Efficient iterative solvers for saddle-point problems in liquid crystal modelling

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Direct or Iterative Solvers?

- direct methods (see e.g. HSL library, MUMPS package)
  - efficient for full matrices
  - good for lots of RHS vectors
  - sparse matrices may lead to fill-in
  - node ordering often important
  - storage and CPU restrictions

- iterative methods (e.g. Krylov subspace methods)
  - data structures predetermined
  - no need for special node ordering
  - efficient for extremely large sparse problems
  - last iterate can give a good starting vector
  - some expertise needed
  - lack of robustness

Symmetric Positive Definite Systems

Conjugate Gradients: Hestenes and Stiefel (1952)

CG method constructs iterates

$$\mathbf{x}_k \in \mathbf{x}_0 + \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \ldots, A^{k-1}\mathbf{r}_0\}$$

where $\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k$, with properties

- $\mathbf{x}_k$ minimises $\|\mathbf{x}_k - \hat{\mathbf{x}}\|_A = (\mathbf{x} - \hat{\mathbf{x}})^T A(\mathbf{x} - \hat{\mathbf{x}})$
- uses a three-term recurrence relation

Theorem: The CG method finds $\hat{\mathbf{x}}$ in s steps.

- In exact arithmetic, CG is a direct method!

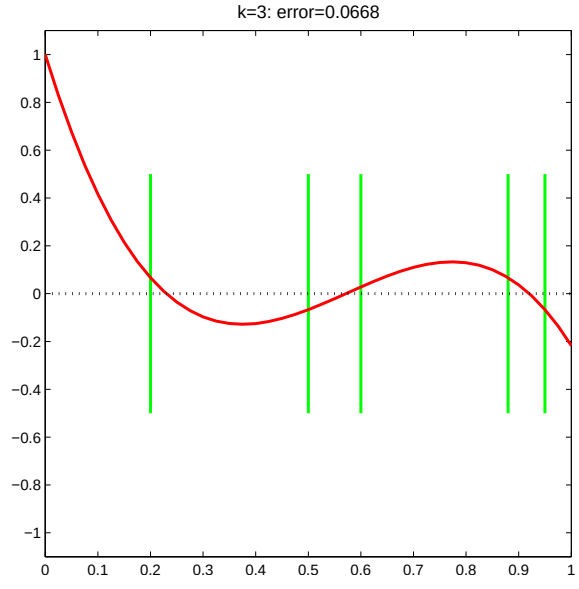
$$\|\mathbf{x}_k - \hat{\mathbf{x}}\|_A \leq \min_{P_k \in \Pi_k^1} \max_i |P_k(\lambda_i)| \|\mathbf{x}_0 - \hat{\mathbf{x}}\|_A$$

Practical Bound

- use Tchebyshev approximation to obtain bound involving the condition number $\kappa = \lambda_{\max}/\lambda_{\min}$
- number of iterations required for convergence to within tolerance ϵ is

$$k \simeq \frac{1}{2} \ln \frac{2}{\epsilon} \sqrt{\kappa}$$

- condition number bound is useful but eigenvalue clustering plays an important role



Symmetric Indefinite Systems

MINRES: Paige and Saunders (1975)

construct iterates $\mathbf{x}_k = \mathbf{x}_0 + V_k \mathbf{y}_k$ with properties

- $\mathbf{x}_k$ minimises $\|\mathbf{r}_k\|_2$
- uses three-term recurrence relation

$$V_k = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k]$$

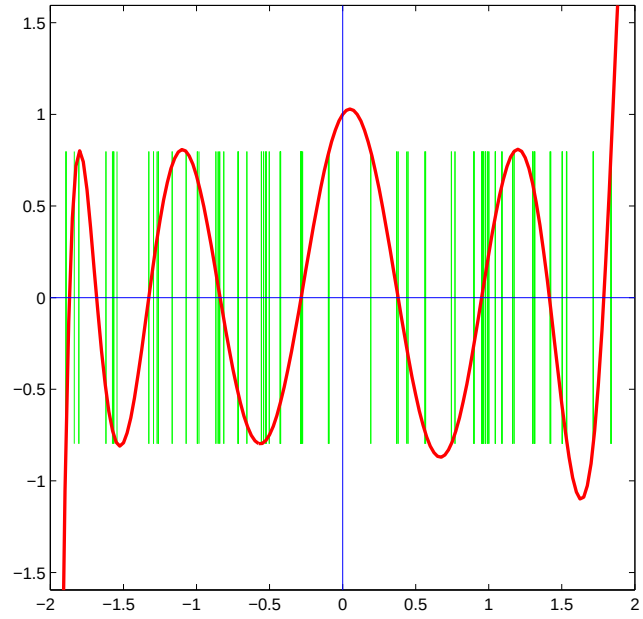
$\mathbf{v}_k$ form an orthonormal basis for $\kappa(A, \mathbf{r}_0, k)$

- use Lanczos method to find $\mathbf{v}_k$
- solve resulting least squares problem for $\mathbf{y}_k$ using Givens rotations and QR factorisation

Convergence of MINRES

- at step k:

$$\|\mathbf{r}_k\|_2 \leq \min_{P_k \in \Pi_k^1} \max_i |P_k(\lambda_i)| \|\mathbf{r}_0\|_2$$



- symmetric intervals: $[-\lambda_{\max}, -\lambda_{\min}] \cup [\lambda_{\min}, \lambda_{\max}]$

$$k \propto \kappa \equiv \frac{\lambda_{\max}}{\lambda_{\min}}$$

Nonsymmetric Systems

GMRES: Saad and Schultz (1986)

Construct iterates $\mathbf{x}_k = \mathbf{x}_0 + V_k \mathbf{y}_k$ with properties

- $\mathbf{x}_k$ minimises $\|\mathbf{r}_k\|_2$
- no short-term recurrence

$$V_k = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k]$$

$\mathbf{v}_k$ form an orthonormal basis for $\kappa(A, \mathbf{r}_0, k)$

- use the Arnoldi method to find $\mathbf{v}_k$
- if A is diagonalisable ($A = X \Lambda X^{-1}$)

$$\|\mathbf{r}_k\|_2 \leq \|X\|_2 \|X^{-1}\|_2 \min_{P_k \in \Pi_k^1} \max_j |P_k(\lambda_j)| \|\mathbf{r}_0\|_2$$

Preconditioning

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

$$M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$$

for some preconditioner M

Choose M so that

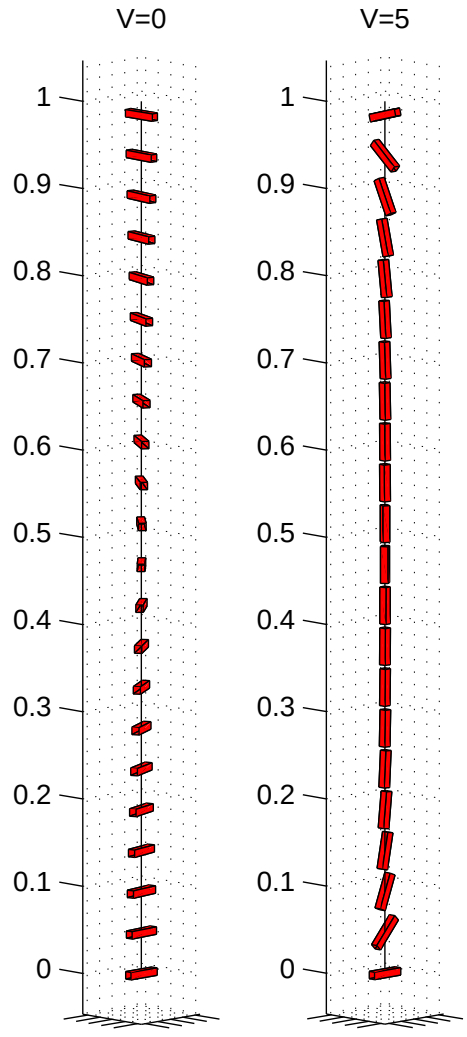
(i) eigenvalues of $M^{-1}A$ are well clustered
(ii) $M\mathbf{u} = \mathbf{r}$ is easily solved

Extreme cases:

- $M = A$: good for (i), bad for (ii)
- $M = I$: good for (ii), bad for (i)

Model Problem: 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



Case 1: Director Model

- director $\mathbf{n} = (u, v, w)$, electric potential U with $E = \dfrac{dU}{dz}$
- 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
- $n = N - 1$ unknowns for each variable u, v, w, U, λ

Constrained Minimisation

$$G = \frac{\Delta z}{2}\left[f(u_1,\ldots,u_n,v_1,\ldots,v_n,w_1,\ldots,w_n,U_1,\ldots,U_n)\right.$$
$$\left. - \lambda_1(u_1^2+v_1^2+w_1^2-1) - \ldots \lambda_n(u_n^2+v_n^2+w_n^2-1)\right]$$

- solve $\nabla \mathbf{G}(\mathbf{x}) = \mathbf{0}$ 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 $\nabla^2 \mathbf{G}(\mathbf{x})$

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

Full Hessian Structure

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

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

- H is symmetric and indefinite
- double saddle-point problem (see e.g. Benzi, Golub and Liesen, Acta Numerica 2005)

Nullspace Method

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

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

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

- 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 $\delta\mathbf{n} = \widehat{\delta\mathbf{n}} + Z\mathbf{z}$ where particular solution satisfies $B^T\widehat{\delta\mathbf{n}} = -\nabla_{\lambda} G$
- system size reduced from $5n \times 5n$ to $3n \times 3n$
- additional equations:

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

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

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

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 $I - \mathbf{n}_j \otimes \mathbf{n}_j$, e.g.

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

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

Solving the Reduced System

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

- 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:

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

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

Preconditioned Spectrum

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

- $3n$ 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 $k = 1, \ldots, n-1$

  where σ_k are non-zero singular values of M

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

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

- $\sigma_{\max}$ can be bounded independently of Δz

Iteration Counts

- iterations - 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

- iterations - 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

- times - A: full \, B: reduced \, C: reduced block

N	A	B	C
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

Case 2: $\mathbf{Q}$-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
- basis representation

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

- applied electric field $\mathbf{E}$, electric potential U
- unknowns $q_1, q_2, q_3, q_4, q_5, U$

Free Energy Minimsation

- additional thermotropic energy term
- solve Euler-Lagrange equations

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

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

- 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

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

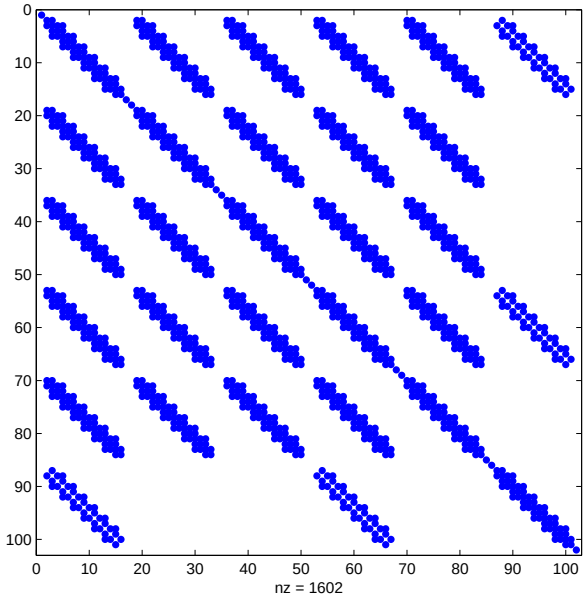
$$\mathcal{K} = \begin{bmatrix} K & & & & & \\ & K & & & & \\ & & K & & & \\ & & & K & & \\ & & & & K & \\ & & & & & \epsilon_0\bar{\epsilon}K \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M & & & & & \\ & M & & & & \\ & & M & & & \\ & & & M & & \\ & & & & M & \\ & & & & & 0 \end{bmatrix}$$

$$\mathcal{N}|_{\mathbf{u}_0} = \begin{bmatrix} N^1_{q1} & N^1_{q2} & N^1_{q3} & N^1_{q4} & N^1_{q5} & E^1_U \\ N^2_{q1} & N^2_{q2} & N^2_{q3} & N^2_{q4} & N^2_{q5} & E^2_U \\ N^3_{q1} & N^3_{q2} & N^3_{q3} & N^3_{q4} & N^3_{q5} & E^3_U \\ N^4_{q1} & N^4_{q2} & N^4_{q3} & N^4_{q4} & N^4_{q5} & E^4_U \\ N^5_{q1} & N^5_{q2} & N^5_{q3} & N^5_{q4} & N^5_{q5} & E^5_U \\ D_{q1} & D_{q2} & D_{q3} & D_{q4} & D_{q5} & D_U \end{bmatrix}$$

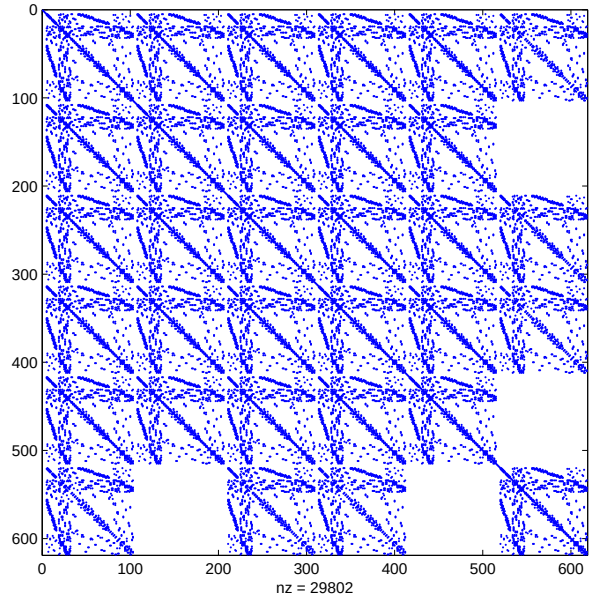
Saddle-point problem

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

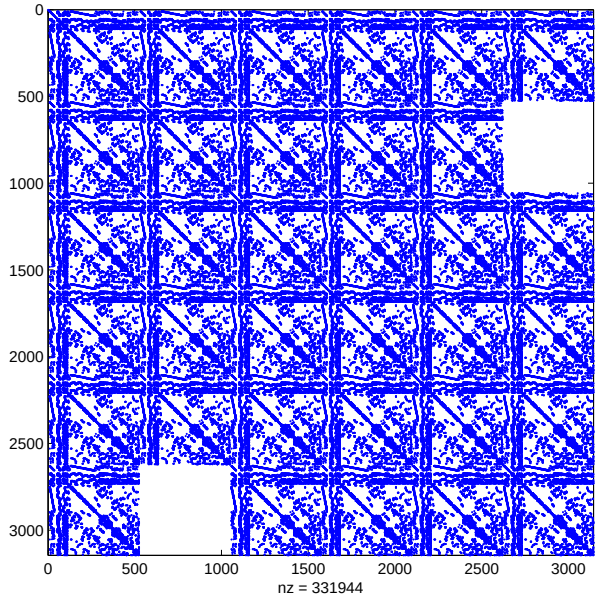
- A is $5n \times 5n$, B_1 is $5n \times n$, B_2 is $n \times 5n$
- nonsymmetric: A can be indefinite, C is positive definite



1D



2D



3D

GMRES Iterations

- 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

$$\mathcal{A} = \begin{bmatrix} A & B_1 \\ B_2 & C \end{bmatrix}, \qquad \mathcal{P} = \begin{bmatrix} \bar{A} & 0 \\ 0 & -\bar{S} \end{bmatrix}$$

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

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

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

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.
- Two 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.

Asymptotic Work Estimates

Iterative method: Conjugate Gradients

Direct method: Gaussian Elimination with band-minimising node ordering

Computational Work

	$d=2$	$d=3$
CG	$O(N^{\frac{3}{2}})$	$O(N^{\frac{4}{3}})$
GE factorise	$O(N^2)$	$O(N^{\frac{7}{3}})$
GE solve	$O(N^{\frac{3}{2}})$	$O(N^{\frac{5}{3}})$

Storage

	$d=2$	$d=3$
CG	$O(N)$	$O(N)$
GE factorise	$O(N^{\frac{3}{2}})$	$O(N^{\frac{5}{3}})$
GE solve	$O(N^{\frac{3}{2}})$	$O(N^{\frac{5}{3}})$

Krylov Subspace Iteration

Solve $A\mathbf{x} = \mathbf{b}$ where

- A is symmetric and positive definite
- A has s distinct (positive) eigenvalues

Minimal polynomial:

$$A^s + m_1 A^{s-1} + \cdots + m_{s-1} A + m_s I = 0$$

so

$$A^{-1} = -\frac{1}{m_s} A^{s-1} - \frac{m_1}{m_s} A^{s-2} - \cdots - \frac{m_{s-1}}{m_s} I$$

$$\hat{\mathbf{x}} = A^{-1}\mathbf{b} \in \mathcal{K}(A, \mathbf{b}, s) \equiv \text{span}\{\mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \ldots, A^{s-1}\mathbf{b}\}$$

Krylov Subspace

Three equivalent problems

1. solve $A\mathbf{x} = \mathbf{b}$

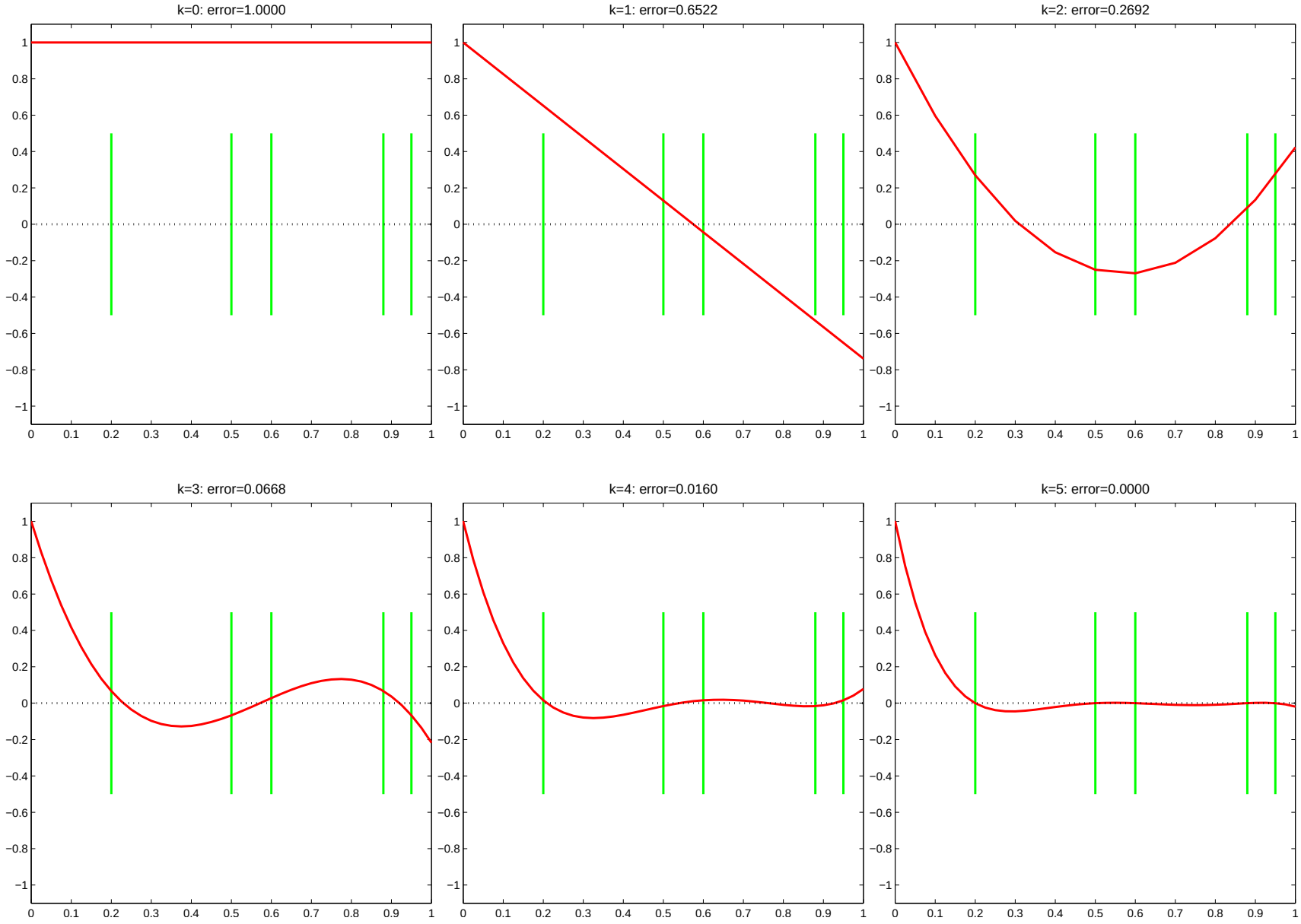
2. minimise $\Phi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T\mathbf{b}$

$$\nabla\Phi(\mathbf{x}) = A\mathbf{x} - \mathbf{b} = \mathbf{0}$$

3. minimise $\|\mathbf{x} - \hat{\mathbf{x}}\|_A$

$$\|\mathbf{v}\|_A = \left\{\mathbf{v}^T A\mathbf{v}\right\}^{\frac{1}{2}}$$

$$(\mathbf{x} - \hat{\mathbf{x}})^T A(\mathbf{x} - \hat{\mathbf{x}}) = \mathbf{b}^T A^{-1}\mathbf{b} + 2\Phi(\mathbf{x})$$


k=0: error=1.0000
k=1: error=0.6522
k=2: error=0.2692
k=3: error=0.0668
k=4: error=0.0160
k=5: error=0.0000

Nonsymmetric Systems

Faber and Manteuffel (1984 & 1987): there is no Krylov type method which retains both

(i) minimisation property

(ii) fixed length recurrence

- Normal Equations
  solve $A^T A\mathbf{x} = A^T\mathbf{b}$ using CG

- Minimum Residual Methods
  retain (i), sacrifice (ii)

- Biorthogonalisation Methods
  retain (ii), sacrifice (i)

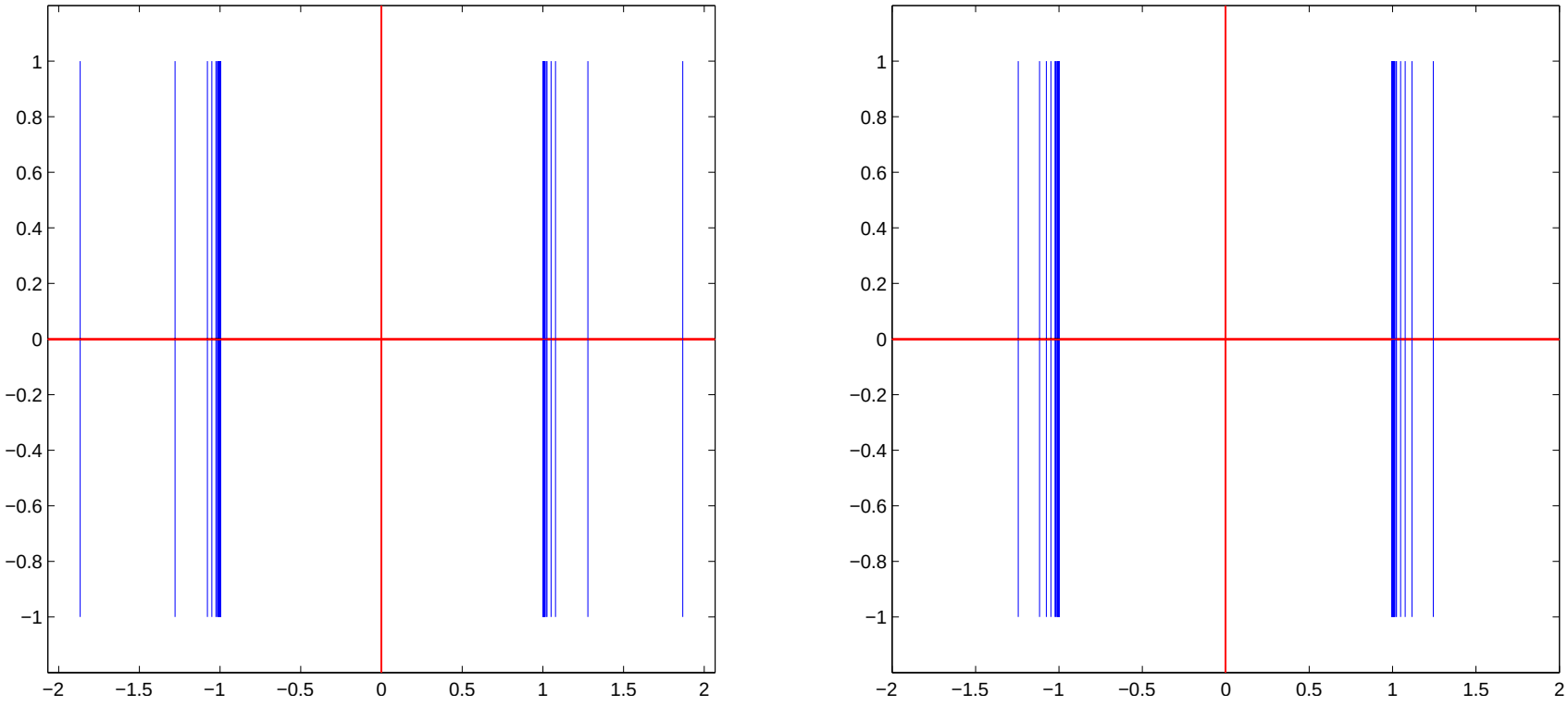
Matrix Conditioning

- 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
	$O(N^4)$	$O(N)$	$O(N^{-3})$	$O(N^{-1})$	$O(N)$

Sample Eigenvalue Plots



eigenvalue plots for $N = 64$, $V = 1.5$
first and last Newton iteration

Elastic Energy

- energy induced by distorting the $\mathbf{Q}$-tensor in space
- energetically favourable for $\mathbf{Q}$ to be constant
- gradients in $\mathbf{Q}$ lead to an increase in energy

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

- parameters L_1 and L_2 related to the Frank elastic constants

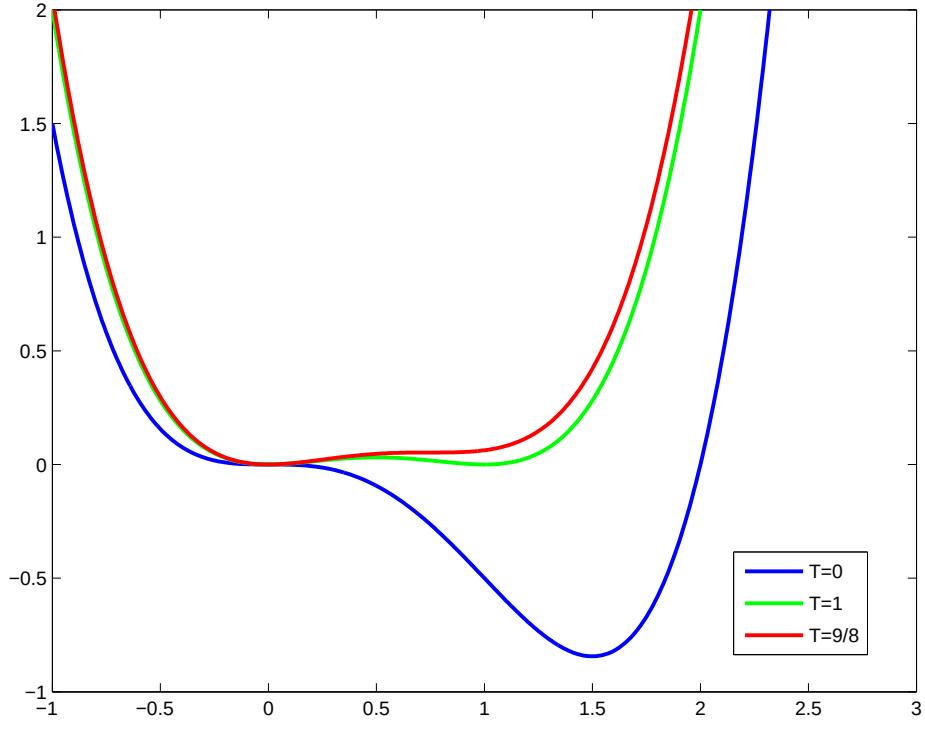
K_1	splay
K_2	twist
K_3	bend
$K_2 + K_4$	saddle-splay

Thermotropic Energy

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

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

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



Electrostatic energy

- applied electric field $\mathbf{E}$, electric potential U

$$\mathbf{E} = -\nabla U$$

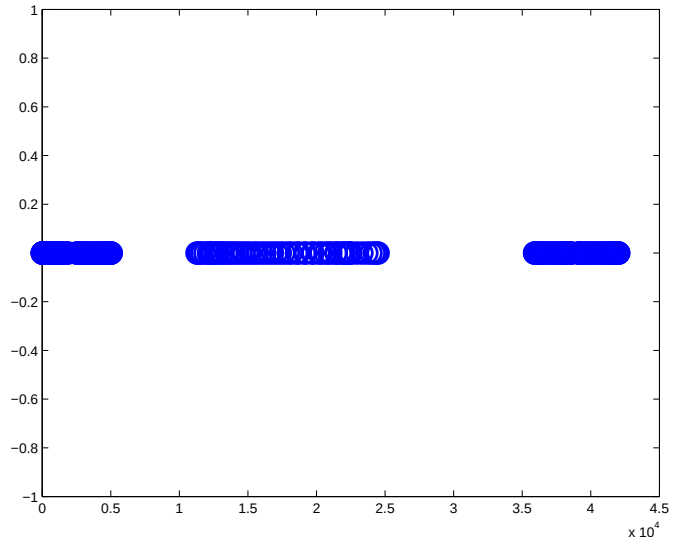
- electric displacement

$$\mathbf{D} = -\epsilon_0(\bar{\epsilon}\mathbf{I} + \Delta\epsilon^*\mathbf{Q})\nabla U$$

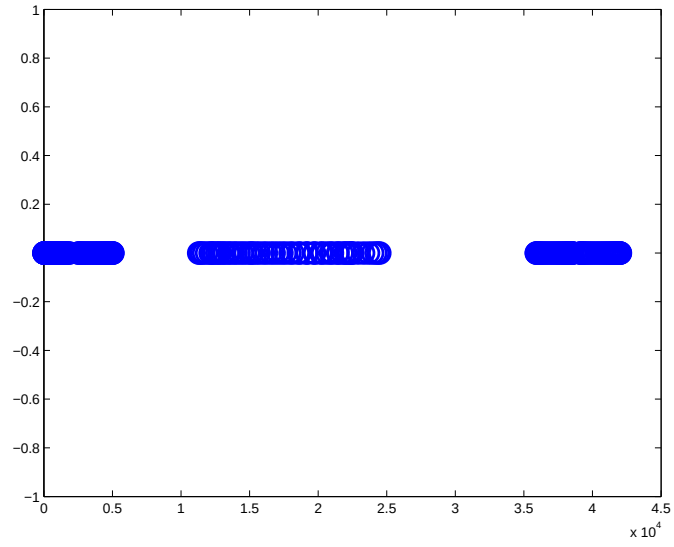
average permittivity $\bar{\epsilon}$, dielectric anisotropy $\Delta\epsilon^*$

$$F_{electrostatic} = -\frac{1}{2}\mathbf{D}\cdot\mathbf{E}$$

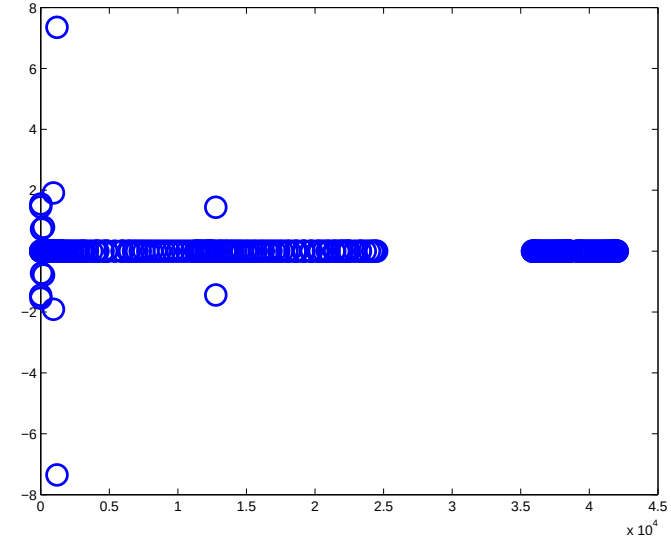
Eigenvalues



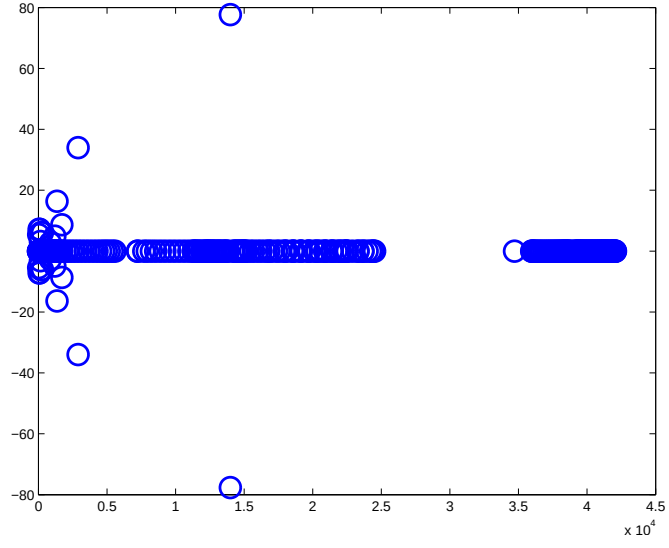
$V = 0$



$V = 0.5$

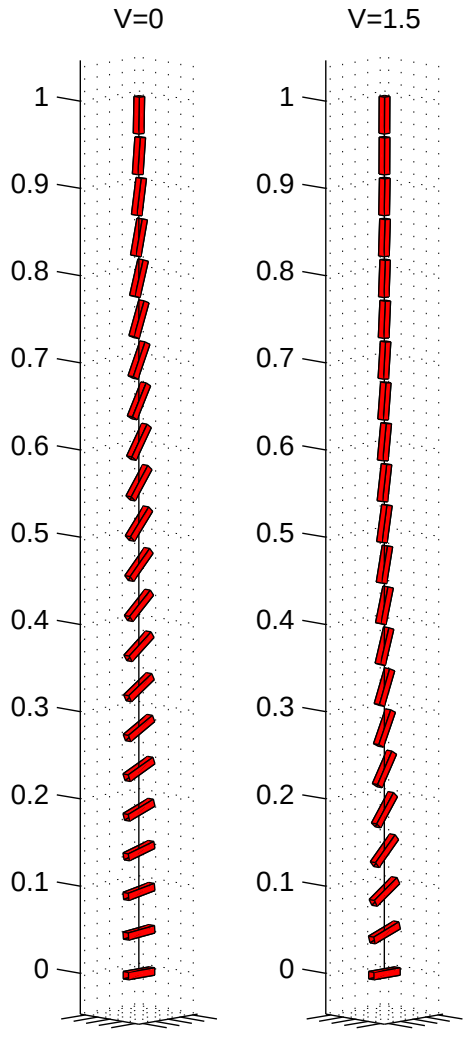


$V = 1.5$

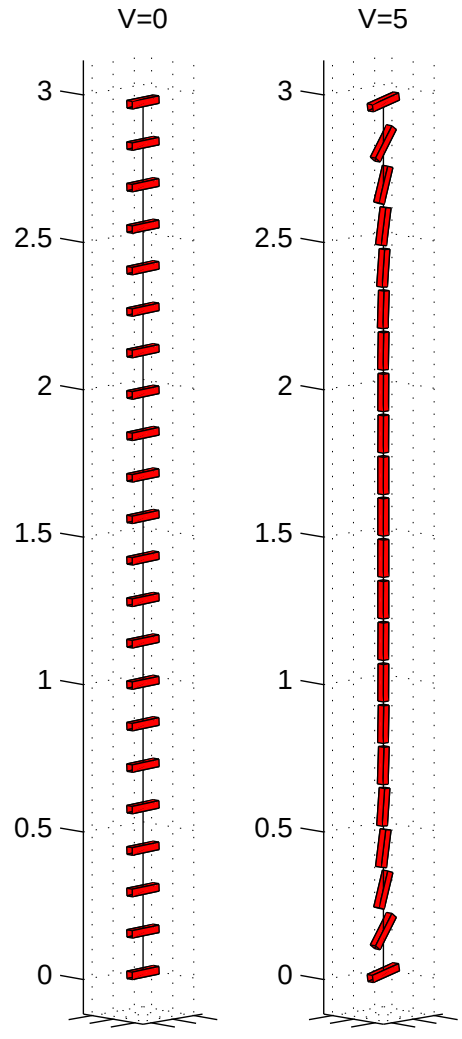


$V = 5$

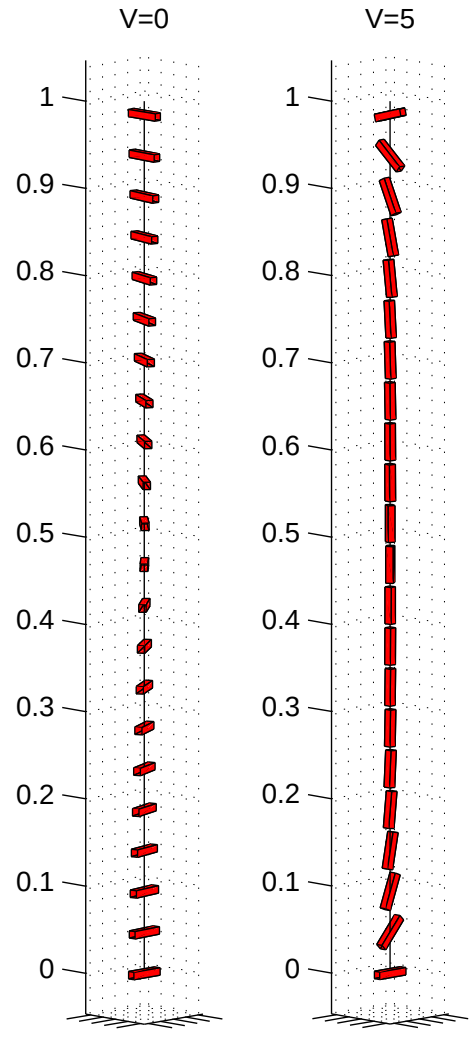
Liquid Crystal Problems



HAN cell



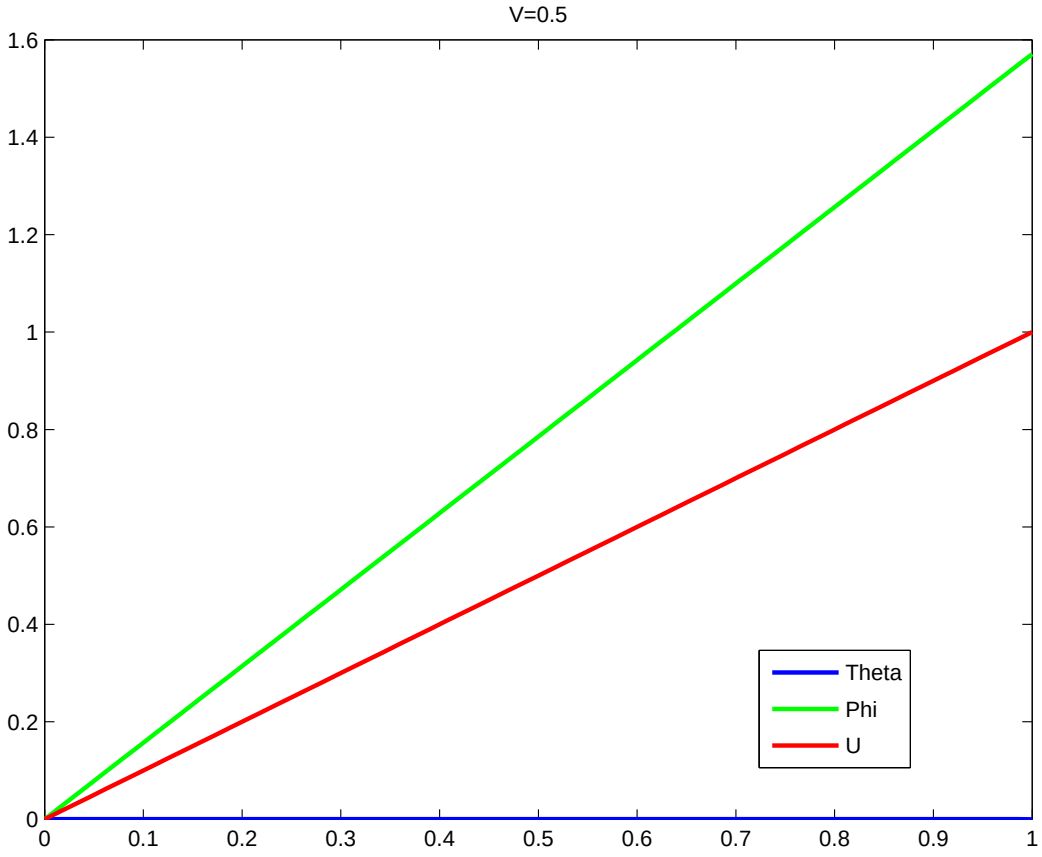
Pi cell

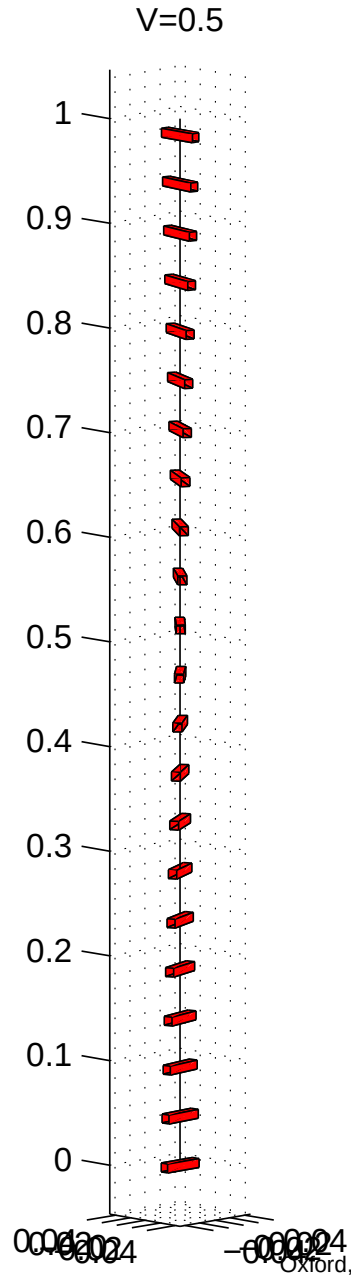


TND cell

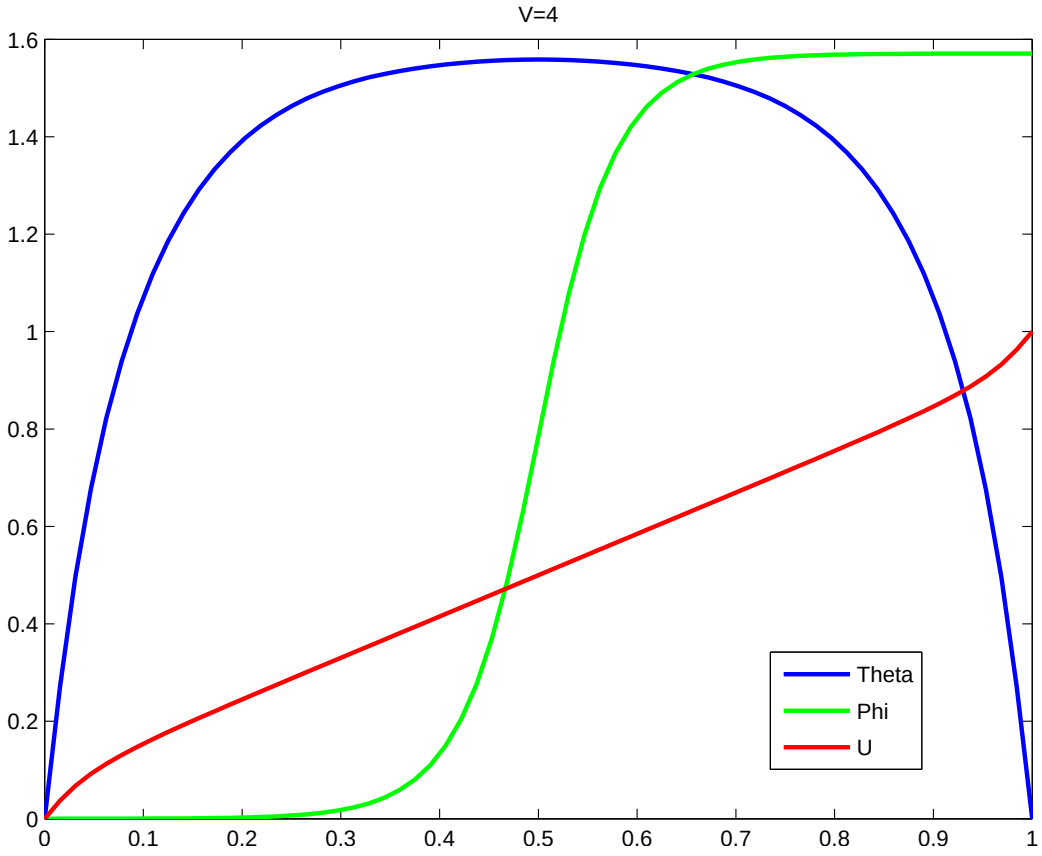
Off State

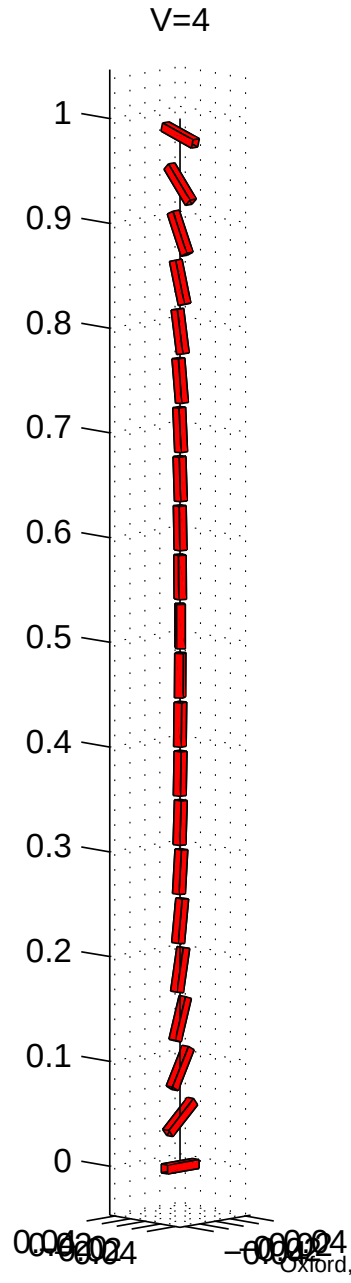
$$\theta(z) \equiv 0, \qquad \phi(z) = \frac{\pi}{2} z, \qquad U(z) = z$$





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

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