Efficient iterative solvers for director-based models of LCDs

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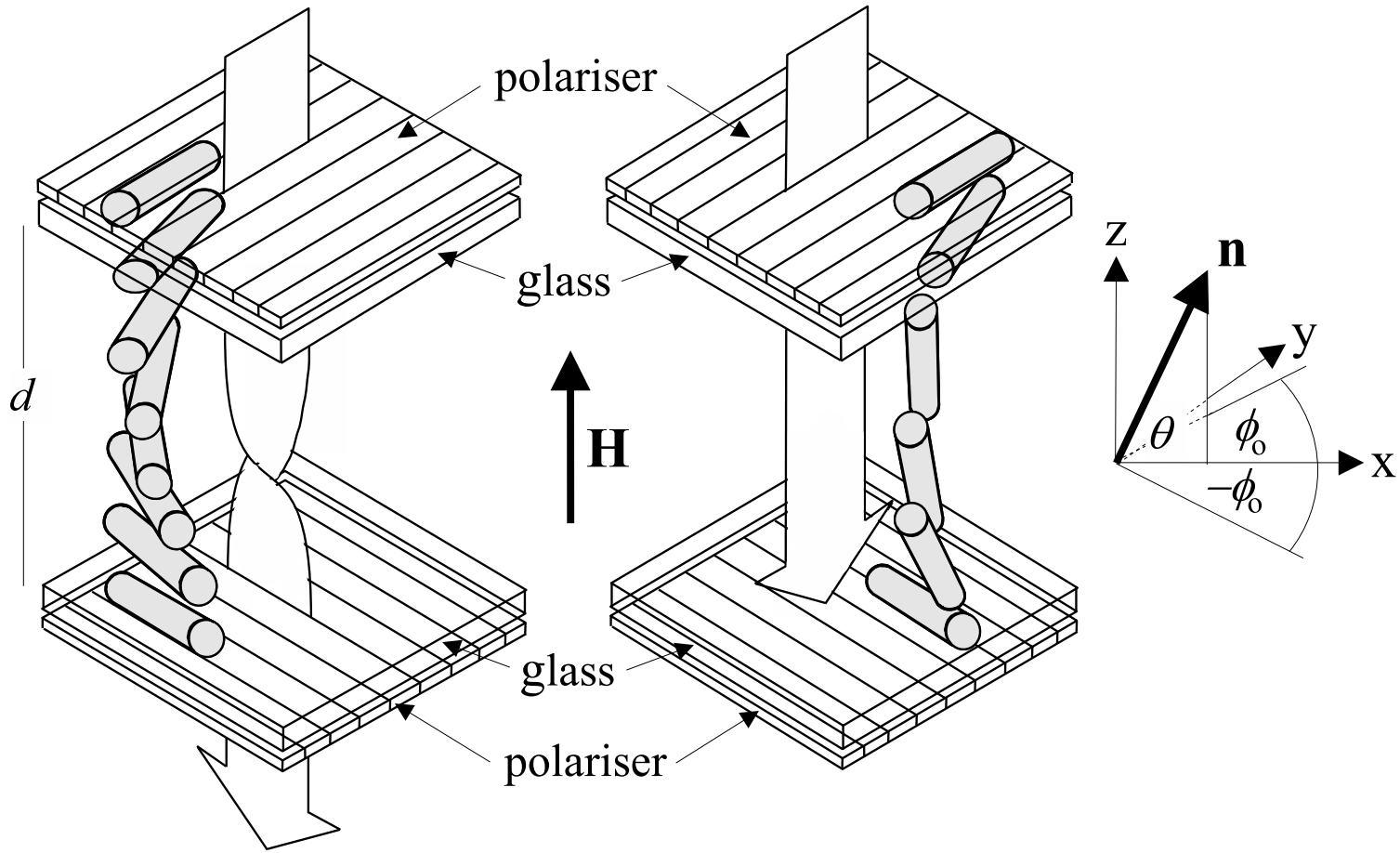
Liquid Crystal Displays

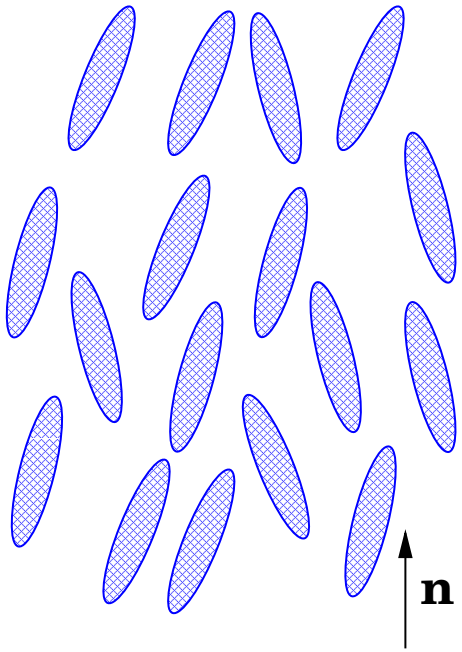


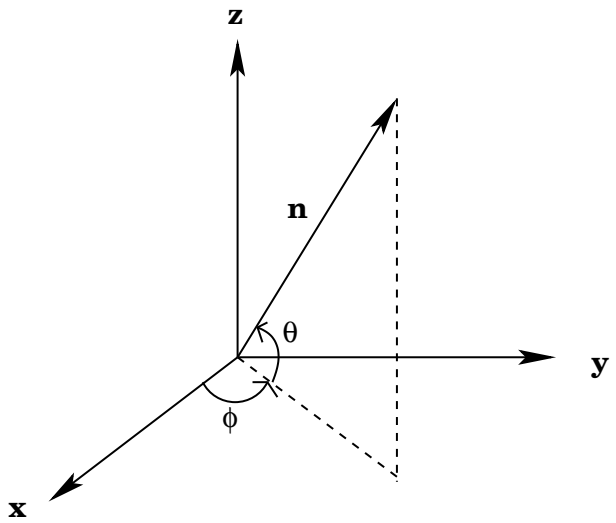
(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$

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

- order parameter: measure of orientational order

$$S = \frac{1}{2} < 3\cos^2\theta_m - 1 >$$

Finding Equilibrium Configurations

- minimise the free energy

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

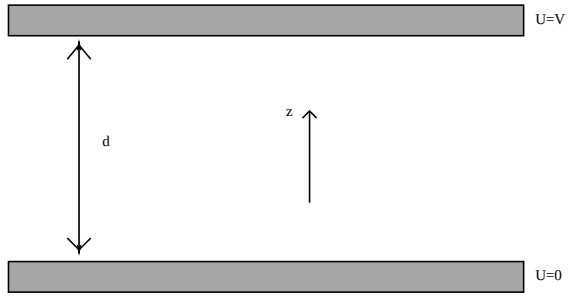
$$F_{bulk} = F_{elastic} + F_{electrostatic}$$

- solutions with least energy are physically relevant

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

Model Problem: Twisted Nematic Device

- two parallel plates distance d apart



- strong anchoring parallel to plate surfaces ($\mathbf{n}$ fixed)
- rotate one plate through $\pi/2$ radians
- electric field $\mathbf{E} = (0, 0, E(z))$, voltage V

Equilibrium Equations

- director $\mathbf{n} = (u, v, w)$, electric potential U: $E = \dfrac{dU}{dz}$
- unknowns u, v, w, U, constraint $|\mathbf{n}| = 1$
- 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

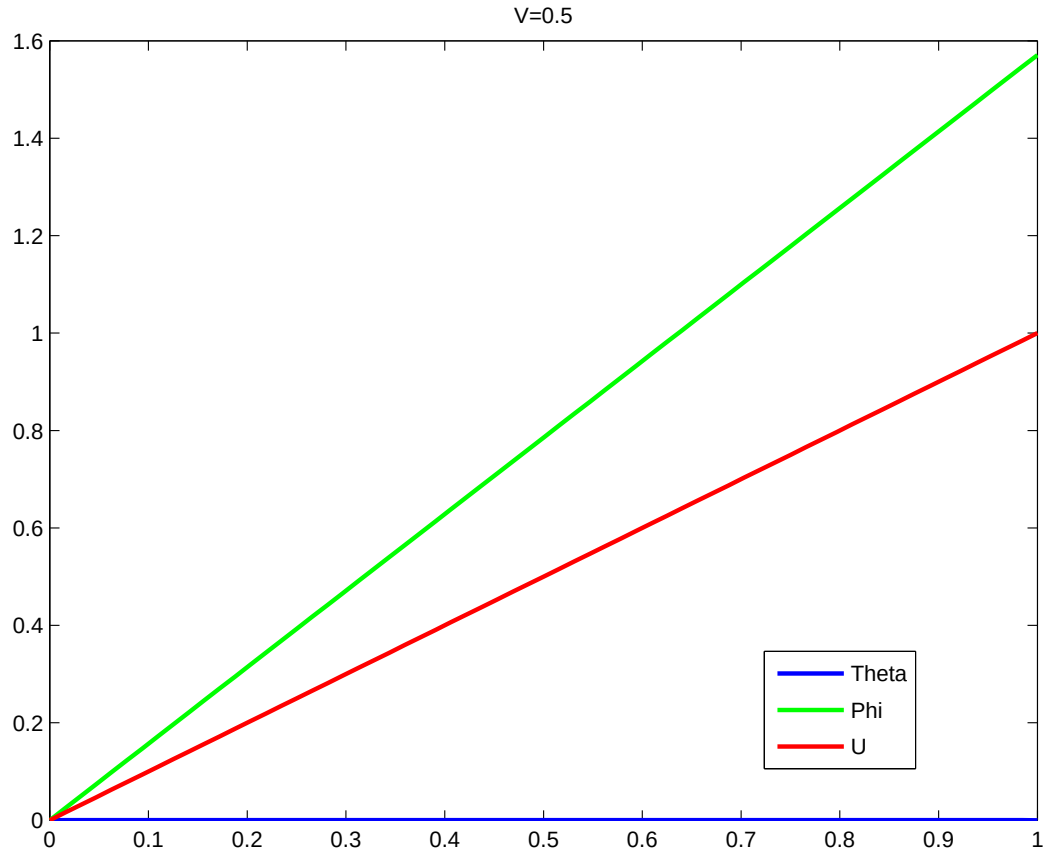
$$\alpha^2 = \frac{\epsilon_0 \epsilon_a V^2}{K \pi^2}, \qquad \beta = \frac{\epsilon_\perp}{\epsilon_a}$$

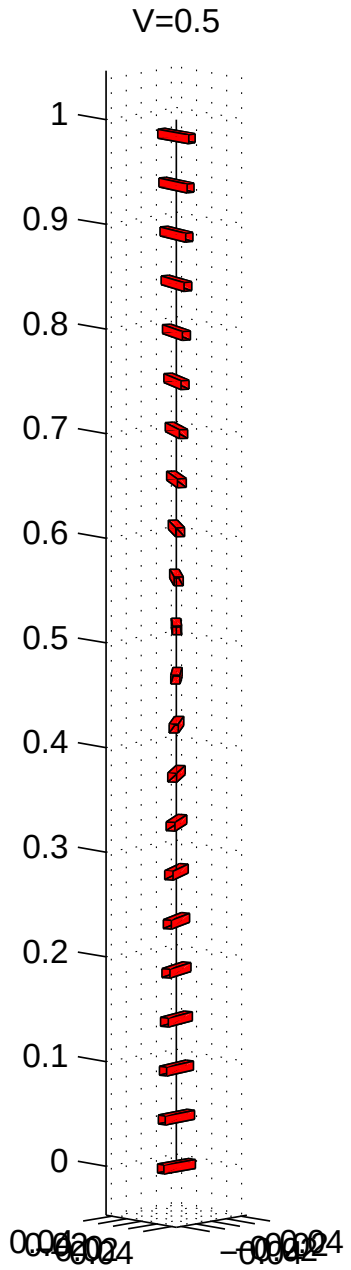
- boundary conditions:

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

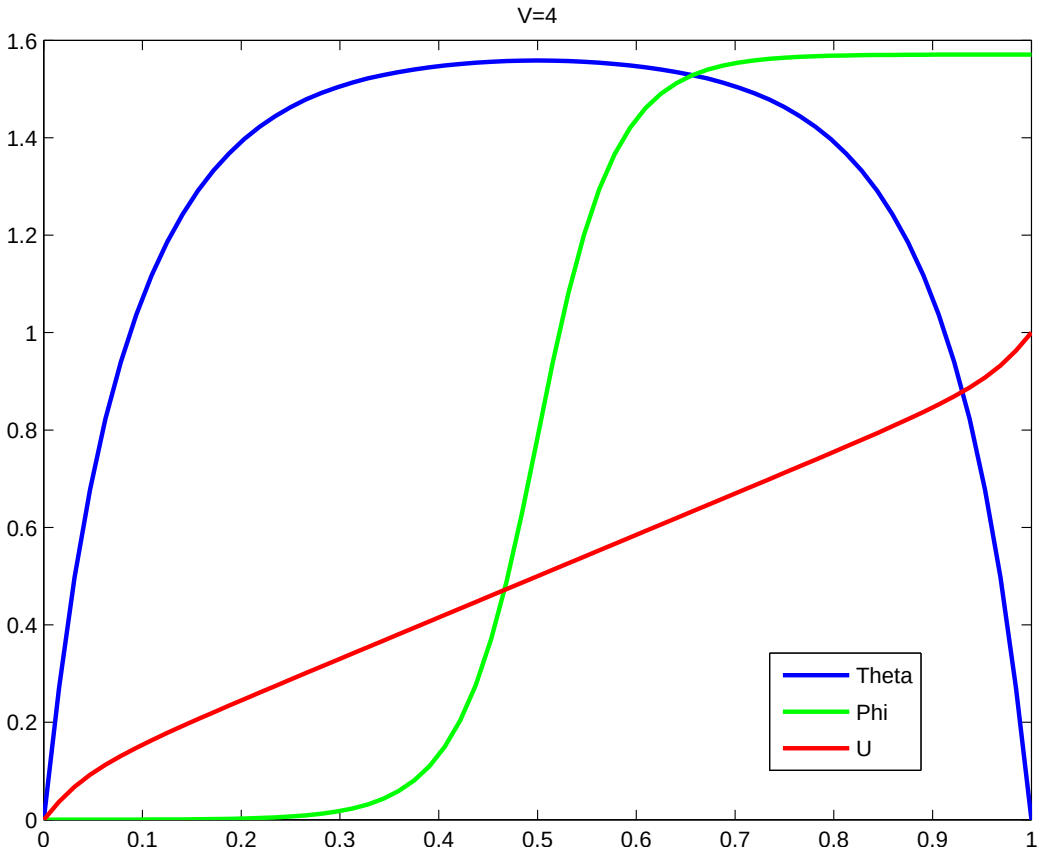
Off State

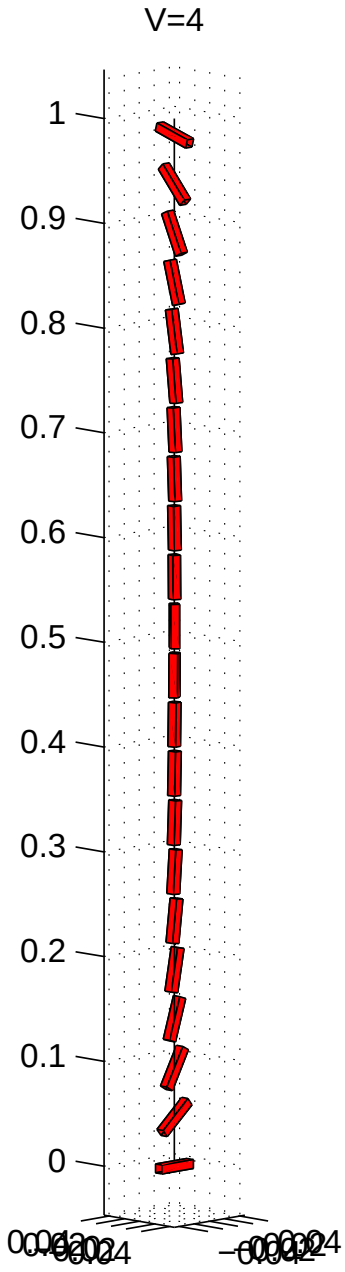
$$\theta(z) \equiv 0, \qquad \phi(z) = \frac{\pi}{2} z, \qquad U(z) = z$$





On State

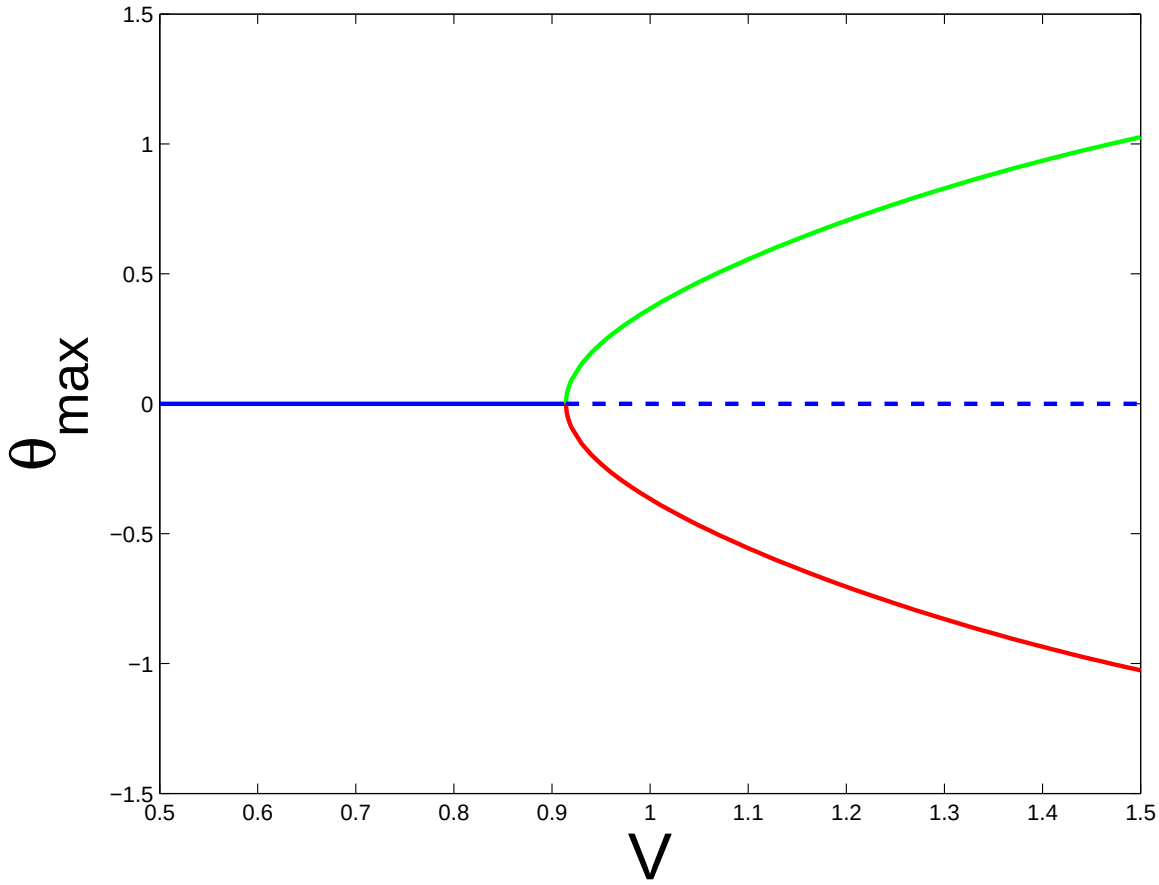

V=4
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Theta
Phi
U


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

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



Constrained Minimisation I

- grid of $N+1$ points z_k a distance Δz apart, $n = N-1$ unknowns for each variable
- discrete free energy (linear finite elements)

$$F \simeq \frac{\Delta z}{2} f(u_1, \ldots, u_n, v_1, \ldots, v_n, w_1, \ldots, w_n, U_1, \ldots, U_n)$$

- minimise F subject to pointwise constraint

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

- constraints are applied via Lagrange multipliers: minimise

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

Constrained Minimisation II

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

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

- use Newton's method: solve

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

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

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

Hessian Components 1

- $\nabla^2_{\mathbf{nn}}\mathbf{G} = A$

$$A = \begin{bmatrix} \nabla^2_{\mathbf{uu}}\mathbf{G} & 0 & 0 \\ 0 & \nabla^2_{\mathbf{vv}}\mathbf{G} & 0 \\ 0 & 0 & \nabla^2_{\mathbf{ww}}\mathbf{G} \end{bmatrix}$$

A is positive definite iff $V < V_c$

- $\nabla^2_{\mathbf{UU}}\mathbf{G} = -C$

C is tridiagonal and positive definite

- $\nabla^2_{\mathbf{nU}}\mathbf{G} = D$

$$D = \frac{\alpha^2\pi^2}{\Delta z} \begin{bmatrix} 0 \\ 0 \\ D_w \end{bmatrix}$$

D has complex eigenvalues in conjugate pairs

Hessian Components 2

- $\nabla^2_{\mathbf{n}\lambda}\mathbf{G} = B$

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

- $B^T B = \Delta z^2 I_n$ when constraints are satisfied

- $\mathrm{rank}(B) = \mathrm{rank}(B^T) = \mathrm{rank}(BB^T) = \mathrm{rank}(B^T B) = n$

Full Newton System

$$\begin{bmatrix} A & B & D \\ B^T & 0 & 0 \\ D^T & 0 & -C \end{bmatrix} \begin{bmatrix} \delta\mathbf{n} \\ \delta\lambda \\ \delta\mathbf{U} \end{bmatrix} = \begin{bmatrix} -\nabla_{\mathbf{n}} G \\ -\nabla_{\lambda} G \\ -\nabla_{\mathbf{U}} G \end{bmatrix}$$

saddle-point problem

- iteration: Newton (outer), MINRES (inner)
- for symmetric eigenvalue intervals

$$[-\lambda_M, -\lambda_m] \cup [\lambda_m, \lambda_M]$$

no. of MINRES iterations required for convergence is

$$k \propto \frac{\lambda_M}{\lambda_m}$$

Minres iterations for full system

N	d	off state ($\alpha = 0.5\alpha_c$) first step	off state ($\alpha = 0.5\alpha_c$) last step	on state ($\alpha = 1.5\alpha_c$) first step	on state ($\alpha = 1.5\alpha_c$) last step
32	155	226	499	291	691
64	315	728	2,004	1,172	3,571
128	635	2,680	8,528	4,106	17,498
256	1,275	10,253	41,666	15,727	85,784
512	2,555	38,809	194,753	57,499	$>$200,000
1,024	5,115	150,376	$>$200,000	$>$200,000	$>$200,000

- doubling N quadruples iteration count

Nullspace Method I

$$A\delta\mathbf{n} + B\delta\lambda + D\delta\mathbf{U} = -\nabla_{\mathbf{n}} G \quad (1)$$

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

$$D^T\delta\mathbf{n} - C\delta\mathbf{U} = -\nabla_{\mathbf{U}} G \quad (3)$$

- write solution of (2) as $\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{z}$
  - nullspace matrix $Z \in \mathbb{R}^{3n\times 2n}$ with $B^T Z = Z^T B = 0$
  - $Z\mathbf{z} \in \mathbb{R}^{2n}$ lies in nullspace of B^T
  - particular solution satisfies $B^T\widehat{\delta\mathbf{n}} = -\nabla_{\lambda} G$

- find $\widehat{\delta\mathbf{n}}$ via $\widehat{\delta\mathbf{n}} = -B(B^T B)^{-1}\nabla_{\lambda} G$

Nullspace Method II

- reduced system:

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

- recover full solution from

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

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

Nullspace of B^T

- use eigenvectors of orthogonal projection $I - \mathbf{n}_j \otimes \mathbf{n}_j$
- construct orthonormalised vectors

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

- form nullspace matrix

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

Minres iterations for reduced system

N	d	off state ($\alpha = 0.5\alpha_c$) first step	off state ($\alpha = 0.5\alpha_c$) last step	on state ($\alpha = 1.5\alpha_c$) first step	on state ($\alpha = 1.5\alpha_c$) last step
32	93	59	128	90	172
64	189	187	418	285	557
128	381	660	1,456	1,004	2,002
256	765	2,562	5,455	3,650	7,043
512	1,533	9,983	21,393	13,907	26,504
1,024	3,069	41,267	80,778	55,563	81,821
2,048	6,141	171,385	$>$200,000	$>$200,000	$>$200,000

- doubling N quadruples iteration count

Preconditioning

Idea: instead of solving $\mathcal{H}\mathbf{x} = \mathbf{b}$, solve

$$\mathcal{P}^{-1}\mathcal{H}\mathbf{x} = \mathcal{P}^{-1}\mathbf{b}$$

for some preconditioner $\mathcal{P}$

Choose $\mathcal{P}$ so that

(i) eigenvalues of $\mathcal{P}^{-1}\mathcal{H}$ are well clustered
(ii) $\mathcal{P}\mathbf{u} = \mathbf{r}$ is easily solved

Extreme cases:

- $\mathcal{P} = \mathcal{H}$: good for (i), bad for (ii)
- $\mathcal{P} = I$: good for (ii), bad for (i)

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

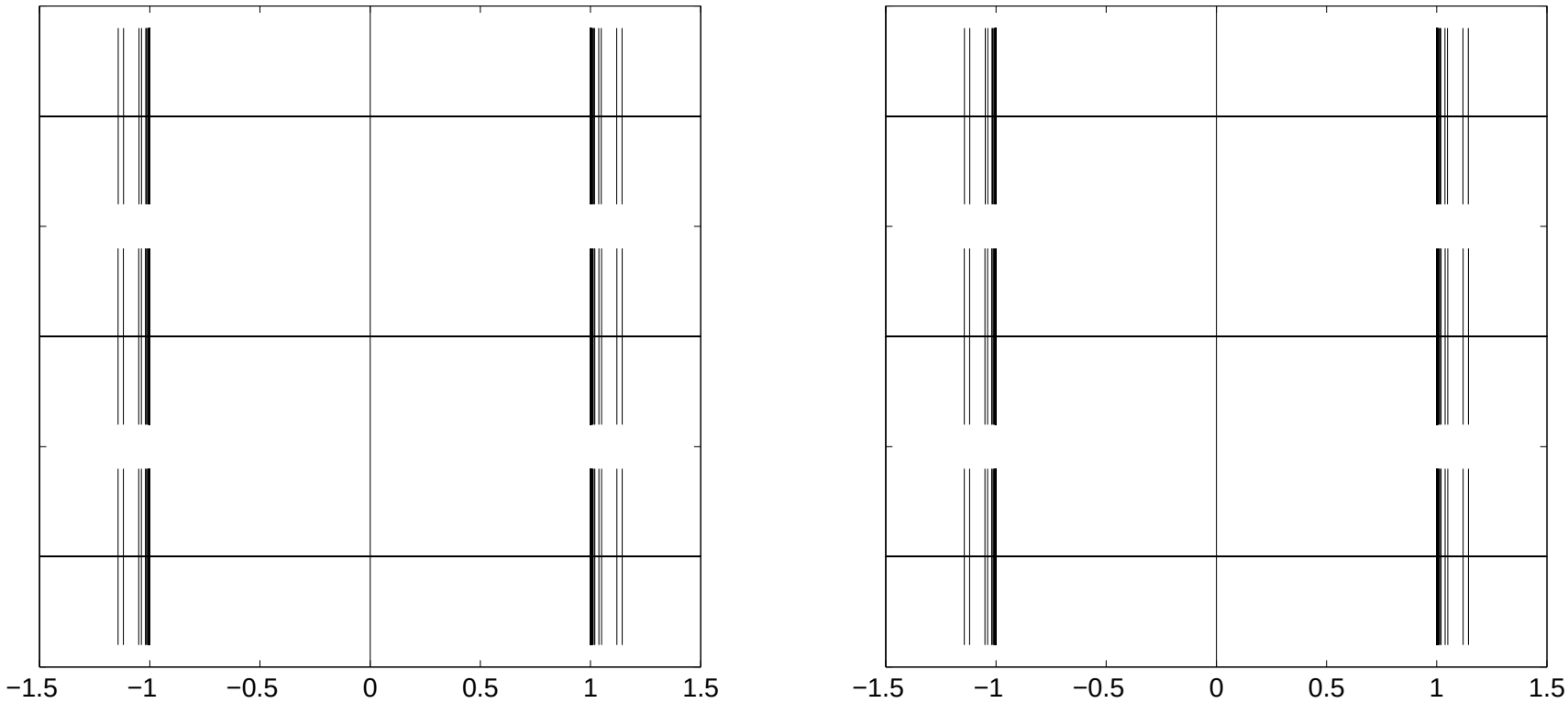
(i) 1 with multiplicity $n+1$
(ii) -1 with multiplicity 1
(iii) $\pm\sqrt{1+\sigma_k^2}$ for $k = 1, \ldots, n-1$

$\sigma_k \equiv$ singular value of M

Sample Eigenvalue Plots

- eigenvalues in two symmetric intervals

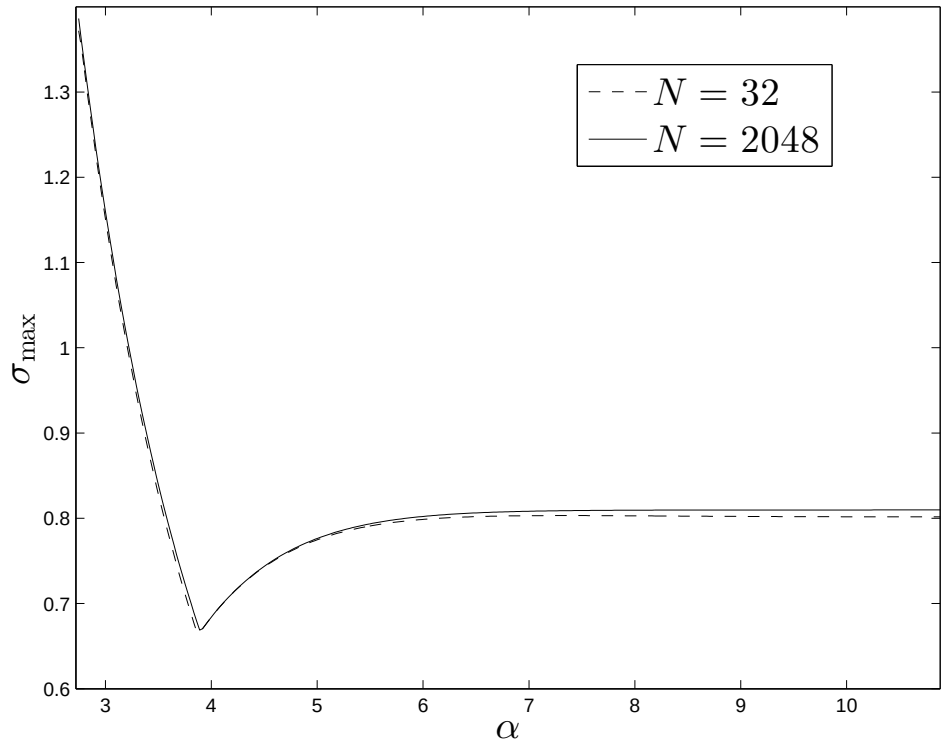
$$[-\beta, -1] \cup [1, \beta], \qquad \beta = \sqrt{1 + \sigma_{\max}^2}$$



eigenvalue plots for $N = 32, 64, 128$
first and last Newton iteration

Estimate of MINRES convergence

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



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

Iteration Counts

N	off state ($\alpha = 0.5\alpha_c$)		on state ($\alpha = 1.5\alpha_c$)	
	first step	last step	first step	last step
32	4	1	5	7
64	4	1	5	7
128	4	1	5	7
256	4	1	5	7
512	4	1	5	7
1,024	4	1	5	7
2,048	4	1	5	7
4,096	4	1	5	7
8,192	4	1	5	7
16,384	4	1	5	7
32,768	4	1	5	7
65,536	4	1	5	7

Non-“ideal” versions?

- 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 ($\alpha = 0.5\alpha_c$)		on state ($\alpha = 1.5\alpha_c$)		off state ($\alpha = 0.5\alpha_c$)		on state ($\alpha = 1.5\alpha_c$)	
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 and other issues

- Nullspace method plus ideal block preconditioner works very well for this simple 1D director model.
- We have also proposed a modified outer iteration (the Renormalized Newton Method) with $\mathbf{n}$ normalised onto the constraint manifold at each iterative step.
- Overall this gives an efficient solution algorithm for repeated solution of liquid crystal director models.
- Nullspace ideas also apply for full 2D and 3D problems.
- Issues remain re how to precondition $Z^T A Z$ for these more general cases.
- Use of spectrally equivalent preconditioned iteration looks promising.

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THANKS!

Computing Time

- elapsed time in seconds (tic/toc)

N	full direct	reduced direct	ideal block	ideal constraint
1,024	9.95e-02	9.70e-02	3.48e-01	3.08e-01
2,048	1.42e-01	1.36e-01	5.32e-01	8.35e-01
4,096	2.91e-01	2.79e-01	1.05e$+00$	2.73e$+00$
8,192	6.02e-01	5.90e-01	2.20e$+00$	9.74e$+00$
16,384	1.42e$+00$	1.29e$+00$	4.69e$+00$	3.80e$+01$
32,768	3.36e$+00$	2.75e$+00$	9.70e$+00$	8.25e$+02$
65,536	9.27e$+00$	7.41e$+00$	2.53e$+01$	—