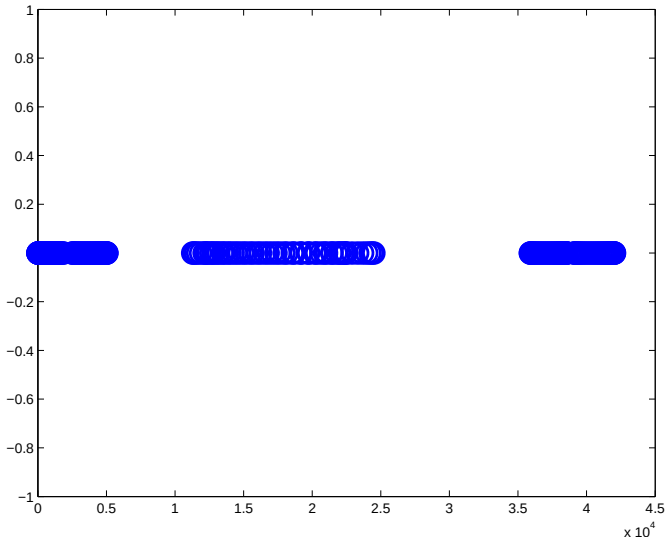
GMRES Iterations

- right preconditioning
- convergence tolerance 1e-8

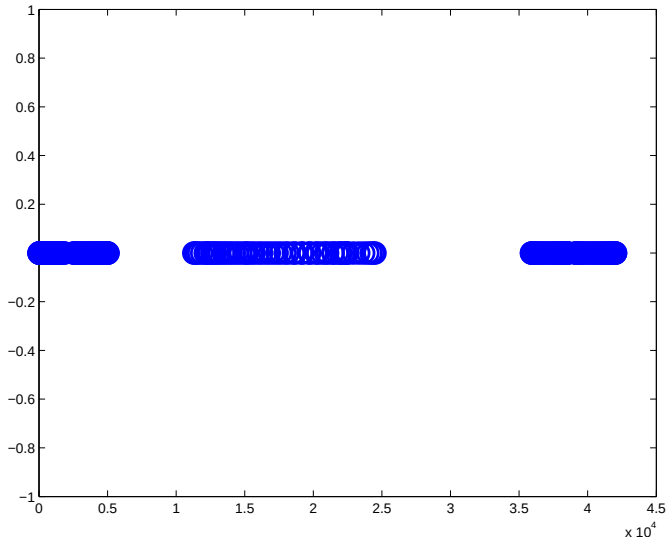
N_{el}	N_{dof}	$V = 0$	$V = 0.5$	$V = 1.5$	$V = 5$
16	198	129	151	141	141
32	390	245	298	270	228
64	774	327	430	349	274
128	1542	372	546	441	395
256	3078	594	985	800	720
512	6150	1108	1821	1557	1408

- many (almost) multiple eigenvalues

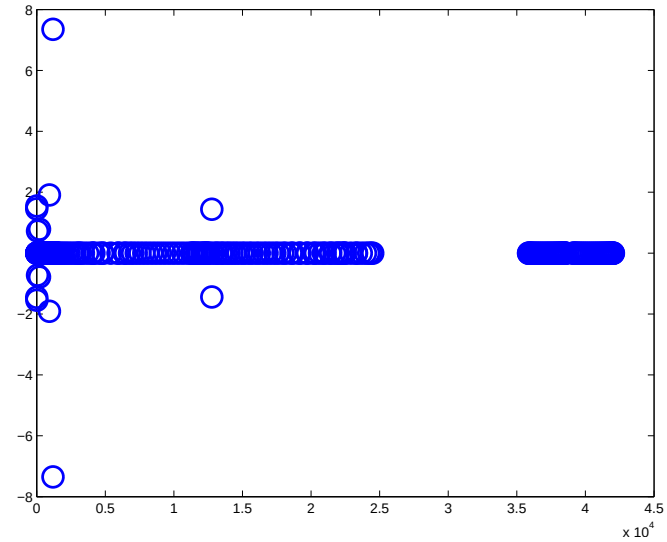
Eigenvalues



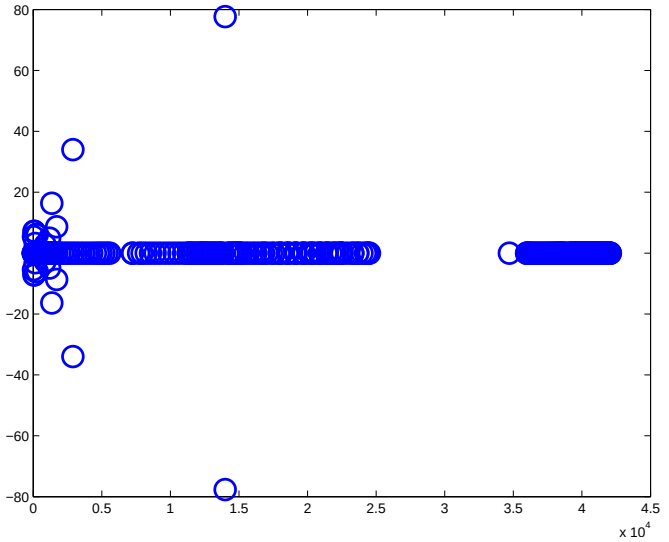
$V = 0$



$V = 0.5$



$V = 1.5$



$V = 5$

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

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

Approximation for A

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

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

- unstructured grids of triangles
- hierarchic finite elements of degree two

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

N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
618	1	9	12	19
1782	1	9	12	21
7746	1	8	12	15

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

N_{dof}	$0V$	$0.5V$	$1.5V$	$5V$
618	166	177	205	218
1782	167	190	235	266
7746	177	196	237	274

Observations

- $\mathbf{Q}$-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 shows promise:
  - Possibility of convergence independent of the mesh parameter.
  - Cheap to implement using direct solve/factorisation.
- Further analysis and experiments needed.

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THANKS FOR YOUR ATTENTION!