Preconditioned Newton-like solvers for liquid crystal director models

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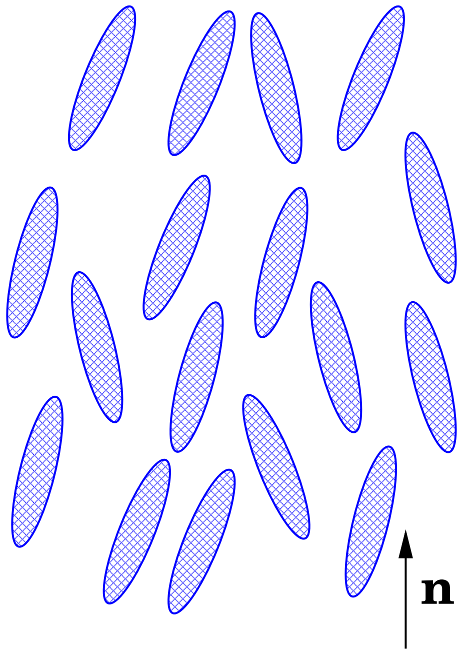
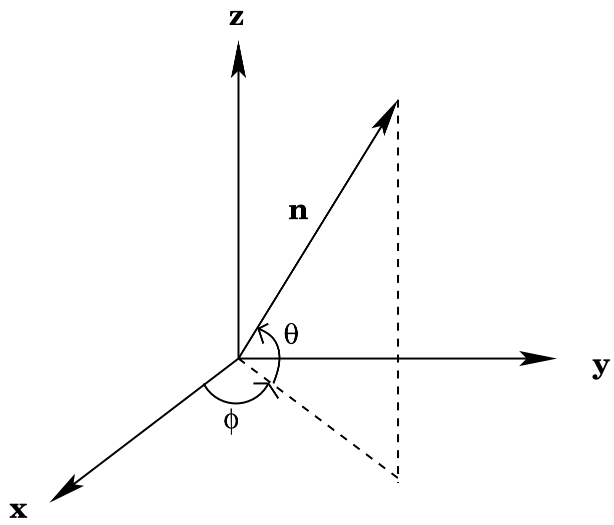
Modelling: Director-Based Models





- director: average direction of molecular alignment

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

- switch between stable states by altering applied voltage, magnetic field, boundary conditions, . . .

Free Energy

$$\mathcal{F}[\mathbf{n}, U] = \int_\Omega [W_e(\mathbf{n}, \nabla\mathbf{n}) - W_E(\mathbf{n}, \nabla U)]$$

- Distortional elastic energy:

$$W_e = \frac{1}{2}K|\nabla\mathbf{n}|^2 = \frac{1}{2}\sum_{i,j=1}^{3}\left(\frac{\partial n_i}{\partial x_j}\right)^2$$

Oseen-Frank model, equal elastic constants

- Electrostatic energy:

$$W_E = \frac{1}{2}\boldsymbol{\epsilon}(\mathbf{n})\nabla U \cdot \nabla U$$

dielectric tensor $\boldsymbol{\epsilon}$, electrostatic potential U

Finding Equilibrium Configurations

- Want equilibria with least free energy: find

$$\min_{|\mathbf{n}|=1} \max_{U} \mathcal{F}[\mathbf{n}, U]$$

- Lagrangian: $L(\mathbf{n}, \mathbf{U}, \boldsymbol{\lambda}) = f(\mathbf{n}, \mathbf{U}) + \sum_{j=1}^{n} \boldsymbol{\lambda}_j g_j(\mathbf{n})$

$$g_j(\mathbf{n}) := \frac{1}{2}(|\mathbf{n}_j|^2 - 1)$$

- Newton step:

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

$$A = \nabla^2_{\mathbf{nn}} L, \quad B = \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L, \quad C = -\nabla^2_{\mathbf{UU}} L, \quad D = \nabla^2_{\mathbf{nU}} L$$

Nullspace Method

- Required:
  - particular solution $\widehat{\boldsymbol{\delta}\mathbf{n}} = -B(B^TB)^{-1}\nabla_{\boldsymbol{\lambda}}L$
  - nullspace matrix Z such that $B^TZ = \mathcal{O}$

- Reduced system:

$$\begin{bmatrix} Z^TAZ & Z^TD \\ D^TZ & -C \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} Z^T(\nabla_{\mathbf{n}}L + A\widehat{\boldsymbol{\delta}\mathbf{n}}) \\ \nabla_{\mathbf{U}}L + D^T\widehat{\boldsymbol{\delta}\mathbf{n}} \end{bmatrix}$$

- Recover update:

$$\boldsymbol{\delta}\mathbf{n} = \widehat{\boldsymbol{\delta}\mathbf{n}} + Z\mathbf{p}, \qquad \boldsymbol{\delta\lambda} = -(B^TB)^{-1}B^T(\nabla_{\mathbf{n}}L + A\boldsymbol{\delta}\mathbf{n} + D\boldsymbol{\delta}\mathbf{U})$$

Constructing Z

$$B = \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L = [\nabla_{\mathbf{n}} g_1, \ldots, \nabla_{\mathbf{n}} g_n] = \begin{bmatrix} \mathbf{n}_1 & & \\ & \ddots & \\ & & \mathbf{n}_n \end{bmatrix}$$

- at each node, form an orthogonal triple $\mathbf{l}_j$, $\mathbf{m}_j$, $\mathbf{n}_j$
- nullspace matrix:

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

- $B^T Z = \mathcal{O}, \quad Z^T B = \mathcal{O}$
- $B^T B$ and $Z^T Z$ are diagonal and nonsingular

Geometric Interpretation

- Decomposition $\boldsymbol{\delta}\mathbf{n} = \widehat{\boldsymbol{\delta}\mathbf{n}} + Z\mathbf{p}$ has local components
  - parallel to $\mathbf{n}_j$:

$$(\widehat{\boldsymbol{\delta}\mathbf{n}})_j = \frac{1}{2}\left(\frac{1 - |\mathbf{n}_j|}{|\mathbf{n}_j|^2}\right)\mathbf{n}_j, \qquad j = 1, \ldots, n.$$

  - perpendicular to $\mathbf{n}_j$:

$$(Zp)_j = p_j \mathbf{l}_j + \mathbf{q}_j \mathbf{m}_j, \qquad \mathbf{p} = [p_1, q_1, \ldots, p_n, q_n]^T.$$

- New local directors satisfy $|\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j| \geq 1$.
- Successive Newton iterates generally exceed the pointwise unit-vector normalization, approaching it in the limit as the Newton iteration converges.

Renormalised Newton

- Set $\boldsymbol{\lambda} = -B^T \nabla_{\mathbf{n}} f$.
- Solve

$$\begin{bmatrix} Z^T A Z & Z^T D \\ D^T Z & -C \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} Z^T \nabla_{\mathbf{n}} f \\ \nabla_{\mathbf{U}} f \end{bmatrix}.$$

- Update and normalise:

$$\delta \mathbf{n} = Z\mathbf{p}, \qquad \mathbf{n}_{ij} = \frac{\mathbf{n}_{ij} + \boldsymbol{\delta}\mathbf{n}_{ij}}{|\mathbf{n}_{ij} + \boldsymbol{\delta}\mathbf{n}_{ij}|}$$

- $B^T B$ and $Z^T Z$ are identity matrices
- Locally quadratic convergence.

2D Model Problem

- Equal-elastic constant free energy functional with no field on unit square - Harmonic Mapping problem

$$\min_{|\mathbf{n}|=1} \mathcal{F}[\mathbf{n}]$$

$$\mathcal{F}[\mathbf{n}] = \frac{1}{2}\int_\Omega |\nabla \mathbf{n}|^2 d\Omega = \frac{1}{2}\int_\Omega [|\nabla u|^2 + |\nabla v|^2 + |\nabla w|^2] d\Omega$$

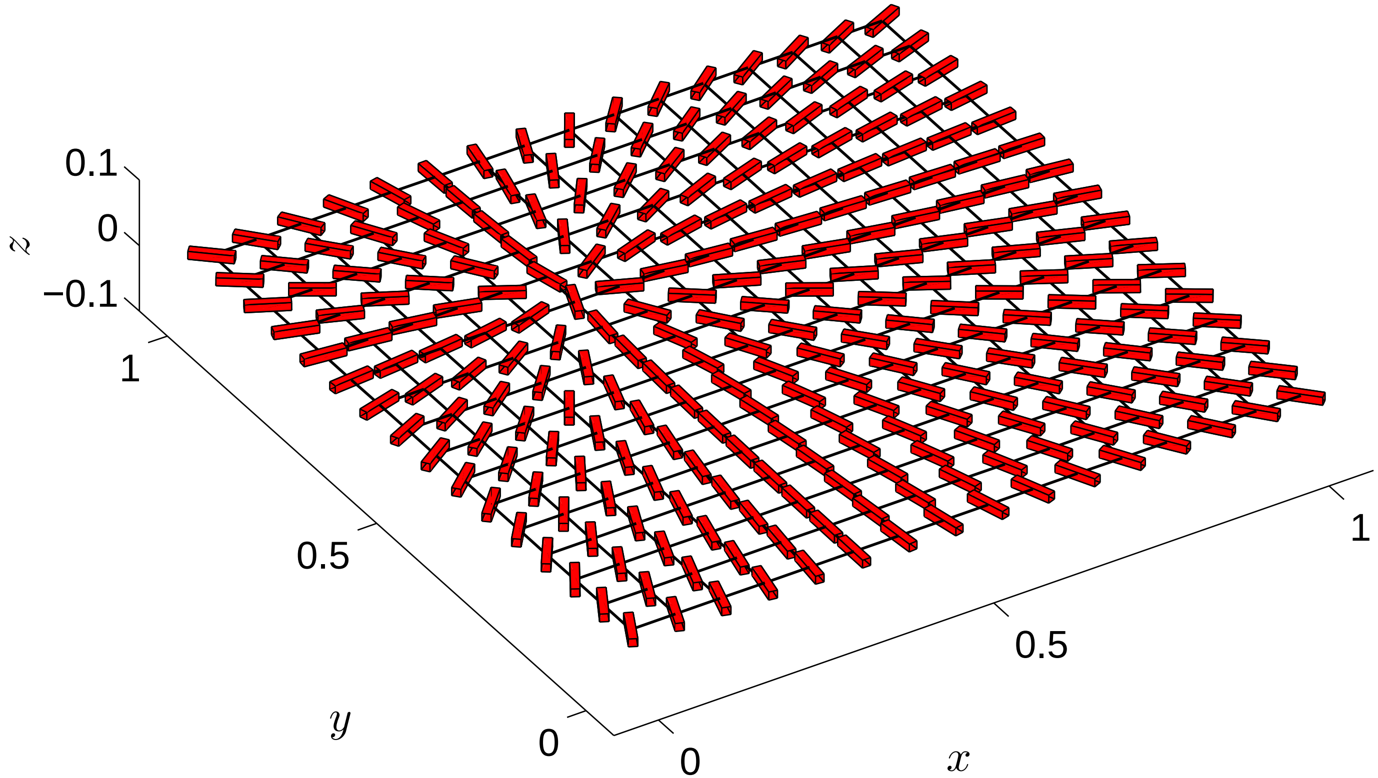
$$\mathbf{n} = u(x,y)\mathbf{e}_x + v(x,y)\mathbf{e}_y + w(x,y)\mathbf{e}_z$$

- Boundary conditions for a line disclination.

$$\mathbf{n} = \mathbf{n}_b \text{ on } \partial\Omega, \qquad \mathbf{n}_b = \frac{(x-x_d)\mathbf{e}_x + (y-y_d)\mathbf{e}_y}{\sqrt{(x-x_d)^2 + (y-y_d)^2}}$$

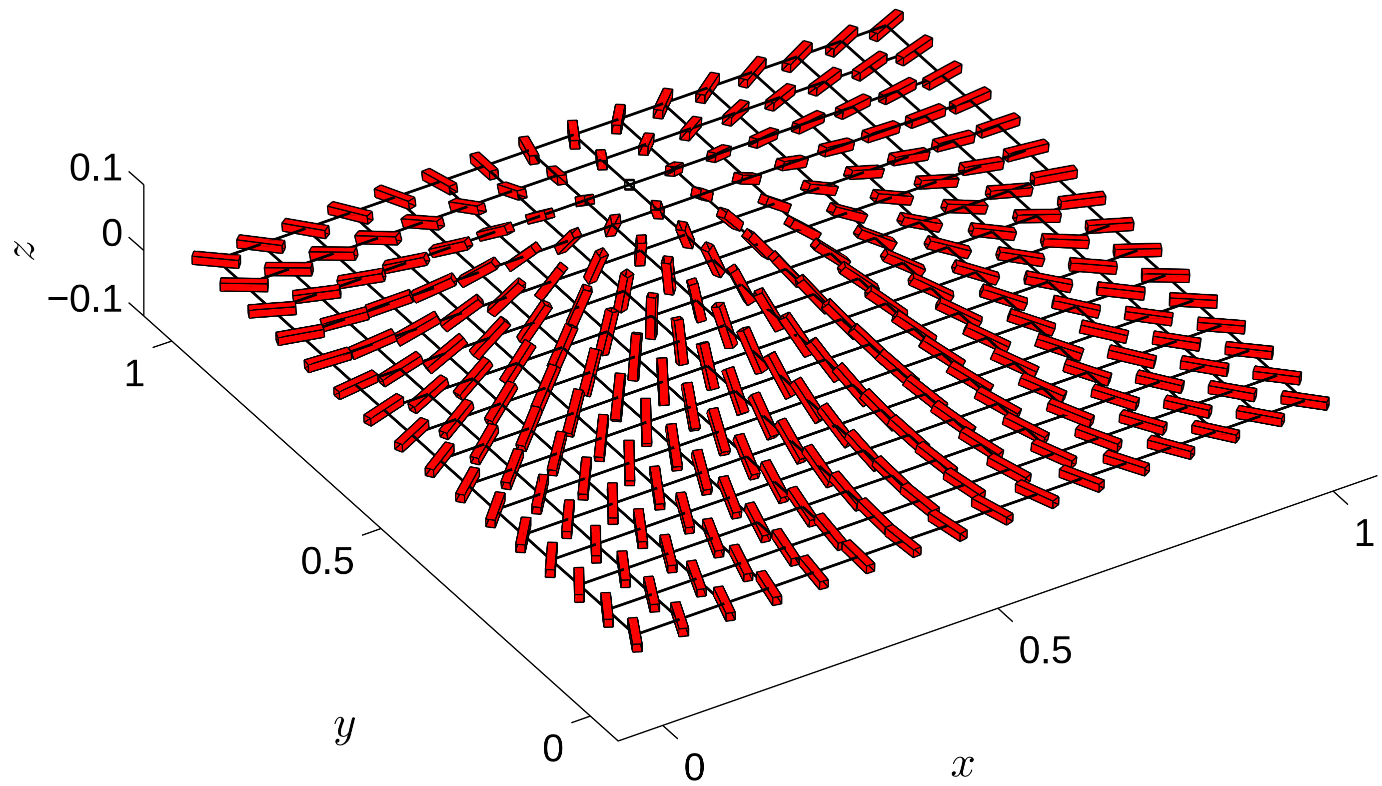
$$(x_d, y_d) = (1/3, 2/3)$$

Equilibrium Director Fields



- Locally unstable planar solution
- Singularity: disclination line

Equilibrium Director Fields



- Locally stable upward “escape” solution
- Locally stable downwards “escape” solution

Nonlinear Iteration

- Full Newton:

$$\begin{bmatrix} A & B \\ B^T & \mathcal{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{\delta}\mathbf{n} \\ \boldsymbol{\delta\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla_{\mathbf{n}} L \\ \nabla_{\boldsymbol{\lambda}} L \end{bmatrix}, \qquad A = A_0 + \boldsymbol{\Lambda}(\boldsymbol{\lambda})$$

$$\mathbf{n} \leftarrow \mathbf{n} + \boldsymbol{\delta}\mathbf{n}, \quad \boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \boldsymbol{\delta\lambda}$$

- Renormalised Newton:

$$\boldsymbol{\lambda} = -B^T \nabla_{\mathbf{n}} f$$

$$Z^T A Z \mathbf{p} = -Z^T \nabla_{\mathbf{n}} f, \quad \boldsymbol{\delta}\mathbf{n} = Z\mathbf{p}$$

$$\mathbf{n}_{ij} \leftarrow \frac{\mathbf{n}_{ij} + \boldsymbol{\delta}\mathbf{n}_{ij}}{|\mathbf{n}_{ij} + \boldsymbol{\delta}\mathbf{n}_{ij}|}$$

Iteration Counts

n	defect solution		defect-free solution	
	Newton iterations	RN iterations	Newton iterations	RN iterations
4	16	—	7	6
8	7	7	7	6
16	—	8	7	6
32	—	11	12	7
64	11	9	—	7
128	10	9	11	8
256	8	9	9	8
512	9	9	9	8

Typical computing times

- defect-free solution
- Matlab direct solver

		Newton		Renormalized	
n	N	size	time	size	time
4	9	36	3.50(-3)	18	3.00(-3)
8	49	196	5.50(-3)	98	5.00(-3)
16	225	900	1.64(-2)	450	1.24(-2)
32	961	3,844	6.73(-2)	1,922	4.42(-2)
64	3,969	15,876	4.52(-1)	7,938	2.33(-1)
128	16,129	64,516	2.71$(+0)$	32,258	1.21$(+0)$
256	65,025	260,100	1.83$(+1)$	130,050	6.71$(+0)$
512	261,121	1,044,484	1.66$(+2)$	522,242	3.55$(+1)$

Condition numbers

$$M_1 = \begin{bmatrix} A & B \\ B^T & \mathcal{O} \end{bmatrix}, \qquad M_2 = Z^T A Z$$

n	defect solution		defect-free solution	
	$\mathrm{cond}(M_1)$	$\mathrm{cond}(M_2)$	$\mathrm{cond}(M_1)$	$\mathrm{cond}(M_2)$
4	7.07(+01)	1.79(+01)	8.66(+01)	2.21(+01)
8	1.68(+02)	5.57(+01)	1.30(+02)	8.93(+01)
16	3.01(+02)	2.55(+02)	4.55(+02)	3.47(+02)
32	1.57(+03)	1.22(+03)	1.71(+03)	1.39(+03)
64	3.79(+04)	3.37(+04)	6.77(+03)	5.72(+03)
128	2.13(+04)	1.89(+04)	2.70(+04)	1.89(+04)
256	7.90(+04)	7.02(+04)	1.08(+05)	8.81(+04)
512	3.56(+05)	3.17(+05)	4.31(+05)	3.52(+05)

Minres Iteration Counts

- Newton: standard Newton with full matrix M_1
- Nullspace: standard Newton with reduced matrix M_2
- RN: renormalised Newton with reduced matrix M_2

	defect solution			defect-free solution		
n	Newton	nullspace	RN	Newton	nullspace	RN
4	28.7	13.3	-	27.2	13.0	10.9
8	102.7	26.0	26.1	96.1	30.2	28.2
16	-	-	54.4	230.8	59.3	56.6
32	-	-	111.9	489.0	129.2	109.9
64	1100.5	245.1	238.8	-	-	211.4
128	2039.6	446.1	424.9	2093.5	464.9	410.7

- average MINRES iterations per Newton step

Preconditioning

- *Nash and Sofer, SIMAX 17, 1996*: try

$$M_2 = Z^T A Z, \qquad P_2^{-1} = Z^T P^{-1} Z$$

$$P^{-1} A \simeq I$$

- Here $\quad A = A_0 + \Lambda(\boldsymbol{\lambda}), \quad A_0 = \nabla^2_{\mathbf{nn}} f$

$$\Lambda = \begin{bmatrix} \Lambda_1 & & \\ & \ddots & \\ & & \Lambda_n \end{bmatrix}, \quad \Lambda_j = \begin{bmatrix} \lambda_j & & \\ & \lambda_j & \\ & & \lambda_j \end{bmatrix}$$

- A_0 is symmetric and positive definite.

Preconditioners Based On A_0

n	$P^{-1} = A_0^{-1}$ nullspace	$P^{-1} = A_0^{-1}$ RN	$P^{-1} \equiv$ AMG solve nullspace	$P^{-1} \equiv$ AMG solve RN
4	9.0	8.1	8.9	8.1
8	9.3	7.7	9.5	7.6
16	10.8	7.9	11.0	7.9
32	24.4	8.2	34.3	8.3
64	-	8.2	-	8.6
128	24.9	7.9	30.5	8.1

- average MINRES iterations per Newton step
- 3 PCG iterations with an AMG preconditioner (HSL_MI20)

Summary: Nonlinear Iteration

- Because of the ease of constructing B and Z, reduced Hessian methods are very effective here.
- The Renormalized Newton scheme has smaller system size, less time per iteration, fewer iterations required, and more robust (quadratic) convergence.
- The resulting structure can be further exploited in terms of preconditioning.
- The ideas here are not tied to a particular problem or discretisation, and extend to 3D.
- The techniques should be useful in a variety of settings in which such constraints appear, including computational micromagnetics (cf. the Truncated Newton method).

What's next?

- For more complicated physical problems, reduced coefficient matrix is

$$\begin{bmatrix} Z^T A Z & Z^T D \\ D^T Z & -C \end{bmatrix}$$

- Block diagonal preconditioners (analysed for 1D problems in *Ramage and Gartland, Jr, SISC 35, 2013*) should be effective.

- Good preconditioners for $Z^T A Z$ still needed: renormalisation should help.