Efficient preconditioned iterative solvers for director-based models of nematic liquid crystals

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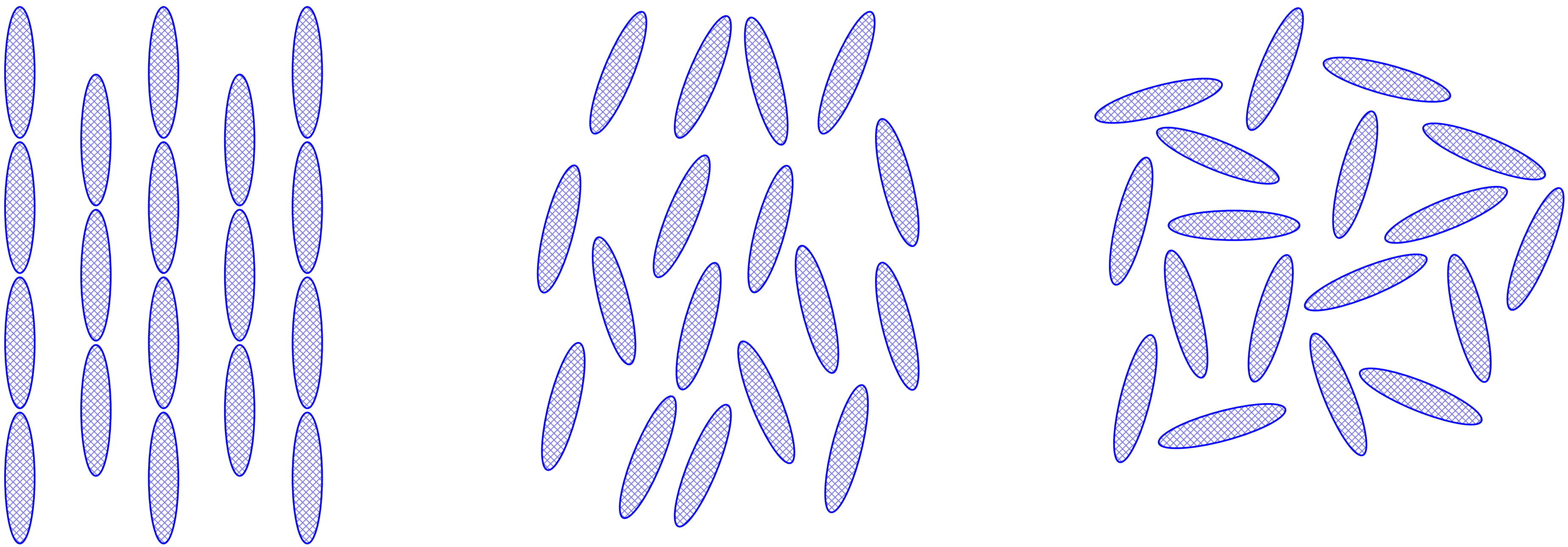
Liquid Crystals

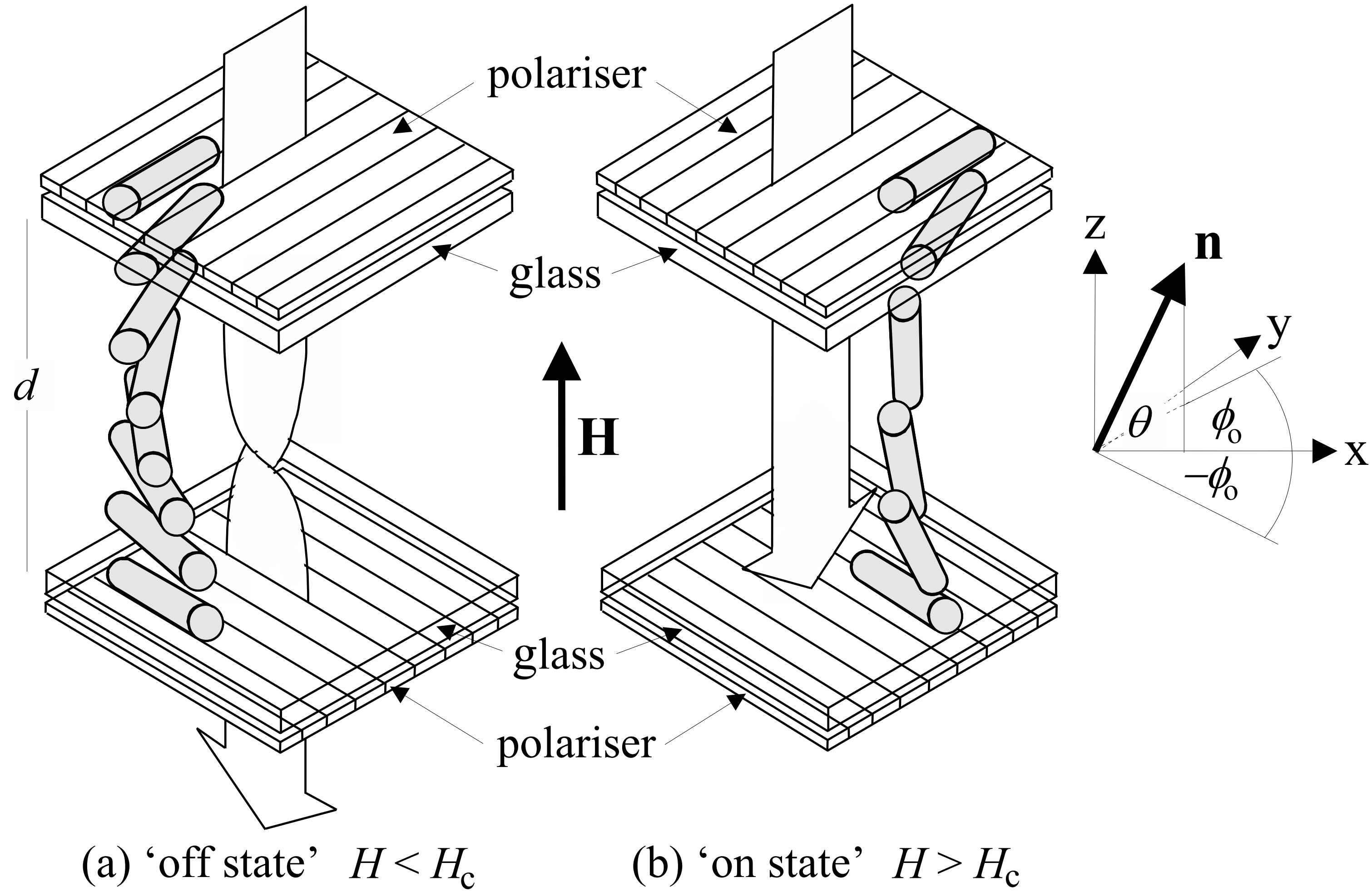
- occur between solid crystal and isotropic liquid states



solid | liquid crystal | liquid

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

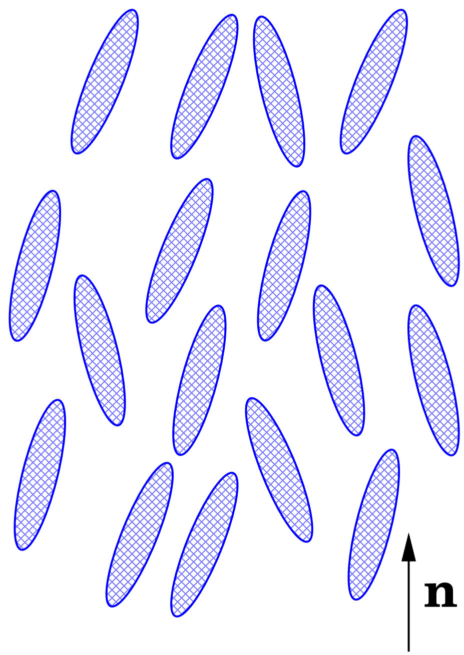
Liquid Crystal Displays

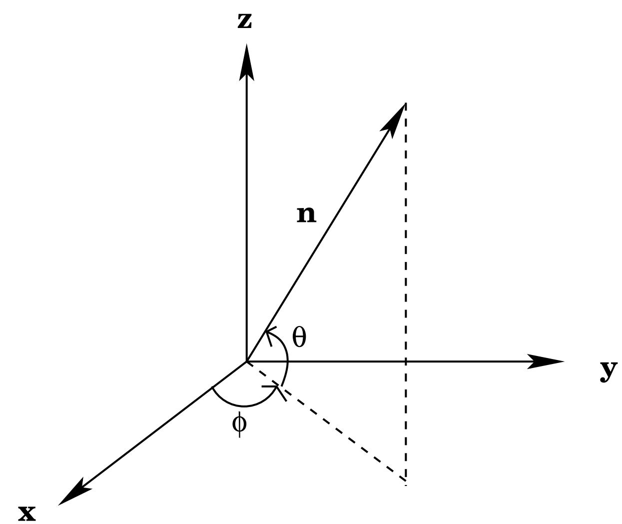


twisted nematic device

Static and Dynamic Continuum Theory of Liquid Crystals,
Iain W. Stewart (2004)

Modelling: Director-based Models





- director: average direction of molecular alignment

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

- $\mathbf{n}$ varies with space and time

$$\theta \equiv \theta(x, y, z, t), \quad \phi \equiv \phi(x, y, z, t)$$

Finding Equilibrium Configurations

- minimise the free energy

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

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

- elastic energy

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

- electrostatic energy

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

Equilibrium Equations

- nondimensionalised equilibrium equations on $z \in [0, 1]$

$$F = \frac{1}{2} \int_0^1 \left[(u_z^2 + v_z^2 + w_z^2) - \alpha^2 \pi^2 (\beta + w^2) U_z^2 \right] \, dz$$

- dimensionless parameters:

$$\alpha^2 = \frac{\epsilon_0 \epsilon_a V^2}{K \pi^2}, \qquad \beta = \frac{\epsilon_\perp}{\epsilon_a}$$

- director $\mathbf{n} = (u, v, w)$, electric potential U: $E = -\frac{dU}{dz}$

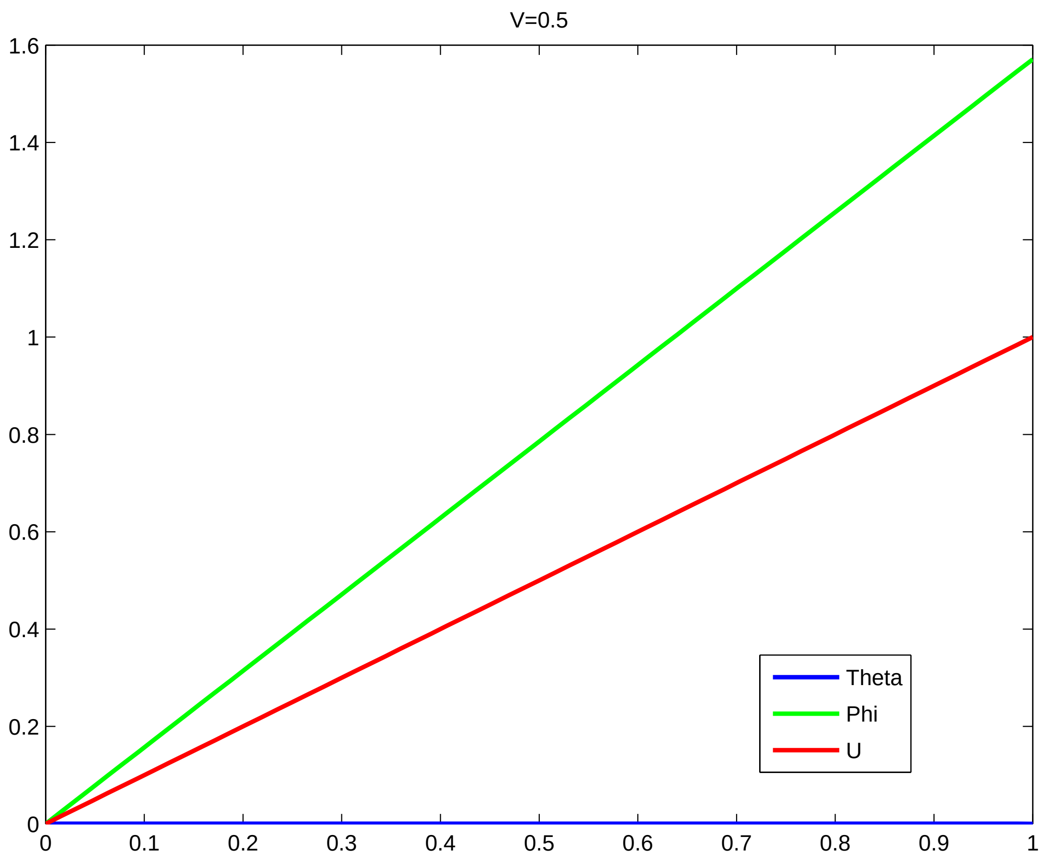
- boundary conditions:

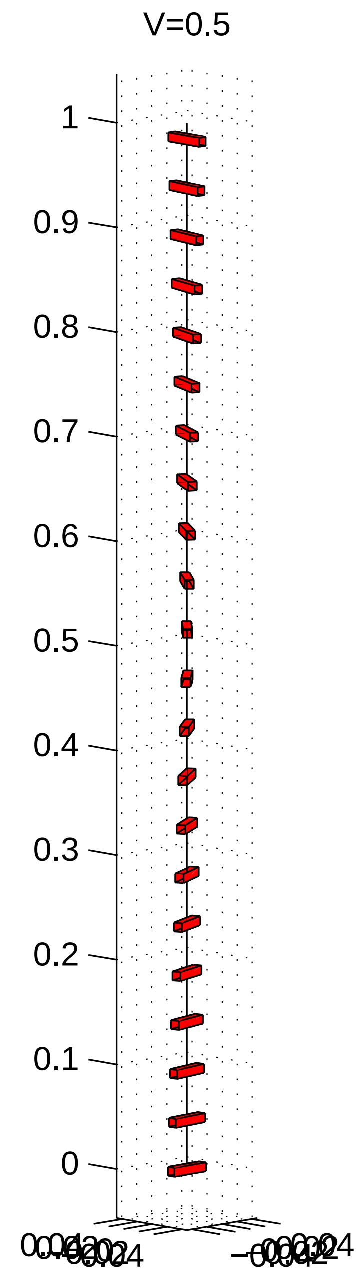
at $z = 0$: $\mathbf{n} = (1, 0, 0)$, at $z = 1$: $\mathbf{n} = (0, 1, 0)$

- unknowns u, v, w, U

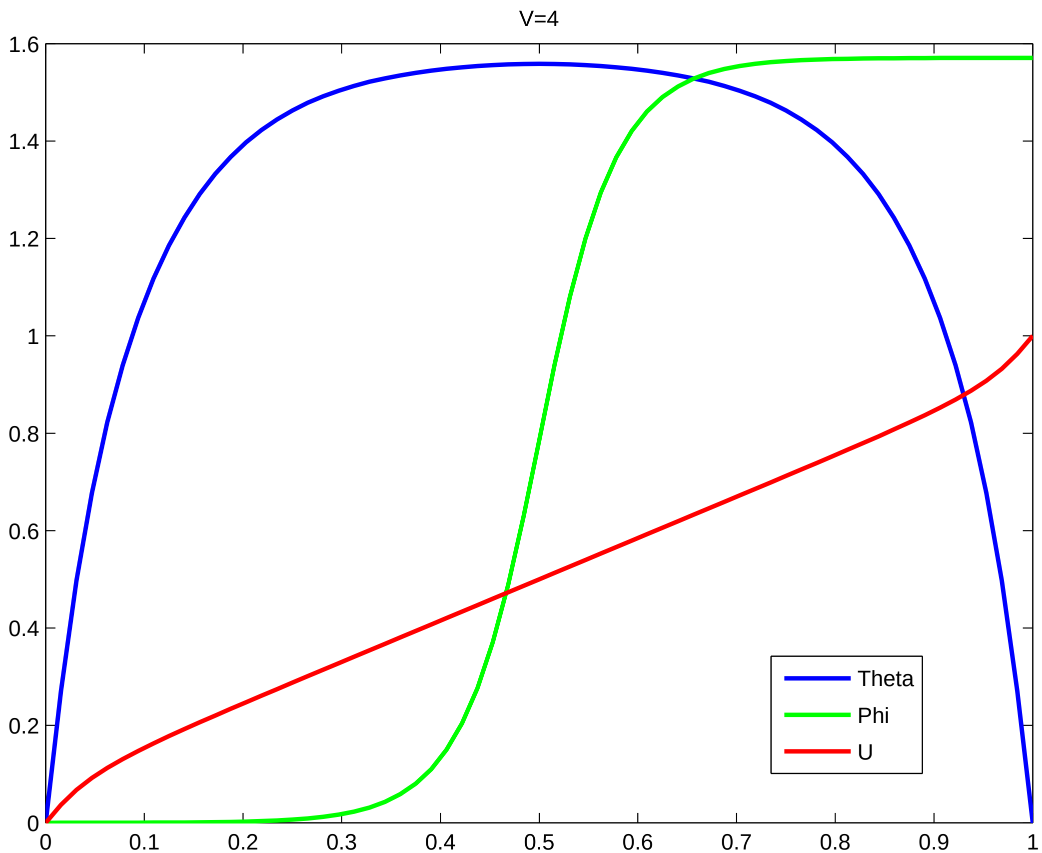
Off State

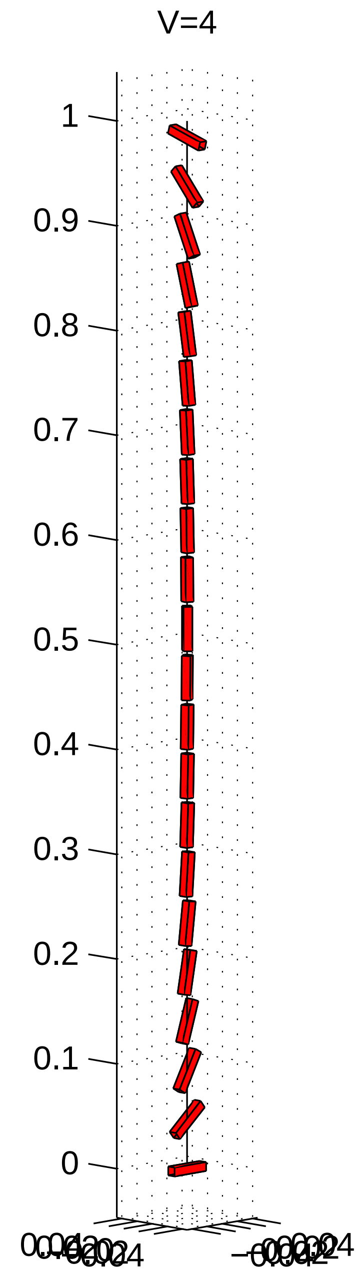
$$\theta(z) \equiv 0, \qquad \phi(z) = \frac{\pi}{2} z, \qquad U(z) = z$$





On State

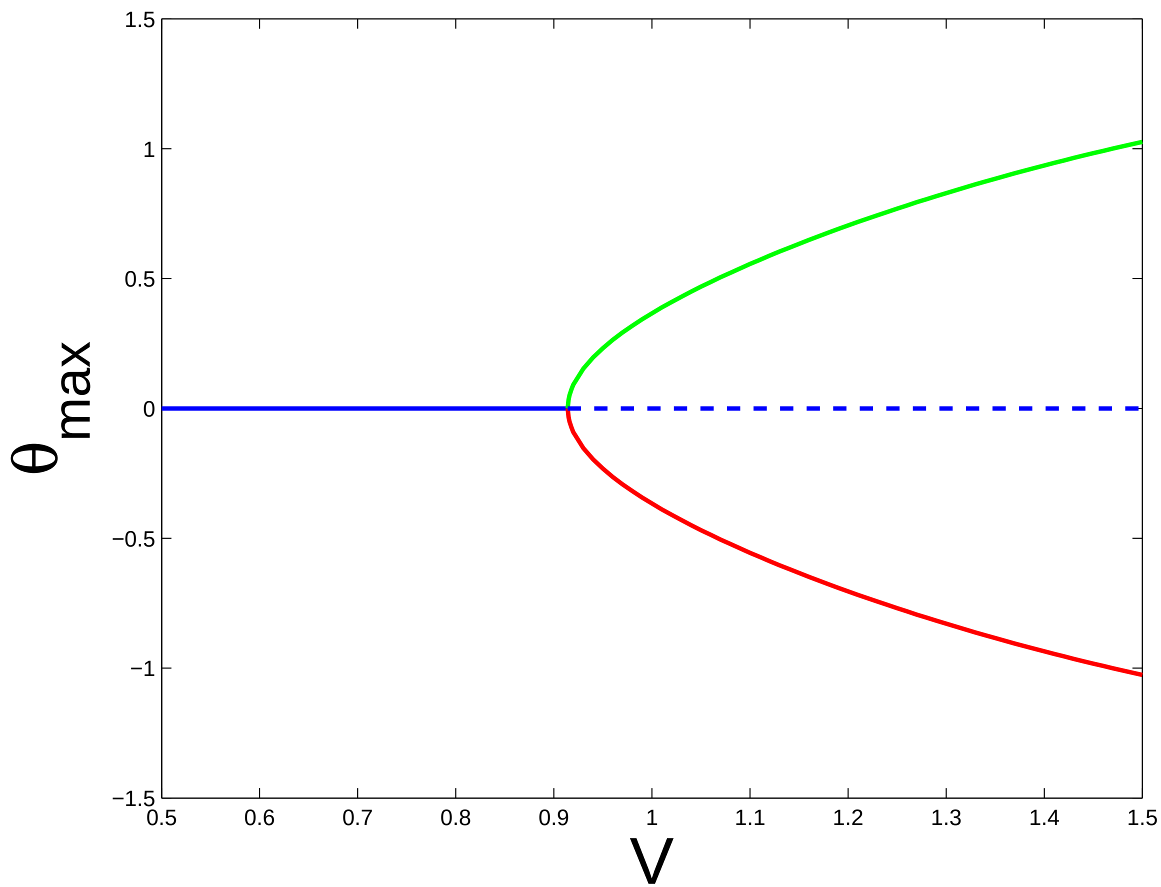

V=4
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Theta
Phi
U


V=4
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

Critical Voltage

- switching occurs at

$$V_c = \frac{\pi}{2}\sqrt{\frac{3K}{\epsilon_0\epsilon_a}}$$



Discrete Free Energy

- grid of $N+1$ points z_k a distance Δz apart, $n = N-1$ unknowns for each variable

- piecewise linear approximation, weighted average

$$
\begin{aligned}
F \;\; &\simeq \;\; \frac{\Delta z}{2} \sum_{k=0}^{N-1} \left\{ \left[\frac{u_{k+1} - u_k}{\Delta z} \right]^2 + \left[\frac{v_{k+1} - v_k}{\Delta z} \right]^2 + \left[\frac{w_{k+1} - w_k}{\Delta z} \right]^2 \right. \\
&- \;\; \left. \alpha^2 \pi^2 \left(\beta + \left[\frac{w_k^2 + w_{k+1}^2}{2} \right] \right) \left[\frac{U_{k+1} - U_k}{\Delta z} \right]^2 \right\}
\end{aligned}
$$

- equivalent to mid-point finite differences, linear finite elements

Constrained Minimisation

- minimise F subject to pointwise constraint

$$u_j^2 + v_j^2 + w_j^2 = 1, \qquad j = 1, \ldots, n$$

- constraints applied via Lagrange multipliers: minimise

$$G = \frac{\Delta z}{2} \left[f - \ldots - \lambda_j (u_j^2 + v_j^2 + w_j^2 - 1) - \ldots \right]$$

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

  $N + 1$ gridpoints $\Rightarrow n = N - 1$ unknowns

- use Newton's method: $5n \times 5n$ Hessian $\nabla^2 \mathbf{G}(\mathbf{x})$

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

Hessian Components

- matrix notation: $\nabla^2_{\mathbf{nn}}\mathbf{G} = A \qquad A \in \mathbb{R}^{3n\times 3n}$
- A is block diagonal with symmetric tridiagonal blocks
- A can be indefinite

- matrix notation: $\nabla^2_{\mathbf{n}\lambda}\mathbf{G} = B \qquad B \in \mathbb{R}^{3n\times n}$
- $B = -\Delta z[B_u, B_v, B_w]^T$, B_u,B_v,B_w are diagonal
- $B^T B = \Delta z^2 I_n$ when constraints are satisfied

- matrix notation: $\nabla^2_{\mathbf{UU}}\mathbf{G} = -C \qquad C \in \mathbb{R}^{n\times n}$
- C is symmetric positive definite and tridiagonal

- matrix notation: $\nabla^2_{\mathbf{nU}}\mathbf{G} = D \qquad D \in \mathbb{R}^{3n\times n}$
- $D = k[0, 0, D_w]^T$, D_w is tridiagonal, $\mathrm{rank}(D) = n - 1$

Iterative solution

- full Hessian matrix:

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

saddle-point problem

- outer iteration: Newton's method tol=$1e-4$
- inner iteration: MINRES tol=$1e-4$

- Hessian is poorly conditioned:

$$\kappa(H) = O(N^4)$$

Nullspace Method

- Idea: use information about nullspace of B to eliminate constraint blocks

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

- write solution of (2) as $\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{z}$ where columns of $Z \in \mathbb{R}^{3n\times 2n}$ form a basis for $\mathcal{N}(B^T)$
- reduced $3n \times 3n$ system:

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

- $B^T B$ is diagonal so solves with $(B^T B)^{-1}$ are cheap

Nullspace of B^T

- permute entries of B:

$$B = -\Delta z\, \mathtt{diag}(\mathbf{n}_1, \mathbf{n}_2, \ldots, \mathbf{n}_n), \quad \mathbf{n}_j = [u_j, v_j, w_j]^T$$

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

$$\mathbf{l}_j = \frac{1}{\sqrt{u_j^2 + v_j^2}} \begin{bmatrix} -v_j \\ u_j \\ 0 \end{bmatrix}, \qquad \mathbf{m}_j = \frac{1}{\sqrt{u_j^2 + v_j^2}} \begin{bmatrix} -u_j w_j \\ -v_j w_j \\ u_j^2 + v_j^2 \end{bmatrix}$$

- at least one of u_j, v_j, w_j nonzero as $|\mathbf{n}_j| = 1$
- $3n \times 2n$ nullspace matrix

$$Z = \mathtt{diag}([\mathbf{l}_1, \mathbf{m}_1], [\mathbf{l}_2, \mathbf{m}_2], \ldots, [\mathbf{l}_n, \mathbf{m}_n])$$

Solving the Reduced System

- write $\bar{A} = Z^T A Z$ and $\bar{D} = Z^T D$:

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

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

- preconditioned matrix:

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

$$M = C^{-1/2} \bar{D} \bar{A}^{-1/2}$$

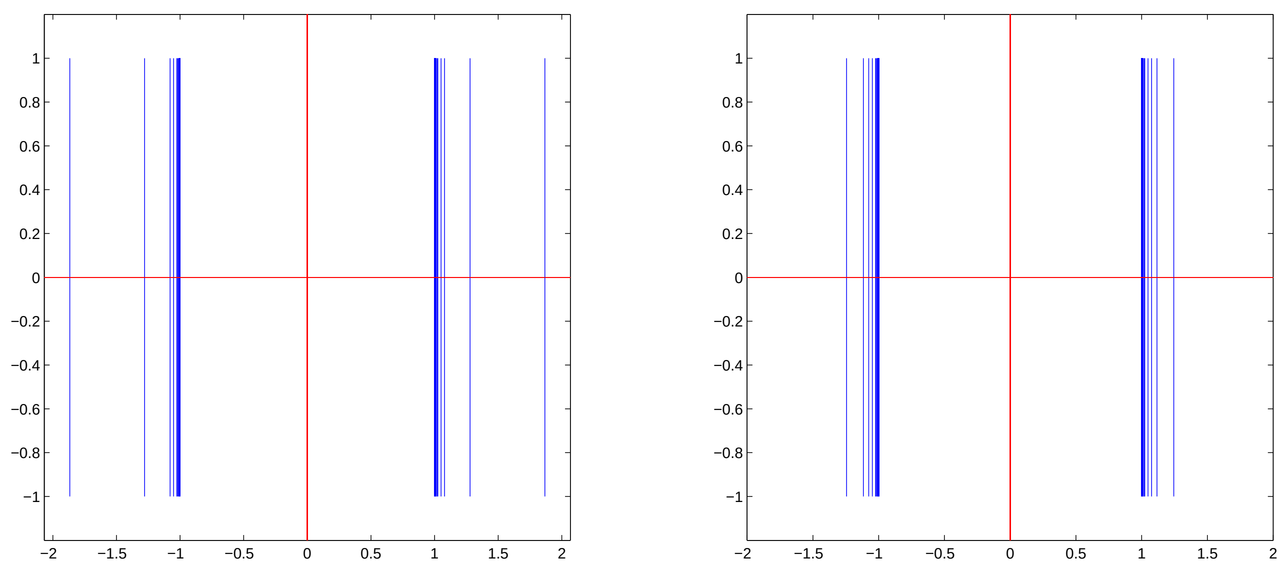
- off state: $M = 0$

Preconditioned Spectrum

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

- non-zero singular values σ_k, $k = 1, \ldots, n-1$
- 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	$k = 1, \ldots, n-1$



sample eigenvalue plots for $N = 64$

Estimate of MINRES convergence

- eigenvalues in two symmetric intervals

$$[-\beta, -1] \cup [1, \beta], \qquad \beta = \sqrt{1 + \sigma_{\max}^2}$$

N	first Newton step	last Newton step
32	1.3563e+00	1.5472e+00
64	1.3579e+00	1.5479e+00
128	1.3583e+00	1.5481e+00
256	1.3584e+00	1.5482e+00

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

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

- for $\epsilon = 1e - 4$, $k \simeq 6$

Iteration Counts

- diagonal scaling

N	8	16	32	64	128	256
first Newton step	15	40	117	382	1293	5126
last Newton step	37	134	414	1617	7466	34755

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- reduced block preconditioning

N	8	16	32	64	128	256
first Newton step	5	5	5	5	5	5
last Newton step	5	5	5	5	5	5

- independent of problem size and Newton iteration

Computing Time

- elapsed time (tic/toc)
- A: full direct, B: reduced direct, C: reduced block

N	A	B	C
8	7.54e-02	7.17e-02	2.85e-03
16	7.67e-03	7.37e-03	2.60e-03
32	1.11e-02	1.06e-02	3.51e-03
64	1.67e-02	1.56e-02	4.95e-03
128	3.55e-02	3.30e-02	8.62e-03
256	1.18e-01	1.26e-01	1.26e-02
512	4.89e-01	4.40e-01	2.26e-02
1024	1.40e+00	1.37e+00	4.64e-02
2048	5.25e+00	5.15e+00	1.12e-01
4096	2.11e+01	2.12e+01	1.78e-01

Summary and Conclusions

- The reduced block preconditioner is very efficient for this problem.
- The nullspace method seems to be ideal for dealing with the unit vector constraint.
- Although this example features a 1D cell, the same method should work well for more complicated liquid crystal cells as the orientation space and unit vector constraint is exactly the same.
- The reduced block preconditioner is cheap to invert here: hopefully approximate solves (e.g. multigrid) can be used for other problems with less structure.

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THANKS!

Diagonal Preconditioning

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

$$\mathcal{D} = \begin{bmatrix} D_A & 0 & 0 \\ 0 & \Delta z^3\, I & 0 \\ 0 & 0 & D_C \end{bmatrix} \qquad \begin{aligned} D_A &= \texttt{diag}(A) \\ D_C &= \texttt{diag}(C) \end{aligned}$$

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- estimated condition of $\mathcal{D}^{-1}H$ is $O(N^2)$

$$\lambda_{\min} = -2, \;\; \lambda_s = O(N^{-2}), \;\; \lambda_{s+1} = O(N^{-2}), \;\; \lambda_{\max} = 2$$