Augmented Lagrangian Preconditioners for Oseen–Frank models in cholesteric liquid crystals

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1. Introduction

Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ be an open, bounded domain with Lipschitz boundary $\partial\Omega$. Denote K_1, K_2, K_3, q_0 as the splay, twist, bend constants and the preferred pitch for cholesteric liquid crystals (LC), respectively.

① Oseen–Frank models (seek the **director** $\mathbf{n} \in \mathbb{R}^d$):

$$\min_{\mathbf{n}\in\mathbf{H}^1(\Omega)} \quad J(\mathbf{n}) = \int_\Omega \frac{K_1}{2}|\nabla\cdot\mathbf{n}|^2 + \frac{K_2}{2}|\mathbf{n}\cdot(\nabla\times\mathbf{n}) + q_0|^2 + \frac{K_3}{2}|\mathbf{n}\times(\nabla\times\mathbf{n})|^2 \mathrm{d}x,$$

subject to $\mathbf{n}\cdot\mathbf{n} = 1$ a.e. in Ω and $\mathbf{n} = \mathbf{g} \in H^{1/2}(\partial\Omega)$ on $\partial\Omega$.

② The augmented problem using Augmented Lagrangian methods (AL):

$$\mathcal{L}(\mathbf{n}, \lambda) = J(\mathbf{n}) + \langle\lambda, n\cdot n - 1\rangle_0 + \frac{\gamma}{2}\langle\mathbf{n}\cdot\mathbf{n} - 1, \mathbf{n}\cdot\mathbf{n} - 1\rangle_0.$$

③ The matrix form of the k-th Newton iteration (by Newton linearization + discretization):

$$\mathcal{A}\begin{bmatrix}u\\p\end{bmatrix} := \begin{bmatrix}A+\gamma B_* & B^T\\ B & 0\end{bmatrix}\begin{bmatrix}u\\p\end{bmatrix} = \begin{bmatrix}f\\g\end{bmatrix},$$

where $(u, p) \in V_h \times W_h \subset \mathbf{H}_0^1(\Omega) \times L^2(\Omega)$ and

$$B_* \sim 4\langle\mathbf{n}_k\cdot\delta\mathbf{n}, \mathbf{n}_k\cdot\delta\lambda\rangle_0 + 2\langle\mathbf{n}_k\cdot\mathbf{n}_k - 1, \delta\mathbf{n}\cdot\delta\lambda\rangle_0.$$

④ Schur complement reduction:

$$\mathcal{A} \Rightarrow \begin{bmatrix}A+\gamma B_* & B^T\\ 0 & S\end{bmatrix},$$

with the Schur complement $S = -B(A+\gamma B_*)^{-1}B^T =: -BA_\gamma^{-1}B^T$.

Our **GOAL** is to design a preconditioner $\mathcal{P}^{-1} = \begin{bmatrix}I & -\tilde{A}_\gamma^{-1}B^T\\ 0 & I\end{bmatrix}\begin{bmatrix}\tilde{A}_\gamma^{-1} & 0\\ 0 & \tilde{S}^{-1}\end{bmatrix}\begin{bmatrix}I & 0\\ -B\tilde{A}_\gamma^{-1} & I\end{bmatrix} \approx \mathcal{A}^{-1}$.

2. Methods

Treat $\tilde{S}^{-1}$: Schur complement approximation

- Motivated by [2], we first have
$$S^{-1} \approx \hat{S}^{-1} = -(BA^{-1}B^T)^{-1} - \gamma M_\lambda^{-1}.$$
- To approximate the $BA^{-1}B^T$ part, we now prove:

Theorem: For equal-constant ($K = K_1 = K_2 = K_3$) nematic ($q_0 = 0$) LC problems, the Schur complement matrix $BA^{-1}B^T$ arising from the Newton-linearized system is spectrally equivalent to the Lagrange multiplier mass matrix M_λ.

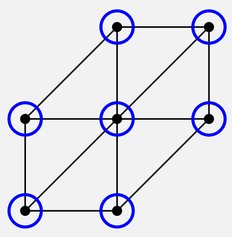
- Thus, our approximation to S^{-1} is
$$\tilde{S}^{-1} = -(1+\gamma)M_\lambda^{-1}.$$

Treat $\tilde{A}_\gamma^{-1}$: Robust multigrid methods

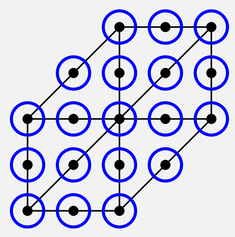
- Kernel-capturing condition [3] (for the decomposition $V_h = \sum_{i=1}^M V_i$):
$$\mathcal{N}_h = \sum_{i=1}^M (V_i \cap \mathcal{N}_h). \tag{1}$$

Here, the kernel is $\mathcal{N}_h = \{\mathbf{u}_h \in V_h : \mathbf{n}_k\cdot\mathbf{u}_h = 0 \text{ a.e.}\}$.

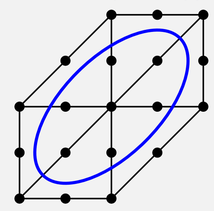
Examples of relaxation satisfying (1) (black dots represent degrees of freedom (dofs)):



(Point-block patch in $\mathbb{P}_1$)



(Point-block patch in $\mathbb{P}_2$)



(Star patch in $\mathbb{P}_2$)

We denote the solver by **ALMG-PBJ** when choosing the point-block patch relaxation in the multigrid (MG) algorithm.

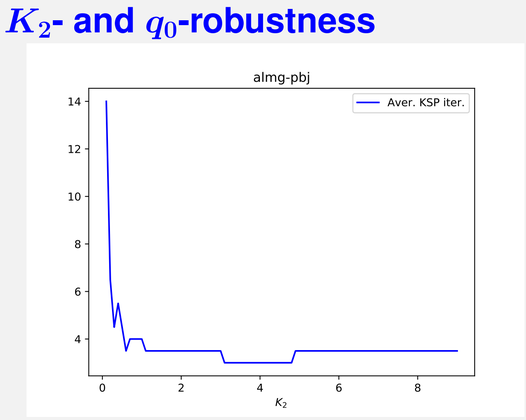
3.1 Result 1: Parameter robustness

- **γ- and h-robustness**

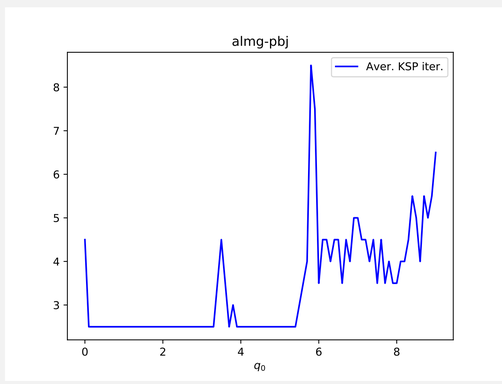
		γ			
#refs	#dofs	10^4	10^5	10^6	10^7
1	19,933	4.00(4)	3.75(4)	3.25(4)	3.25(4)
2	78,810	4.80(5)	3.75(4)	3.25(4)	3.25(4)
3	313,408	9.40(5)	3.60(5)	3.25(4)	3.25(4)
4	1,249,980	18.00(5)	6.00(5)	3.50(4)	3.00(4)
5	4,992,628	32.80(5)	11.20(5)	4.75(4)	3.00(4)
6	19,955,940	58.60(5)	21.40(5)	7.60(5)	3.50(4)

Table 1: The average number of linear iterations (the number of nonlinear iterations).

- **K_2- and q_0-robustness**



(K_2-continuation)



(q_0-continuation)

Figure 1: Plot of the average number of linear iterations w.r.t. K_2 and q_0 with step size 0.1.

3.2 Result 2: Efficiency

ALMG-PBJ is about three times faster than MGVanka [1].

Runtime (in minutes) of ALMG-PBJ vs. MGVanka						
#refs	1	2	3	4	5	6
#dofs	19,933	78,810	313,408	1,249,980	4,992,268	19,955,940
MGVanka	0.02	0.05	0.15	0.61	2.30	10.98
ALMG-PBJ	0.02	0.03	0.05	0.14	0.56	3.72

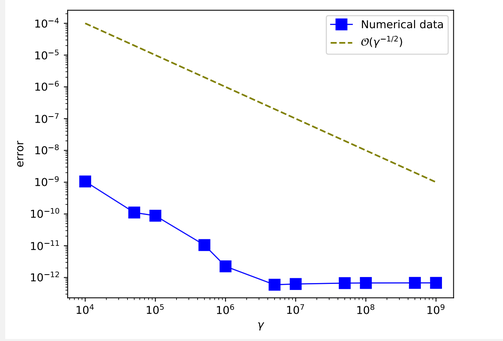
3.3 Result 3: Improvement of constraints

We can show

$$\|\mathbf{n}_h\cdot\mathbf{n}_h - 1\|_0 \le \mathcal{O}(\gamma^{-1/2}),$$

by assuming that

- $\mathbb{P}_1$-$\mathbb{P}_1$ finite element pair is used;
- the Dirichlet boundary data g is constant.



Remarks: Our test model in this poster is the cholesteric LC model in an ellipse, see [1]; for further details about this poster, see [4].

4. Conclusions

- Our proposed AL-based preconditioner is robust and efficient.
  - ▷ AL can not only help control the Schur complement, but also improve the discrete constraint as $\gamma \to \infty$.
  - ▷ Multigrid algorithms with patchwise (star or point-block) relaxations solve the top-left block robustly.

5. References

[1] D. B. Emerson, P. E. Farrell, J. H. Adler, S. P. MacLachlan and T. J. Atherton, *Computing equilibrium states of cholesteric liquid crystals in elliptical channels with deflation algorithms*, Liquid Crystals, 45(3), 2018, 341-350.

[2] P. E. Farrell, L. Mitchell and F. Wechsung, *An augmented Lagrangian preconditioner for the 3D stationary incompressible Navier–Stokes equations at high Reynolds number*, SIAM Journal on Scientific Computing, 41(5), 2019, A3073–A3096.

[3] J. Schöberl, *Multigrid methods for a parameter dependent problem in primal variables*, Numerische Mathematik, 84(1), 1999, 97-119.

[4] J. Xia, P. E. Farrell and F. Wechsung. *Augmented Lagrangian preconditioners for Oseen–Frank models in cholesteric liquid crystals*, in preparation.

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