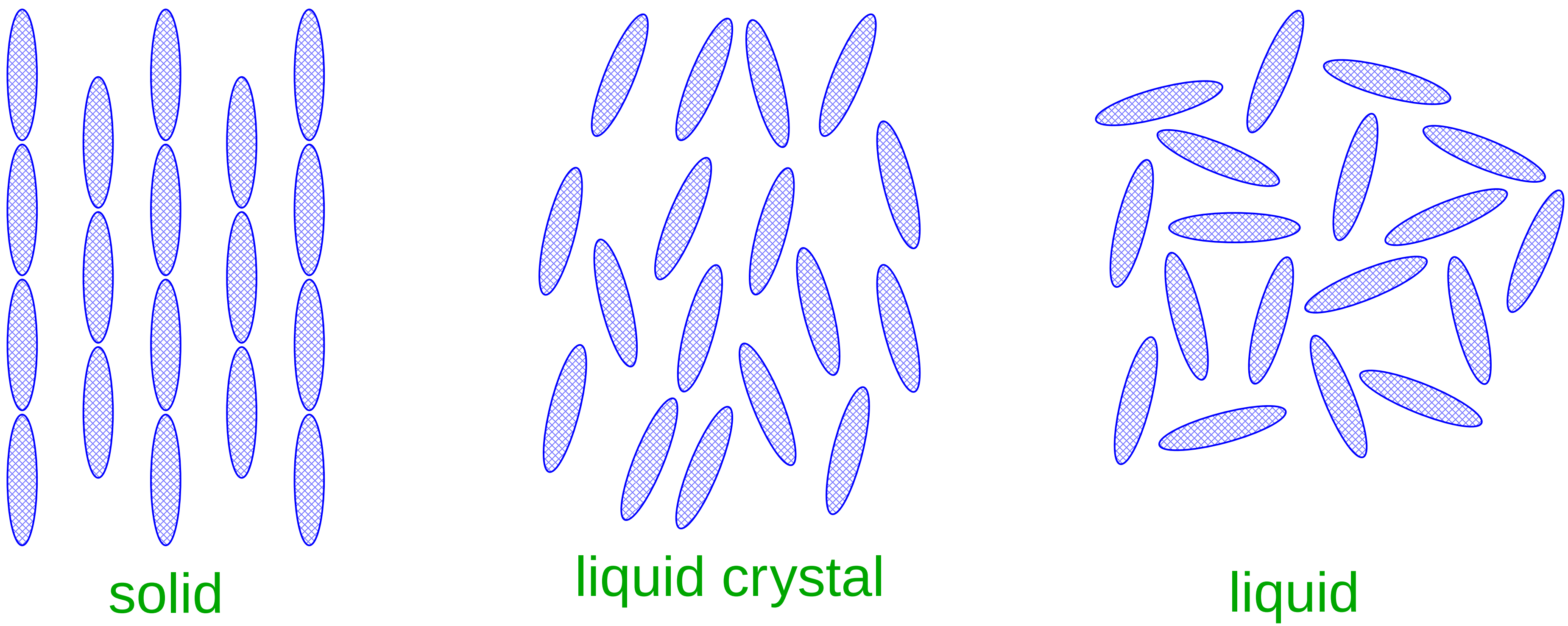
Saddle point problems in liquid crystal modelling

Alison Ramage
Mathematics and Statistics
University of Strathclyde
Glasgow, Scotland

Eugene C. Gartland, Jr.
Mathematics
Kent State University
Ohio, USA

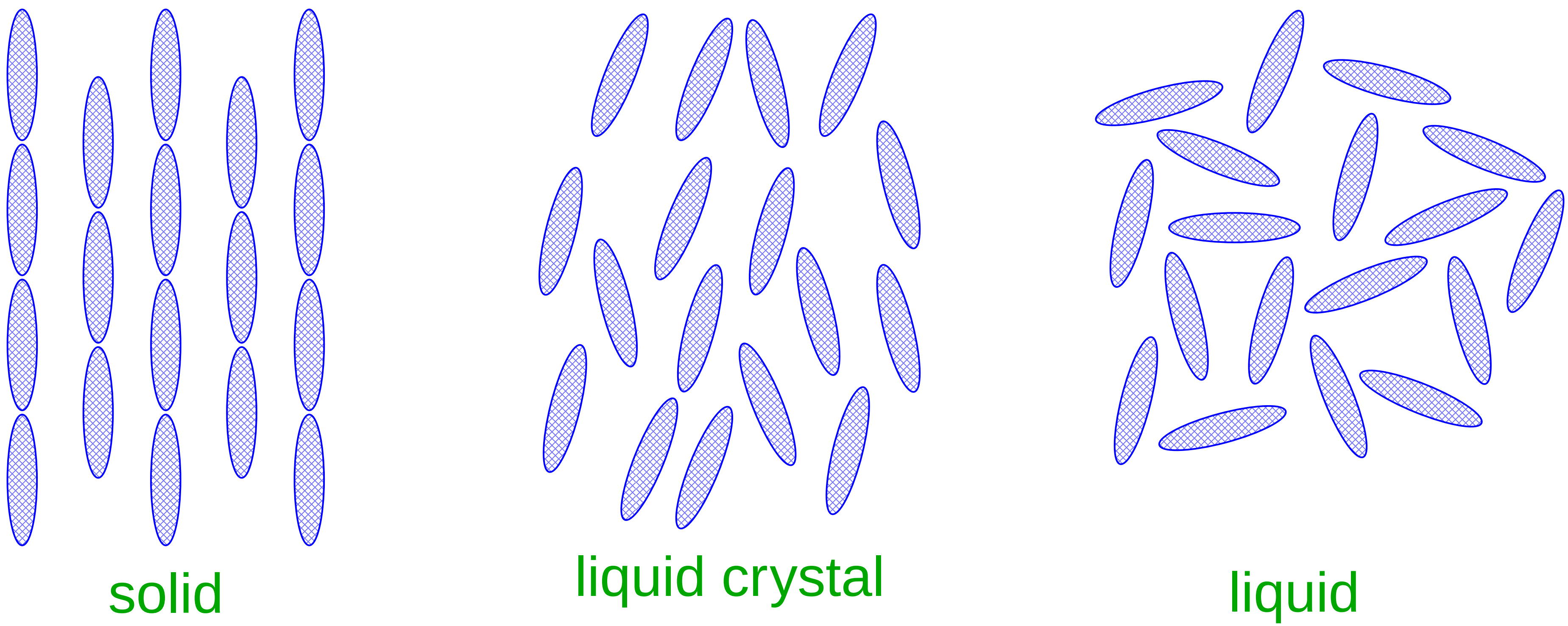
Liquid Crystals

- occur between solid crystal and isotropic liquid states



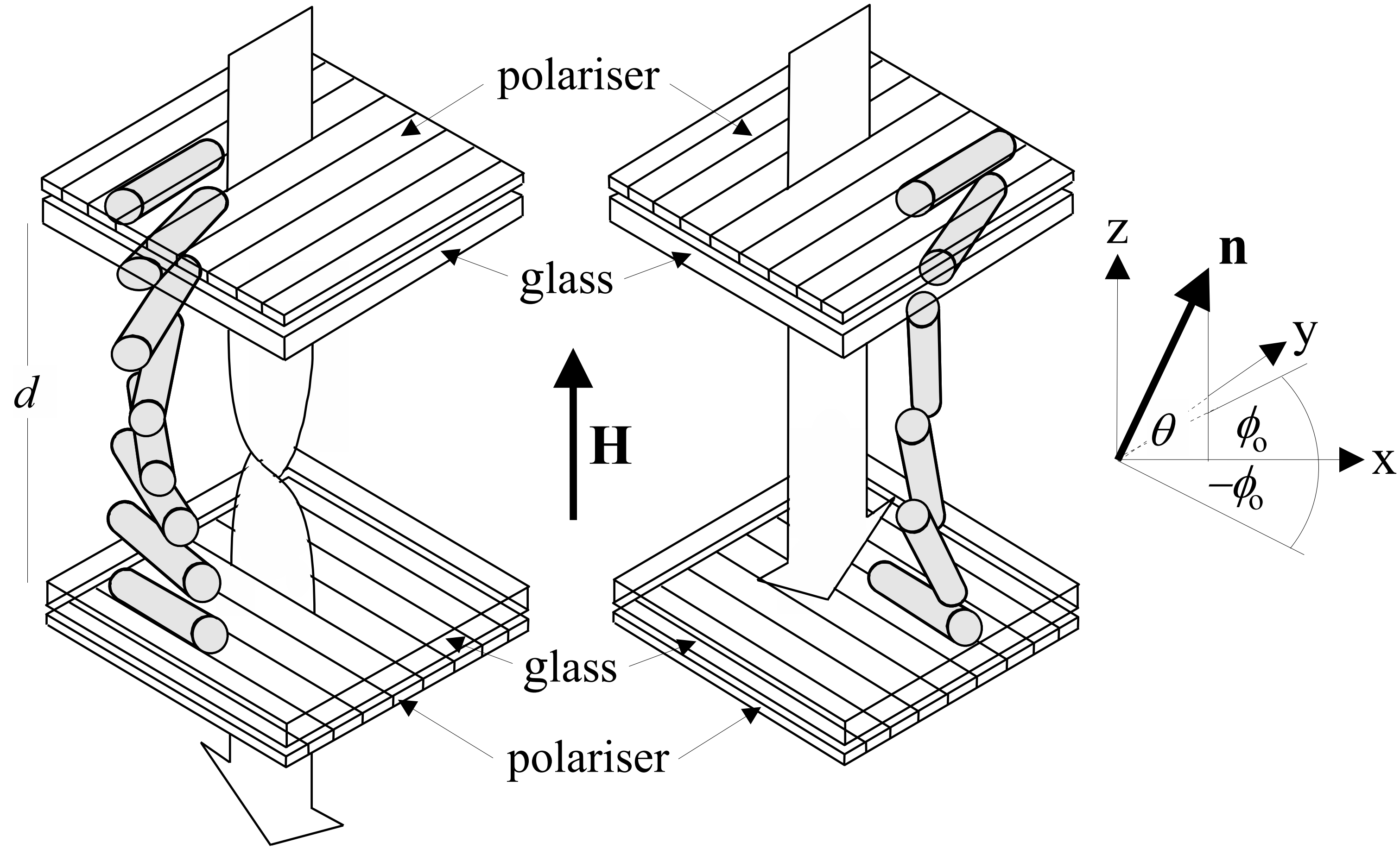
Liquid Crystals

- occur between solid crystal and isotropic liquid states



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

Liquid Crystal Displays

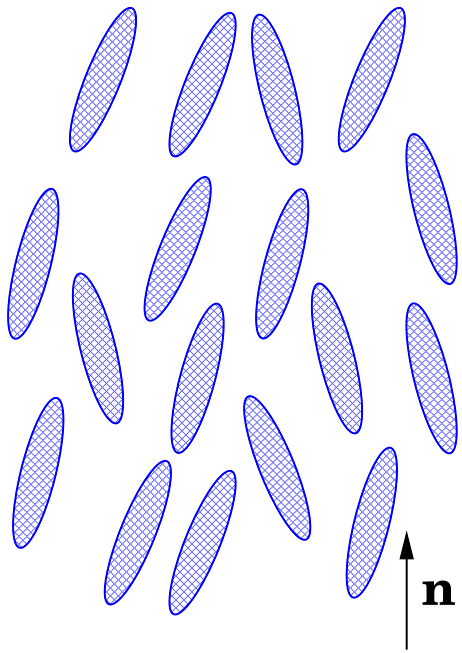


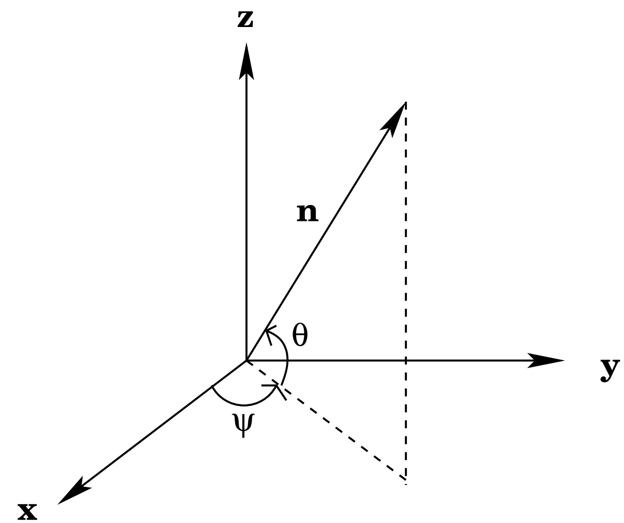
(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$

twisted nematic device

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

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

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

Finding Equilibrium Configurations

- minimise the free energy

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

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

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

Finding Equilibrium Configurations

- minimise the free energy

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

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

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

- solutions with least energy are physically relevant

Elastic Energy

- Frank-Oseen elastic energy

$$
\begin{aligned}
F_{elastic} &= \frac{1}{2}K_1(\nabla\cdot\mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 \\
&+ \frac{1}{2}K_3(\mathbf{n}\times\nabla\times\mathbf{n})^2 \\
&+ \frac{1}{2}(K_2+K_4)\nabla\cdot[(\mathbf{n}\cdot\nabla)\mathbf{n}-(\nabla\cdot\mathbf{n})\mathbf{n}]
\end{aligned}
$$

- Frank elastic constants

K_1	splay
K_2	twist
K_3	bend
K_2+K_4	saddle-splay

One-Constant Approximation

- set

$$K = K_1 = K_2 = K_3, \qquad K_4 = 0$$

One-Constant Approximation

- set

$$K = K_1 = K_2 = K_3, \qquad K_4 = 0$$

- vector identities

$$(\nabla \times \mathbf{n})^2 = (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + (\mathbf{n} \times \nabla \times \mathbf{n})^2$$

$$\nabla(\mathbf{n} \cdot \mathbf{n}) = 0$$

$$\left[(\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2\right] + \nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}] = \|\nabla \mathbf{n}\|^2$$

One-Constant Approximation

- set

$$K = K_1 = K_2 = K_3, \qquad K_4 = 0$$

- vector identities

$$(\nabla \times \mathbf{n})^2 = (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + (\mathbf{n} \times \nabla \times \mathbf{n})^2$$

$$\nabla(\mathbf{n} \cdot \mathbf{n}) = 0$$

$$\left[(\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2\right] + \nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}] = \|\nabla \mathbf{n}\|^2$$

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

Electrostatic Energy

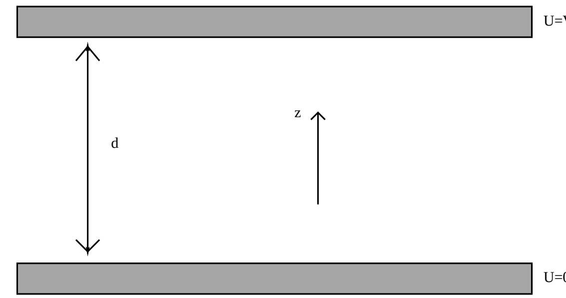
- applied electric field $\mathbf{E}$ of magnitude E
- electrostatic energy

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

- dielectric anisotropy $\epsilon_a = \epsilon_\parallel - \epsilon_\perp$
- permittivity of free space ϵ_0

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 1

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

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

- director $\quad \mathbf{n} = (u, v, w)$, $\quad |\mathbf{n}| = 1$

- electric potential U: $\quad E = \dfrac{dU}{dz}$

- unknowns $\quad u$, v, w, U

Alternative Model: Q-tensor Theory

- tensor order parameter

$$Q = \sqrt{\frac{3}{2}} S \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right)$$

- symmetric tensor

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

$$tr(Q) = 0, \qquad tr(Q^2) = S^2$$

- five unknowns q_1, q_2, q_3, q_4, q_5

Equilibrium Equations 2

- nondimensionalise: $\bar{z} = \frac{z}{d}, \qquad \bar{U} = \frac{U}{V}$

- 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

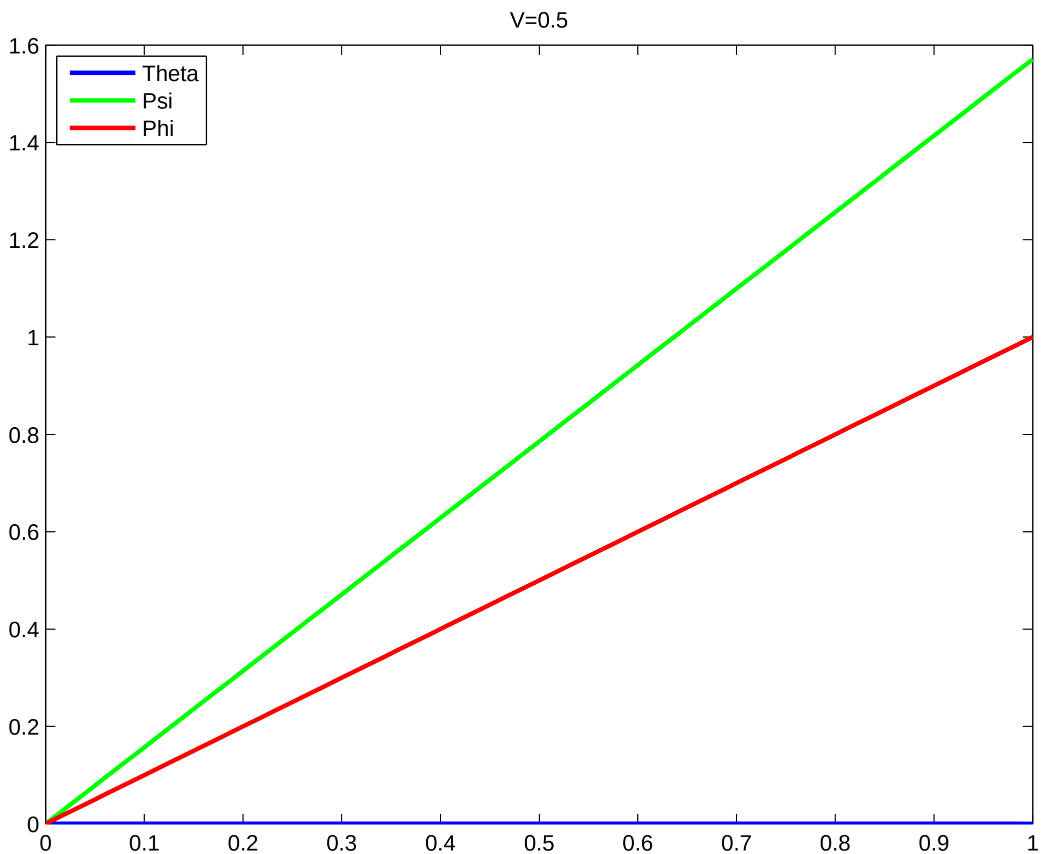
$$\alpha^2 = \frac{\epsilon_0 \epsilon_a V^2}{K \pi^2}, \qquad \beta = \frac{\epsilon_\perp}{\epsilon_a}$$

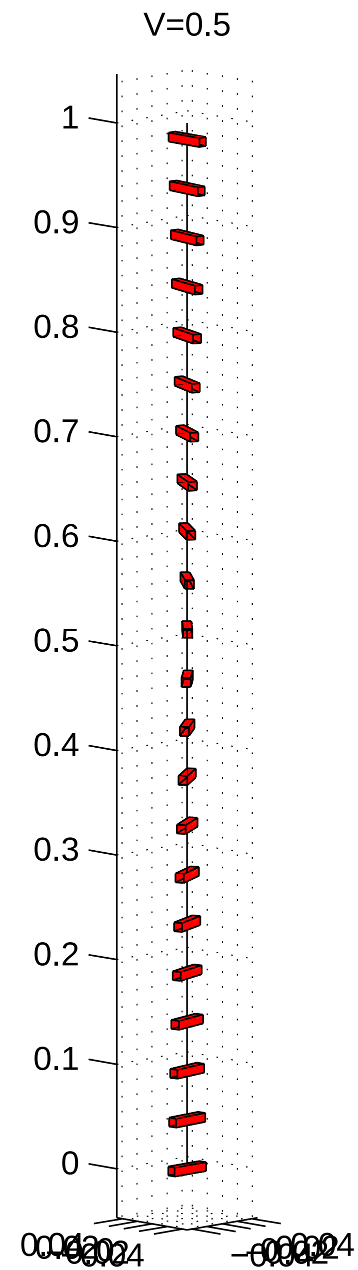
- boundary conditions:

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

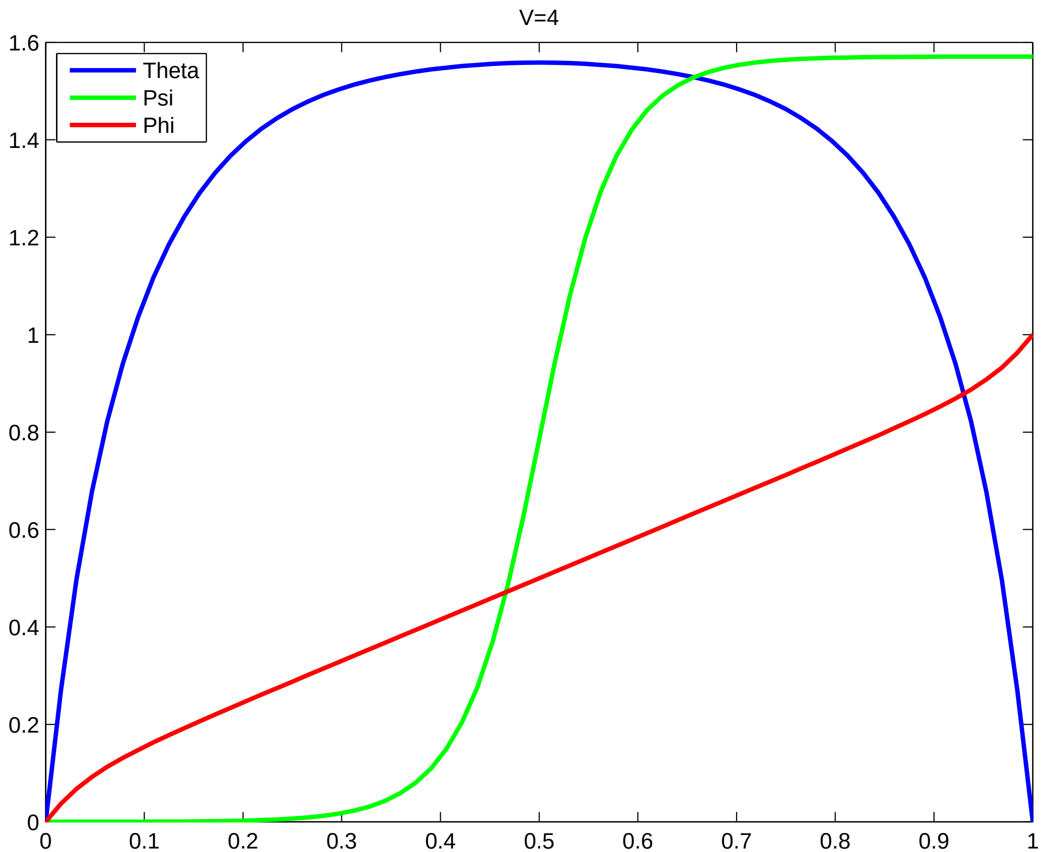
Off State

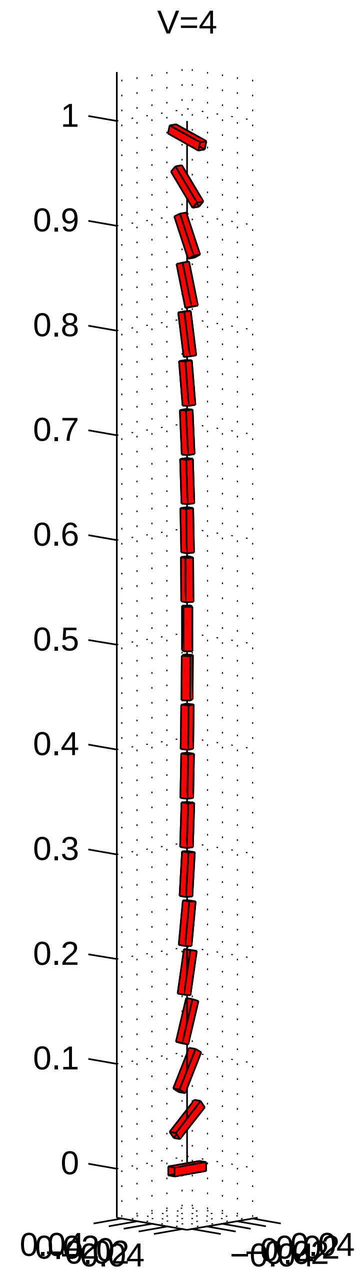
$$\theta(z) \equiv 0, \qquad \phi(z) = \frac{\pi}{2} z, \qquad U(z) = z$$





On State

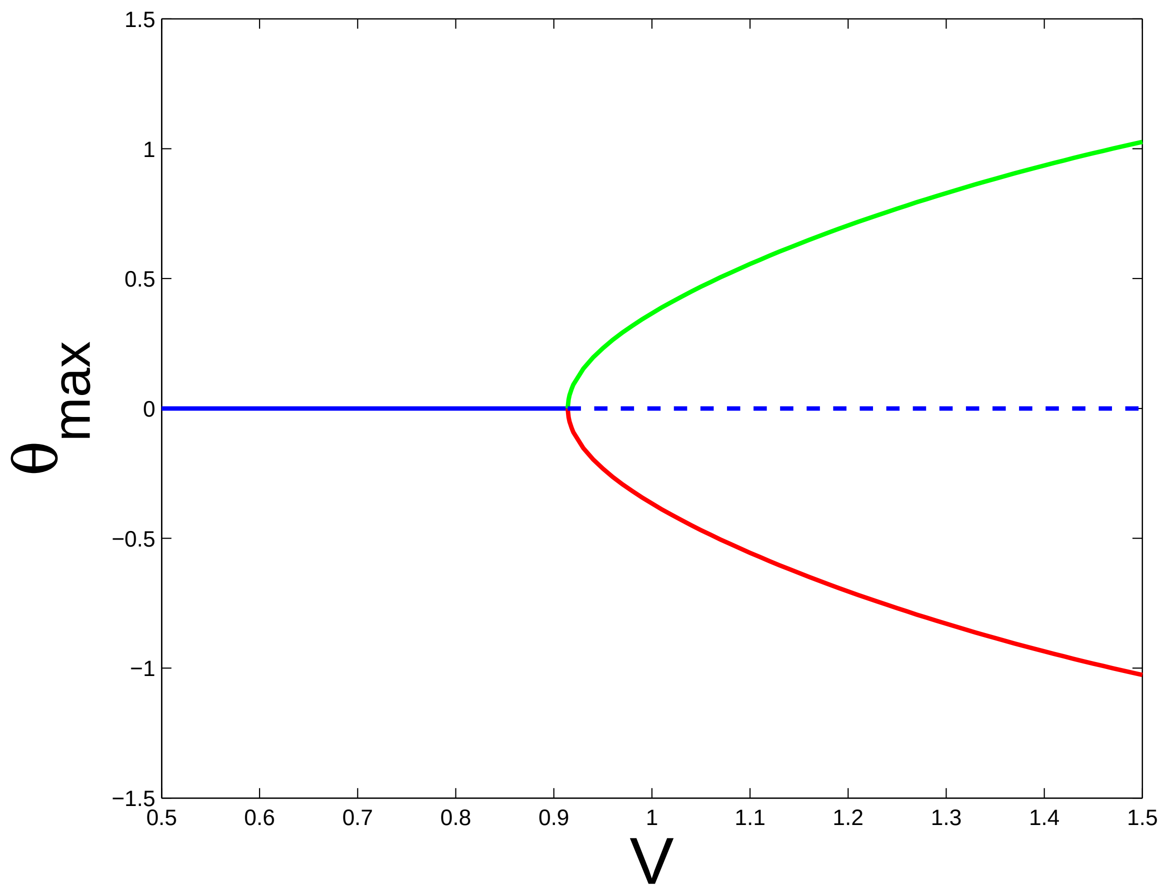

V=4
Theta
Psi
Phi
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
0.1
0.3
0.5
0.7
0.9


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

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 I

- discrete free energy

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

- 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

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

Constrained Minimisation II

- set $$\frac{\partial G}{\partial u_k}, \frac{\partial G}{\partial v_k}, \frac{\partial G}{\partial w_k}, \frac{\partial G}{\partial U_k}, \frac{\partial G}{\partial \lambda_k}$$ equal to zero

Constrained Minimisation II

- set $$\frac{\partial G}{\partial u_k}, \frac{\partial G}{\partial v_k}, \frac{\partial G}{\partial w_k}, \frac{\partial G}{\partial U_k}, \frac{\partial G}{\partial \lambda_k}$$ equal to zero

- 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

Constrained Minimisation II

- set $\dfrac{\partial G}{\partial u_k}, \dfrac{\partial G}{\partial v_k}, \dfrac{\partial G}{\partial w_k}, \dfrac{\partial G}{\partial U_k}, \dfrac{\partial G}{\partial \lambda_k}$ equal to zero

- 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

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

Constrained Minimisation II

- set $\dfrac{\partial G}{\partial u_k}, \dfrac{\partial G}{\partial v_k}, \dfrac{\partial G}{\partial w_k}, \dfrac{\partial G}{\partial U_k}, \dfrac{\partial G}{\partial \lambda_k}$ equal to zero

- 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

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

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

- A_{uu}, A_{vv} and A_{ww} are $n \times n$ symmetric tridiagonal blocks

Hessian Components 1

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

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

- A_{uu}, A_{vv} and A_{ww} are $n \times n$ symmetric tridiagonal blocks
- $A_{uu} = A_{vv} = \frac{1}{\Delta z}\mathtt{tri}(-1, 2 - \Delta z^2 \lambda_j, -1)$
- $A_{ww} = \frac{1}{\Delta z}\mathtt{tri}(-1, 2 - \Delta z^2 \lambda_j - \gamma_j, -1)$

$$\gamma_j = \frac{\alpha^2 \pi^2}{2}[(U_{j+1} - U_j)^2 + (U_j - U_{j-1})^2]$$

Eigenvalues of A

- off state: first Newton step, linear U, constant λ

$$\lambda_j = \lambda = \frac{4}{\Delta z^2} \sin^2 \left(\frac{\pi \Delta z}{4} \right)$$

- block matrices are Toeplitz

Eigenvalues of A

- off state: first Newton step, linear U, constant λ

$$\lambda_j = \lambda = \frac{4}{\Delta z^2} \sin^2\left(\frac{\pi \Delta z}{4}\right)$$

- block matrices are Toeplitz

- $\sigma_{\min}(A_{uu}) = \sigma_{\min}(A_{vv}) \simeq \frac{3\pi^2}{4}\Delta z > 0$

A_{uu} and A_{vv} are positive definite

- $\sigma_{\min}(A_{ww}) \simeq \left(\frac{3\pi^2}{4} - \alpha^2\pi^2\right)\Delta z$

A_{ww} is positive definite iff $V < V_c$

Eigenvalues of A

- off state: first Newton step, linear U, constant λ

$$\lambda_j = \lambda = \frac{4}{\Delta z^2} \sin^2\left(\frac{\pi \Delta z}{4}\right)$$

- block matrices are Toeplitz

- $\sigma_{\min}(A_{uu}) = \sigma_{\min}(A_{vv}) \simeq \frac{3\pi^2}{4}\Delta z > 0$

A_{uu} and A_{vv} are positive definite

- $\sigma_{\min}(A_{ww}) \simeq \left(\frac{3\pi^2}{4} - \alpha^2\pi^2\right)\Delta z$

A_{ww} is positive definite iff $V < V_c$

- number of negative eigenvalues increases with V

Hessian Components 2

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

- the $3n \times n$ matrix B has structure

$$B = -\Delta z \begin{bmatrix} B_u \\ B_v \\ B_w \end{bmatrix}, \qquad \begin{array}{l} B_u = \texttt{diag}(\mathbf{u}) \\ B_v = \texttt{diag}(\mathbf{v}) \\ B_w = \texttt{diag}(\mathbf{w}) \end{array}$$

Hessian Components 2

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

- the $3n \times n$ matrix B has structure

$$B = -\Delta z \begin{bmatrix} B_u \\ B_v \\ B_w \end{bmatrix}, \qquad \begin{array}{l} B_u = \texttt{diag}(\mathbf{u}) \\ B_v = \texttt{diag}(\mathbf{v}) \\ B_w = \texttt{diag}(\mathbf{w}) \end{array}$$

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

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

Hessian Components 3

- matrix notation: $\nabla^2_{\mathbf{UU}}\mathbf{G} = -C$
- the $n \times n$ matrix C is symmetric and tridiagonal

Hessian Components 3

- matrix notation: $\nabla^2_{\mathbf{UU}}\mathbf{G} = -C$
- the $n \times n$ matrix C is symmetric and tridiagonal
- $C = \dfrac{1}{\Delta z}\texttt{tri}(-a_{j-\frac{1}{2}}, a_{j-\frac{1}{2}} + a_{j+\frac{1}{2}}, -a_{j+\frac{1}{2}})$

$$a_{j-\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_{j-1}^2 + w_j^2)) > 0$$

$$a_{j+\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_j^2 + w_{j+1}^2)) > 0$$

Hessian Components 3

- matrix notation: $\nabla^2_{\mathbf{UU}}\mathbf{G} = -C$
- the $n \times n$ matrix C is symmetric and tridiagonal
- $C = \dfrac{1}{\Delta z}\texttt{tri}(-a_{j-\frac{1}{2}}, a_{j-\frac{1}{2}} + a_{j+\frac{1}{2}}, -a_{j+\frac{1}{2}})$

$$a_{j-\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_{j-1}^2 + w_j^2)) > 0$$

$$a_{j+\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_j^2 + w_{j+1}^2)) > 0$$

- diagonally dominant with positive real diagonal entries

C is positive definite

Hessian Components 4

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

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

- the $n \times n$ matrix D_w is tridiagonal

$$D_w = \texttt{diag}(\mathbf{w})\texttt{tri}(U_j - U_{j-1}, U_{j-1} - 2U_j + U_{j+1}, U_j - U_{j+1})$$

Hessian Components 4

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

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

- the $n \times n$ matrix D_w is tridiagonal

$$D_w = \texttt{diag}(\mathbf{w})\texttt{tri}(U_j - U_{j-1}, U_{j-1} - 2U_j + U_{j+1}, U_j - U_{j+1})$$

- D_w has complex eigenvalues in conjugate pairs and one zero eigenvalue (N even)

- $\mathrm{rank}(D) = n - 1$

Full Hessian Structure

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

$$\nabla^2 \mathbf{G} = \begin{bmatrix} A & B & D \\ B^T & 0 & 0 \\ D^T & 0 & -C \end{bmatrix}$$

saddle-point problem

Four Saddle-Point Problems

- for unknown vector ordered as $\mathbf{x} = [\mathbf{u}, \mathbf{v}, \mathbf{w}, \mathbf{U}, \lambda]$

$$H = \left[\begin{array}{c|cc} A & D & B \\ \hline D^T & -C & 0 \\ B^T & 0 & 0 \end{array}\right] \qquad H = \left[\begin{array}{cc|c} A & D & B \\ D^T & -C & 0 \\ \hline B^T & 0 & 0 \end{array}\right]$$

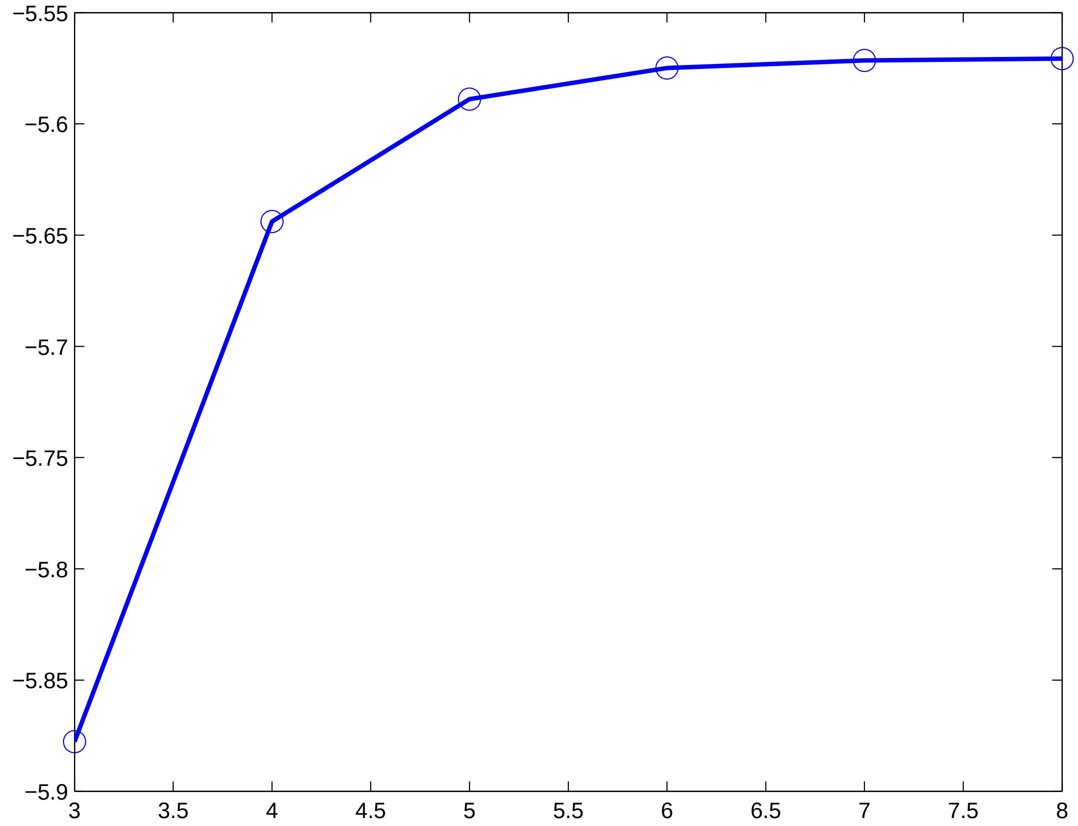
- for unknown vector ordered as $\mathbf{x} = [\mathbf{u}, \mathbf{v}, \mathbf{w}, \lambda, \mathbf{U}]$

$$H = \left[\begin{array}{c|cc} A & B & D \\ \hline B^T & 0 & 0 \\ D^T & 0 & -C \end{array}\right] \qquad H = \left[\begin{array}{cc|c} A & B & D \\ B^T & 0 & 0 \\ \hline D^T & 0 & -C \end{array}\right]$$

double saddle-point structure

Iterative Solution

- outer iteration: Newton's method tol=$1e-4$
- inner iteration: MINRES tol=$1e-4$
- check accuracy by calculating energy of final solution



Matrix Conditioning

- eigenvalues of H lie in $[\lambda_{\min}, \lambda_s] \cup [\lambda_{s+1}, \lambda_{\max}]$
- estimate of matrix conditioning:

N	condest	$\lambda_{\min}(H)$	$\lambda_s(H)$	$\lambda_{s+1}(H)$	$\lambda_{\max}(H)$
8	1.64e+6	-6.68e+2	-5.40e-4	1.88e-1	3.07e+1
16	2.58e+7	-1.44e+3	-6.26e-5	2.19e-1	6.33e+1
32	4.09e+8	-2.98e+3	-7.68e-6	1.28e-1	1.28e+2
64	6.51e+9	-6.07e+3	-9.56e-7	6.60e-2	2.56e+2
128	1.04e+11	-1.23e+4	-1.20e-7	3.33e-2	5.12e+2
256	1.66e+12	-2.46e+4	-1.50e-8	1.67e-2	1.03e+3
	$O(N^4)$	$O(N)$	$O(N^{-3})$	$O(N^{-1})$	$O(N)$

Nullspace Method I

- Newton system:

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

Nullspace Method I

- Newton system:

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

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

Nullspace Method I

- Newton system:

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

- Idea: use information about nullspace of B to eliminate constraint blocks
- use $Z \in \mathbb{R}^{3n \times 2n}$ whose columns form a basis for the nullspace of B^T

$$B^T Z = Z^T B = 0$$

- $\mathrm{rank}(Z) = 2n$

Nullspace Method I

- Newton system:

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

- Idea: use information about nullspace of B to eliminate constraint blocks
- use $Z \in \mathbb{R}^{3n \times 2n}$ whose columns form a basis for the nullspace of B^T

$$B^T Z = Z^T B = 0$$

- $\mathrm{rank}(Z) = 2n$
- system size will reduce from $5n \times 5n$ to $3n \times 3n$

Nullspace Method II

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

Nullspace Method II

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

- write solution of (2) as

$$\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{z}$$

  - particular solution satisfies $B^T \widehat{\delta\mathbf{n}} = -\nabla_{\lambda}$
  - $Z\mathbf{z} \in \mathbb{R}^{2n}$ lies in nullspace of B^T

Nullspace Method II

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

- write solution of (2) as

$$\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{z}$$

  - particular solution satisfies $B^T\widehat{\delta\mathbf{n}} = -\nabla_{\lambda}$
  - $Z\mathbf{z} \in \mathbb{R}^{2n}$ lies in nullspace of B^T

- find $\widehat{\delta\mathbf{n}}$ via $\widehat{\delta\mathbf{n}} = -B(B^TB)^{-1}\nabla_{\lambda}$
- here B^TB is diagonal so solve is cheap

Nullspace Method III

- reduced system:

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

Nullspace Method III

- 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

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

Nullspace Method III

- 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

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

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

Nullspace of B^T I

- permute entries of B:

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

Nullspace of B^T I

- permute entries of B:

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

- eigenvectors of orthogonal projection

$$I - \mathbf{n}_j \otimes \mathbf{n}_j = \begin{bmatrix} 1 - u_j^2 & -v_j u_j & -w_j u_j \\ -u_j v_j & 1 - v_j^2 & -w_j v_j \\ -u_j w_j & -v_j w_j & 1 - w_j^2 \end{bmatrix}$$

will be orthogonal to $\mathbf{n}_j$

Nullspace of B^T II

- eigenvectors of orthogonal projection: e.g.

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

- orthonormalise:

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

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

Nullspace of B^T III

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

Nullspace of B^T III

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

- consider $B^T Z \mathbf{p}$ where $\mathbf{p} = [p_1, q_1, p_2, q_2, \ldots, p_n, q_n]^T$:

$$B^T Z \mathbf{U} = \begin{bmatrix} \mathbf{n}_1^T & & & \\ & \mathbf{n}_2^T & & \\ & & \ddots & \\ & & & \mathbf{n}_n^T \end{bmatrix} \begin{bmatrix} p_1 \mathbf{l}_1 + q_1 \mathbf{m}_1 \\ p_2 \mathbf{l}_2 + q_2 \mathbf{m}_2 \\ \vdots \\ p_n \mathbf{l}_n + q_n \mathbf{m}_n \end{bmatrix} = 0$$

- columns of Z form a basis for nullspace of B^T

Condition of Reduced System

- eigenvalues of H lie in $[\lambda_{\min}, \lambda_s] \cup [\lambda_{s+1}, \lambda_{\max}]$
- estimate of matrix conditioning:

N	condest	$\lambda_{\min}(H)$	$\lambda_s(H)$	$\lambda_{s+1}(H)$	$\lambda_{\max}(H)$
8	1.28e+3	-7.44e+2	-2.13e+1	1.71e+0	3.39e+3
16	1.51e+4	-1.51e+3	-9.77e+0	8.14e-1	1.89e+4
32	2.13e+5	-3.06e+3	-4.77e+0	4.04e-1	1.40e+5
64	3.29e+6	-6.20e+3	-2.37e+0	2.02e-1	1.10e+6
128	4.97e+7	-1.24e+4	-1.18e+0	1.01e-1	8.78e+6
256	7.84e+8	-2.50e+4	-5.91e-1	5.05e-2	7.02e+7
	$O(N^4)$	$O(N)$	$O(N^{-1})$	$O(N^{-1})$	$O(N^3)$

Solving the Reduced System

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

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

Solving the Reduced System

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

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

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

Solving the Reduced System

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

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

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

- preconditioned matrix:

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

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

Preconditioned Spectrum

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

- $M = C^{-1/2}Z^T D(Z^T AZ)^{-1/2}$
- rank(M)=$n-1$
- non-zero singular values σ_k

Preconditioned Spectrum

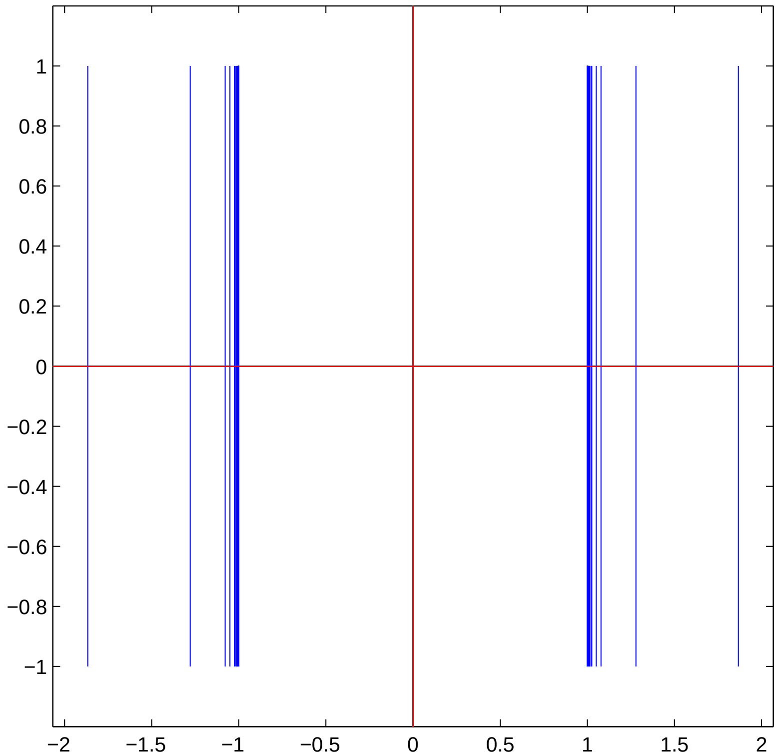
$$\tilde{\mathcal{A}} = \mathcal{G}^{-1/2}\mathcal{A}\mathcal{G}^{-1/2} = \begin{bmatrix} I & M^T \\ M & -I \end{bmatrix}$$

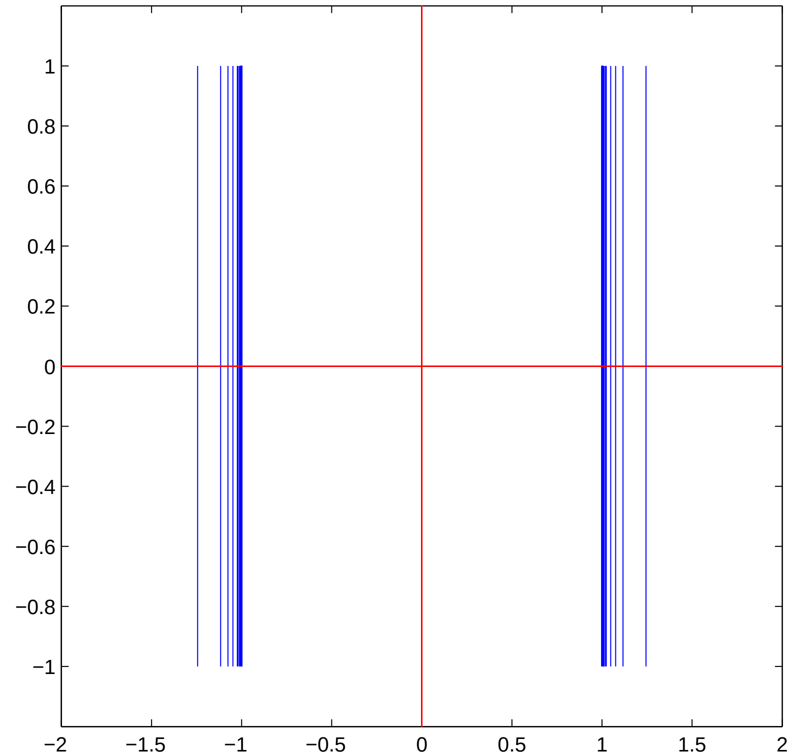
- $M = C^{-1/2} Z^T D (Z^T A Z)^{-1/2}$
- rank(M)=$n-1$
- non-zero singular values σ_k

- $3n$ eigenvalues of $\tilde{\mathcal{A}}$ 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





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

Diagonal Preconditioning

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

$$\mathcal{D} = \begin{bmatrix} D_A & 0 & 0 \\ 0 & \Delta z^3 \, I & 0 \\ 0 & 0 & D_C \end{bmatrix}$$

$$\begin{aligned} D_A &= \texttt{diag}(A) \\ D_C &= \texttt{diag}(C) \end{aligned}$$

Diagonal Preconditioning

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

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

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

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

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

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

- 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

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

Conclusions and the Future

- Reduced block preconditioner is very efficient for this problem.
- Nullspace method is ideal for this simple 1D director model.

Conclusions and the Future

- Reduced block preconditioner is very efficient for this problem.
- Nullspace method is ideal for this simple 1D director model.

- Can the convergence analysis be pushed further?
- Does the same method work well for more complicated liquid crystal cells?
- What about 2D models?
- Reduced block preconditioner is cheap to invert here: could approximate solves (e.g. multigrid) be used for other problems with less structure?

Conclusions and the Future

- Reduced block preconditioner is very efficient for this problem.
- Nullspace method is ideal for this simple 1D director model.

- Can the convergence analysis be pushed further?
- Does the same method work well for more complicated liquid crystal cells?
- What about 2D models?
- Reduced block preconditioner is cheap to invert here: could approximate solves (e.g. multigrid) be used for other problems with less structure?

THANKS!

Iteration Counts

- iteration counts at first Newton step

N	8	16	32	64	128	256
$\mathcal{D}$	15	40	117	382	1293	5126
C_1	13	25	50	98	195	387
C_2	7	9	8	9	7	8

Iteration Counts

- iteration counts at first Newton step

N	8	16	32	64	128	256
$\mathcal{D}$	15	40	117	382	1293	5126
C_1	13	25	50	98	195	387
C_2	7	9	8	9	7	8

- iteration counts at last Newton step

N	8	16	32	64	128	256
$\mathcal{D}$	37	134	414	1617	7466	34755
C_1	22	55	226	635	2259	7166
C_2	6	14	23	43	65	114