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Analysis and approximation of the nematic Helmholtz–Korteweg equation

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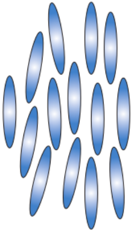
Introduction

- Goal: describe time-harmonic acoustic wave propagation in a nematic liquid crystal
- Korteweg-fluid: $\underline{\underline{\sigma}} = p\underline{\underline{I}} - u_1\rho(\nabla\rho \otimes \nabla\rho)$
- nematic LC can be considered as a Korteweg-fluid:

$$\underline{\underline{\sigma}} = p\underline{\underline{I}} - u_1\rho(\nabla\rho \otimes \nabla\rho) - u_2(\nabla\rho \cdot \boldsymbol{n})\nabla\rho \otimes \boldsymbol{n}$$

→ time harmonic acoustic waves described by the nematic Helmholtz–Korteweg equations!

→ how does the alignment of the nematic field influence the propagation of the acoustic wave?



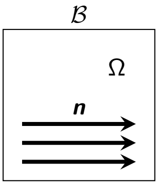
W. Wang, L. Zhang, P. Zhang, *Modelling and computation of liquid crystals.* Acta Numerica, 2021.

Nematic Helmholtz–Korteweg equation[1]

Given $f \in L^2(\Omega)$, find $u : \Omega \to \mathbb{C}$ s.t.

$$\begin{aligned} \alpha\Delta^2 u + \beta\nabla\cdot\nabla(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}) - \Delta u - k^2 u &= f && \text{in } \Omega, \\ \mathcal{B}u &= (0,0) && \text{on } \partial\Omega. \end{aligned}$$

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, bounded Lipschitz domain;
- α, β : constitution parameters;
- $\mathcal{H}$: Hessian;
- $\boldsymbol{n}$: orientation of the nematic field ($\|\boldsymbol{n}\| = 1$);
- $k = \omega/c$: (classic) wave-number;
- $\mathcal{B}$: encodes the boundary conditions;



[1] P.E. Farrell, U. Zerbinati, *Time-harmonic waves in Korteweg and nematic-Korteweg fluids.* arXiv, 2024.

Boundary conditions[2]

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→ 4th-order PDE, so we need two boundary conditions

1. *sound soft:*

$$\mathcal{B}u := \left(u, \Delta u + \frac{\beta}{\alpha}\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}\right)$$

2. *sound hard:*

$$\mathcal{B}u := \left(\partial_{\nu}u, \partial_{\nu}\Delta u + \frac{\beta}{\alpha}\partial_{\nu}(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n})\right)$$

3. *impedance:*

$$\mathcal{B}u := \left(\partial_{\nu}u - i\theta u, \partial_{\nu}\Delta u - i\theta(\frac{\beta}{\alpha}\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n} - \frac{\beta}{\alpha}\partial_{\nu}(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}))\right)$$

→ our analysis covers all cases!

[2] P.E. Farrell, U. Zerbinati, *Time-harmonic waves in Korteweg and nematic-Korteweg fluids.* arXiv, 2024.

Abstract framework

Well-posedness

Let X be a Hilbert space, $a : X \times X \to \mathbb{C}$ be a bounded sesquilinear form & $A \in L(X, X')$ be the associated operator: $\langle Au, v\rangle_{X',X} = a(u, v)\ \forall u, v \in X$.

➔ find $u \in X$ s.t. $Au = f$ in X' is well-posed

$\Leftrightarrow$ A is a bounded isomorphism

$\Leftrightarrow$ A is injective & $\mathrm{ran}(A)$ is closed & A^* injective

$\Leftrightarrow$ $\exists \alpha > 0$ s.t. $\|Au\|_{X'} \geq \alpha \|u\|_X$ for all $u \in X$ & A^* injective

$$\Leftrightarrow \underbrace{\inf_{u\in X} \sup_{v\in X} \frac{|\langle Au, v\rangle_{X',X}|}{\|u\|_X \|v\|_X} \geq \alpha > 0}_{\text{inf-sup condition}^3} \text{ \& } A^* \text{ injective}$$

Theorem (Lax-Milgram)

A is coercive, i.e. $\exists \alpha > 0$ s.t. $\Re\{\langle Au, u\rangle_{X',X}\} \geq \|u\|_X^2 \Rightarrow A$ is a bounded isomorphism

[3] F. Brezzi, *On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers.*, R.A.I.R.O., 1974.

T-coercivity

Simple observation: A bijective $\Leftrightarrow \exists\, T$ bijective s.t. AT is coercive

Definition (T-coercivity[4])

We call $A \in L(X, X')$ *T-coercive* if there exists a bijective operator $T \in L(X)$ s.t. $AT \in L(X, X')$ is coercive, i.e.

$$\Re\{\langle ATu, u\rangle_{X',X}\} \geq \alpha \|u\|_X^2$$

- → T-coercivity equivalent to well-posedness (necessary & sufficient)
- → recover coercivity with $T = \mathrm{Id}$
- → not directly inherited to the discrete level

[4] e.g. P. Ciarlet Jr., *T-coercivity: Application to the discretization of Helmholtz-like problems*. CAMWA, 2012.

Construction of T – Example

For given $k \gg 0$, $f \in L^2(\Omega)$, find $u \in X$ s.t.

$$a(u,v) := e(u,v) - k^2(u,v)_{L^2(\Omega)} = (f,v)_{L^2(\Omega)} \quad \forall v \in X, \tag{P}$$

- ➔ $\{\lambda^{(i)}, e^{(i)}\}_{i\in\mathbb{N}}$ eigenpairs associated with $e(\cdot,\cdot)$, $i_* \in \mathbb{N}$ s.t. $\lambda^{(i_*)} < k^2 < \lambda^{(i_*+1)}$
- ➔ construct $T \in L(X)$ bijective, s.t.

$$Te^{(i)} = \begin{cases} -e^{(i)} & \text{if } i \leq i_*; \\ +e^{(i)} & \text{if } i > i_*. \end{cases}$$

- ➔ can show coercivity of $a(T\cdot,\cdot)$ since

$$a(Te^{(i)}, e^{(i)}) = \begin{cases} k^2 - \lambda^{(i)} & \text{if } i \leq i_* \\ \lambda^{(i)} - k^2 & \text{if } i > i_* \end{cases} > 0.$$

- ➔ what about boundary terms?

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Definition (Compact operator)

We call an operator $K \in L(X, Y)$ *compact* if $\forall$ bounded $(u_n)_{n\in\mathbb{N}} \subset X$, the sequence $(Ku_n)_{n\in\mathbb{N}} \subset Y$ has a convergent subsequence.

Definition (Weak T-coercivity[5])

$A \in L(X, X')$ is called *weakly T-coercive* if there $\exists$ $T \in L(X)$ bijective, $K \in L(X, X')$ compact s.t. $AT + K$ is coercive.

- ➔ i.e. $AT =$ bij. $+$ comp., so AT is Fredholm with index zero!
- ➔ if A is weakly T-coercive and injective, then A is bijective

[5] see e.g., M. Halla, *Galerkin approximation of holomorphic eigenvalue problems: weak T-coercivity and T-compatibility.* Numerische Mathematik, 2021.

→ (weak) T-coercivity not inherited to the discrete level!

Definition (Uniform T$_h$-coercivity)

Let $\{X_h\}_h \subset X$ be a seq. of discrete spaces. We call A uniformly T$_h$-coercive on $\{X_h\}_h$ if there exists a family of bijective operators $\{T_h\}_h$, $T_h \in L(X_h)$ and α_* independent of h s.t.

$$\Re\{(AT_h u_h, u_h)_{X_h}\} \geq \alpha_* \|u_h\|_X^2,$$

Theorem

Let $A \in L(X)$ be injective and $A = B + K$, where $B \in L(X)$ is bijective and $K \in L(X)$ compact. If B is uniformly T_h-coercive on $\{X_h\}_h \subset X$, then there exists $h_0 > 0$ s.t. A is uniformly T_h-coercive on $\{X_h\}_h$ for $h \leq h_0$.

Continuous problem

Weak formulation

We want to find $u \in X$ s.t.

$$a(u,v) = (f,v)_{L^2(\Omega)} \qquad \forall v \in X, \tag{CP}$$

where

$$a(u,v) := \underbrace{\alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}}_{=:e(u,v)} - k^2(u,v)_{L^2(\Omega)}$$
$$+ \langle Ku, v\rangle_{X',X}$$

- ➔ $K \in L(X, X')$ encodes the boundary conditions
- ➔ choice of X depends on BCs:
  sound soft: $X = H_0^2(\Omega) := H^2(\Omega) \cap H_0^1(\Omega)$,
  sound hard & impedance: $X = H^2(\Omega)$

Boundary conditions

- *sound soft*: $K := 0$
- *sound hard*:

$$\langle Ku, v\rangle_{X',X} := -\alpha(\Delta u, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)}$$

- *impedance*:

$$\begin{aligned}\langle Ku, v\rangle_{X',X} :=& -\alpha(\Delta u, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} + \alpha i\theta(\Delta u, v)_{L^2(\partial\Omega)} \\ & + \beta i\theta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, v)_{L^2(\partial\Omega)} - \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} \\ & - i\theta(u, v)_{L^2(\partial\Omega)}\end{aligned}$$

Roadmap

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To show the well-posedness of (CP), we take the following steps:

1. Study the EVP: find $u \in H_0^2(\Omega)$, $\lambda \in \mathbb{C}$ s.t.

$$e(u, v) = \lambda(u, v)_{L^2(\Omega)} \quad \forall v \in H_0^2(\Omega);$$

   ➔ self-adjointness, well-posedness, compact solution operator

2. Construct $T \in L(X)$ bijective and show that $e(\cdot, \cdot) - k^2(\cdot, \cdot)_{L^2(\Omega)}$ is T-coercive;
3. Show that $K \in L(X, X')$ is compact;
4. Show that $\mathcal{A} \in L(X, X')$, $\langle \mathcal{A}u, v\rangle_{X',X} := a(u, v)$, is injective.

} only *sound hard* & *impedance* BCs (steps 3 and 4)

$\Rightarrow$ $\mathcal{A}$ is weakly T-coercive and injective, so (CP) is well-posed.

Continuous Analysis: EVP

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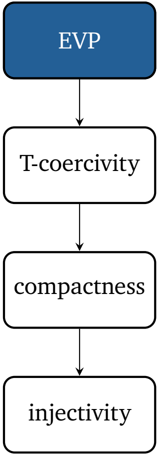
Find $u \in H_0^2(\Omega)$, $\lambda \in \mathbb{C}$ s.t. $e(u,v) = \lambda(u,v)_{L^2(\Omega)}$ for all $v \in H_0^2(\Omega)$,

$$e(u,v) := \alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}.$$

Lemma

If β is sufficiently small, the EVP is well-posed and the solution operator is compact and self-adjoint.

- → self-adjointness of $\beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)}$ by part. Int.
- → coercivity of $e(\cdot,\cdot)$ on $H_0^2(\Omega)$ with C. S. and Poincaré ineq.
- → compactness follows from the compact emb. $H_0^2(\Omega) \hookrightarrow L^2(\Omega)$



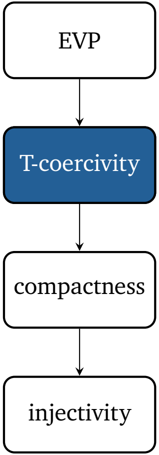
Continuous Analysis: T-coercivity

- $\exists$ eigenpairs $(\lambda^{(i)}, e^{(i)})_{i\in\mathbb{N}}$ of $e(\cdot,\cdot)$ s.t. $(e^{(i)})_{i\in\mathbb{N}}$ forms an orthonormal basis of X
- set $i_* := \min\{i \in \mathbb{N} : \lambda^{(i)} < k^2\}$ and define

$$W := \text{span}_{0\leq i \leq i_*}\{e^{(i)}\}, \qquad T := \text{Id}_X - 2P_W$$

- T bijective & acts on eigenfcts. as $Te^{(i)} = \begin{cases} -e^{(i)} & \text{if } \lambda^{(i)} < k^2; \\ +e^{(i)} & \text{if } \lambda^{(i)} > k^2. \end{cases}$
- We have that

$$e(Tu,u) - k^2(Tu,u)_{L^2} = \sum_{i\leq i_*} C_\lambda(k^2 - \lambda^{(i)})(u^{(i)})^2 + \sum_{i>i_*} C_\lambda(\lambda^{(i)} - k^2)(u^{(i)})^2 \geq \gamma\|u\|_X^2$$

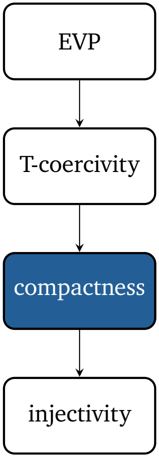


Continuous Analysis: compactness

Estimate each boundary term, e.g. for *sound hard* BCs ($\beta = 0$)

$$
\begin{aligned}
\|Ku\|_{X'} = &\sup_{v \in X \setminus \{0\}} \frac{|\langle Ku, v \rangle_{X',X}|}{\|v\|_{H^2(\Omega)}} \\
\leq &\sup_{v \in X \setminus \{0\}} \frac{|\alpha| \|\gamma_0 \Delta u\|_{L^2(\partial\Omega)} \|\gamma_0 \nabla v \cdot \boldsymbol{\nu}\|_{L^2(\partial\Omega)}|}{\|v\|_{H^2(\Omega)}} \\
\leq &\, C|\alpha| \|\gamma_0 \Delta u\|_{L^2(\partial\Omega)}
\end{aligned}
$$

- last step uses continuity of normal trace operator
- Thus: $\forall (u_n)_{n\in\mathbb{N}} \subset H^2$ s.t. $u_n \overset{H^2}{\rightharpoonup} u \Rightarrow Ku_n \to Ku$, so K is compact
- use similar arguments for $\beta > 0$ & the *impedance* case



Continuous Analysis: injectivity

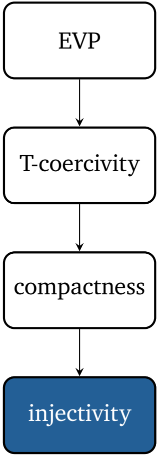
- need to assume that $k^2 \notin \{\lambda^{(i)}\}_{i \in \mathbb{N}}$
- for *impedance* case: take $v \in \ker a(\cdot, \cdot)$, then

$$0 = |-\Im a(v, v)| \geq \left| \frac{\alpha\zeta}{2} \|\Delta v\|^2_{L^2(\partial\Omega)} + \frac{\theta}{2\zeta} \|v\|^2_{L^2(\partial\Omega)} \right|$$

- $\gamma_0 v = 0$ and $\gamma_0 \Delta v = 0$ on $\partial\Omega$, use unique continuation principle to conclude that $v = 0$ in Ω

We have shown:

$\mathcal{A}$ is (weakly) T-coercive and injective $\Rightarrow$ there $\exists! u \in X$ s.t. $a(u, v) = (f, v)_{L^2(\Omega)}$ for all $v \in X$

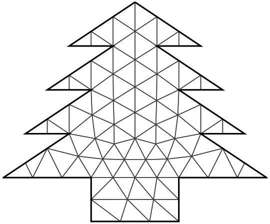


Discrete problem

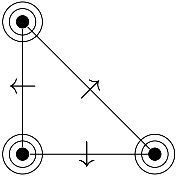
Discretization

Let $\{\mathcal{T}_h\}_h$ be a family of shape regular, quasi-uniform, simplicial triangulations. We choose an H^2-conforming finite element space, $p > 4$:

$$X_h := \{v \in H^2(\Omega) : v|_T \in \mathcal{P}^p(T) \quad \forall T \in \mathcal{T}_h\}$$



- imposing essential BCs for $\mathcal{C}^1$-conf. FEM challenging[6];
- use Nitsche's method to impose BCs (for *sound soft* & *sound hard*, not necessary for *impedance*)



Argyris-element, $p \geq 5$

[6] R.C. Kirby, L. Mitchell, *Code generation for generally mapped finite elements*. ACM TOMS, 2019.

Discrete problem

Find $u_h \in X_h$ s.t. $a_h(u_h, v_h) = (f, v_h)_{L^2(\Omega)}$ for all $v_h \in X_h$, where

$$a_h(u_h, v_h) := a(u_h, v_h) + \epsilon\,(\mathcal{N}_h(u_h, v_h))$$

- $\epsilon = 0$ for *impedance* BCs, $\epsilon = 1$ for *sound soft* BCs
- discrete analysis follows similar steps as the continuous case:
  1. analyse the discrete EVP (with potential Nitsche terms);
  2. construct T_h and show uniform T_h-coercivity;
- for *impedance* BCs ($\epsilon = 0$), we can neglect the compact term
- *sound hard* BCs can be analyzed with similar arguments

Nitsche terms

$$
\begin{aligned}
\mathcal{N}_h(u_h, v_h) :=& \alpha(\nabla(\Delta u_h)\cdot\boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} - (\nabla u_h \cdot \boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} \\
&+\beta(\nabla(\boldsymbol{n}^T(\mathcal{H}u_h)\boldsymbol{n})\cdot\boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)}
\end{aligned}
\quad \Bigg\} \text{ natural boundary terms}
$$

$$
\begin{aligned}
&+\alpha(u_h, \nabla(\Delta v_h)\cdot\boldsymbol{\nu})_{L^2(\partial\Omega)} - (u_h, \nabla v_h \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} \\
&+\beta(u_h, \nabla(\boldsymbol{n}^T(\mathcal{H}v_h)\boldsymbol{n})\cdot\boldsymbol{\nu})_{L^2(\partial\Omega)}
\end{aligned}
\quad \Bigg\} \text{ symmetry terms}
$$

$$
\begin{aligned}
&+\alpha\frac{\eta_1}{h^3}(u_h, v_h)_{L^2(\partial\Omega)} + \frac{\eta_2}{h}(u_h, v_h)_{L^2(\partial\Omega)} \\
&+\beta\frac{\eta_3}{h^3}(u_h, v_h)_{L^2(\partial\Omega)}
\end{aligned}
\quad \Bigg\} \text{ penalty terms}
$$

➔
$$
\begin{aligned}
|\mathcal{N}_h(u_h, u_h)| \gtrsim& -\frac{\alpha\zeta_1}{h^3}\|\Delta u_h\|^2_{L^2(\Omega)} - \frac{\zeta_2}{h}\|\nabla u_h\|^2_{L^2(\Omega)} - \frac{\beta\zeta_3}{h^3}|u|^2_{H^2(\Omega)} \\
&+\left(\frac{\alpha\eta_1}{h^3} - \frac{\alpha}{\zeta_1} + \frac{\eta_2}{h} - \frac{1}{\zeta_2} + \frac{\beta\eta_3}{h^3} - \frac{\beta}{\zeta_3}\right)\|u\|^2_{L^2(\partial\Omega)}
\end{aligned}
$$

Discrete EVP

Find $u_h \in \tilde{X}_h \subseteq X_h$, $\lambda \in \mathbb{C}$, s.t. for all $v_h \in \tilde{X}_h$

$$e_h(u_h, v_h) := e(u_h, v_h) + \epsilon \mathcal{N}_h(u_h, v_h) = \lambda (u_h, v_h)_{L^2(\Omega)}$$

- ➔ $\tilde{X}_h = X_h$ if $\epsilon = 1$, $\tilde{X}_h = X_h \cap \{u_h = 0 \text{ on } \partial\Omega\} \cap \{\Delta u_h = 0 \text{ on } \partial\Omega\}$ if $\epsilon = 0$
- ➔ Discrete norm: $\|u_h\|_\epsilon^2 := |u_h|_{H^2(\Omega)}^2 + |u_h|_{H^1(\Omega)}^2 + \epsilon \|u\|_{L^2(\partial\Omega)}^2$

Lemma

For η_i, $i = 1, 2, 3$, large enough, the bilinear form $e_h(\cdot, \cdot)$ is uniformly coercive on $\tilde{X}_h$ w.r.t. $\|\cdot\|_\epsilon$.

Proof.

Use the estimate for $\mathcal{N}_h(\cdot, \cdot)$ from the previous slide & choose ζ_i small enough, η_i large enough, $i = 1, 2, 3$. □

Discrete T_h-coercivity

- define $T_h \in L(X_h)$ s.t $Te_h^{(i)} = \begin{cases} -e_h^{(i)} & \text{if } i \leq i_*; \\ +e_h^{(i)} & \text{if } i > i_*. \end{cases}$
- as in the continuous case, we have that

$$
\begin{aligned}
&e_h(T_h u_h, u_h) - k^2(T_h u_h, u_h) \\
&= \sum_{0 \leq i \leq i_*} C_{\lambda_h}(k^2 - \lambda_h^{(i)})(u_h^{(i)})^2 + \sum_{i > i_*} C_{\lambda_h}(\lambda_h^{(i)} - k^2)(u_h^{(i)})^2 \geq \gamma \|u_h\|_\epsilon^2,
\end{aligned}
$$

  if h is small enough s.t. $\lambda_h^{(i_*)} < k^2$.
- (there $\exists h_0$ s.t. $\forall h \leq h_0$) $a_h(\cdot, \cdot)$ is uniformly T_h-coercive
- the discrete problem has a unique solution for h small enough

Best approximation

- $a_h(\cdot,\cdot)$ is continuous wrt (stronger) $\|\cdot\|_{h,\epsilon}$-norm:

$$\|u_h\|_{h,\epsilon}^2 := \|u_h\|_\epsilon^2 + \epsilon \left(h^3 \|\nabla(\Delta u_h)\|_{L^2(\partial\Omega)}^2 + h^3 \|\nabla(\boldsymbol{n}^T \mathcal{H} u_h \boldsymbol{n})\|_{L^2(\Omega)}^2 + h \|\nabla u_h\|_{L^2(\partial\Omega)} \right)$$

- a_h is consistent, i.e. $a_h(u - u_n, v_h) = 0$ for all $v_h \in X_h$
- with classical arguments, we can show that

$$\|u - u_h\|_{h,\epsilon} \leq C \inf_{v_h \in X_h} \|u - v_h\|_{h,\epsilon}.$$

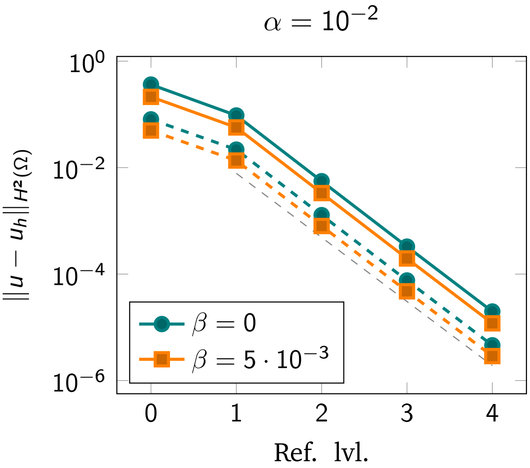
Numerical examples

Manufactured Solution

- plane wave solution $u(\boldsymbol{x}) = e^{i\boldsymbol{d}\cdot\boldsymbol{x}}$, choose $\boldsymbol{d} \in \mathbb{C}^d$ s.t. u solves the nematic Helmholtz–Korteweg eqs.
- for $u \in H^5(\Omega)$, we can construct $I_h : u \to X_h$ s.t.

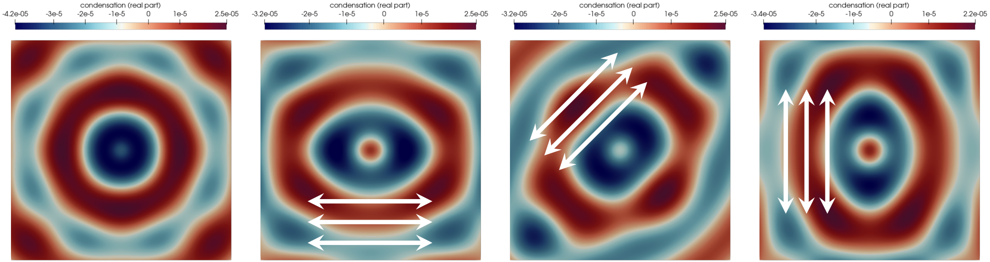
$$\|u - I_h u\|_{H^2(\Omega)} \leq h^3 \|u\|_{H^5(\Omega)}$$

- dashed: $k = 20$, solid: $k = 30$



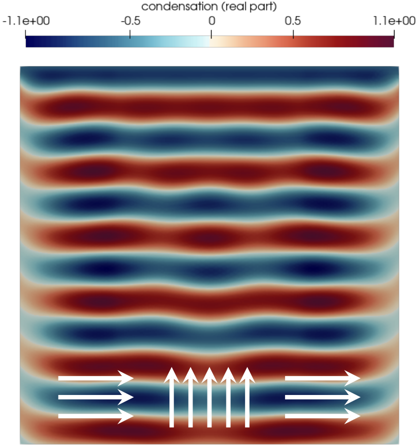
Gaussian pulse

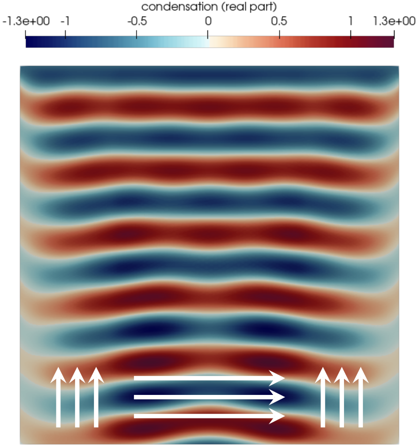
→ rhs: symmetric Gaussian pulse in $(0,0)$, *impedance* BCs, $k = 40$, $\alpha = 10^{-2}$



$\beta = 0$ | $\beta = 5 \cdot 10^{-3}$ | $\beta = 5 \cdot 10^{-3}$ | $\beta = 5 \cdot 10^{-3}$

Mullen-Lüthi-Stephen experiment[7]





[6] M.E. Mullen, B. Lüthi, M.J. Stephen, *Sound velocity in a nematic liquid crystal*. Physics review letters, 1972.

Conclusion

- we showed well-posedness of the (continuous) nematic Helmholtz–Korteweg equations
  - (weak) T-coercivity argument where T flips the sign of 'problematic' eigenfcts.
  - analysis appplies to *sound soft*, *sound hard* & *impedance* BCs
- we analysed the discretization with H^2-conforming FEM
  - imposition of essential BCs through Nitsche's method
  - transfer T-coercivity arguments to the discrete level
- numerical experiments to study the effect of the nematic field on the propagation of acoustic waves

Thank you for your attention!