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Analysis and approximation of the nematic Helmholtz-Korteweg equation

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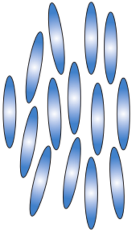
Applied Mathematics Seminar, Pavia, Dec. 10th, 2024

Introduction

- Goal: describe time-harmonic (acoustic) wave propagation in a nematic liquid crystal



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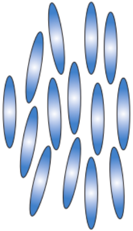

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- nematic LC can be considered as a Korteweg-fluid:

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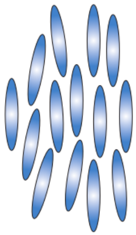

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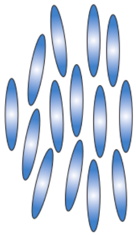
→ time harmonic acoustic waves described by the nematic Helmholtz-Korteweg equations!

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



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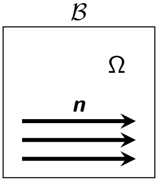
Nematic Helmholtz-Korteweg equation[1]

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

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

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, 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]

➔ 4^{th}-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:*

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

➔ our analysis covers all cases!

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

Abstract framework

Indefiniteness of Helmholtz-like problems

Let X be a separable Hilbert space. For given $k \gg 0$, $f \in L^2(\Omega)$, find $u \in X$ s.t.

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

where $e(\cdot,\cdot)$ is s.t. the eigenvalue problem: find $u \in X$, $\lambda \in \mathbb{C}$ s.t.

$$e(u,v) = \lambda(u,v)_{L^2(\Omega)}$$

is well-posed and the associated solution operator is compact & self-adjoint.

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is well-posed and the associated solution operator is compact & self-adjoint.

- ➔ the eigenfcts. $\{e^{(i)}\}_{i\in\mathbb{N}}$ form an orthonormal basis of X
- ➔ suppose $\exists i_*$ s.t. $\lambda^{(i_*)} < k^2 < \lambda^{(i_*+1)}$, then (P) is indefinite:

$$a(e^{(i_*)}, e^{(i_*)}) = \lambda^{(i_*)} - k^2 < 0 < \lambda^{(i_*+1)} - k^2 = a(e^{(i_*+1)}, e^{(i_*+1)})$$

Well-posedness

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

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

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

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- $\Leftrightarrow$ $\exists \alpha > 0$ s.t. $\|Au\|_X \geq \alpha \|u\|_X$ for all $u \in X$ & A^* injective

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

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

Theorem (Lax-Milgram)

A is coercive, i.e. $\exists \alpha > 0$ s.t. $\Re\{(Au, u)_X\} \geq \|u\|_X^2 \Rightarrow A$ is a bounded isomorphism

T-coercivity

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

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

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Definition (T-coercivity[3])

We call $A \in L(X)$ *T-coercive* if there exists a bijective operator $T \in L(X)$ s.t. AT is coercive, i.e.

$$\Re\{(ATu, u)_X\} \geq \alpha \|u\|_X^2$$

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→ T-coercivity equivalent to well-posedness (necessary & sufficient)

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

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Construction of T – Example

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

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- ➔ construct $T \in L(X)$ bijective, s.t.

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

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

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- what about boundary terms?

Definition (Compact operator)

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

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$A \in L(X)$ is called *weakly T-coercive* if there $\exists$ $T \in L(X)$ bijective, $K \in L(X)$ compact s.t. $AT + K$ is coercive.

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

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The discrete level

➔ (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.

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

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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

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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

$$\begin{aligned} a(u, v) :=& \alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)} - k^2(u, v)_{L^2(\Omega)} \\ &+ (Ku, v)_{H^2(\Omega)} \end{aligned}$$

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

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Boundary conditions

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

$$(Ku, v)_{H^2(\Omega)} := -\alpha(\Delta u, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)}$$

- *impedance*:

$$\begin{aligned}(Ku, v)_{H^2(\Omega)} := &- \alpha(\Delta u, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} + \alpha i\theta(\Delta u, v)_{L^2(\partial\Omega)} \\ &+ \beta i\theta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, v)_{L^2(\partial\Omega)} - \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \nabla v \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} \\ &- i\theta(u, v)_{L^2(\partial\Omega)}\end{aligned}$$

Roadmap

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.

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

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2. Construct $T \in L(X)$ bijective and show that $e(\cdot, \cdot) - k^2(u, v)_{L^2(\Omega)}$ is T-coercive;
3. Show that $K \in L(X)$ is compact;

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   ➔ self-adjointness, well-posedness, compact solution operator
2. Construct $T \in L(X)$ bijective and show that $e(\cdot, \cdot) - k^2(u, v)_{L^2(\Omega)}$ is T-coercive;
3. Show that $K \in L(X)$ is compact;
4. Show that $\mathcal{A} \in L(X)$, $(\mathcal{A}u, v)_{H^2(\Omega)} := a(u, v)$, is injective.

Roadmap

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

Continuous Analysis: EVP

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

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EVP

↓

T-coercivity

↓

compactness

↓

injectivity

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

EVP

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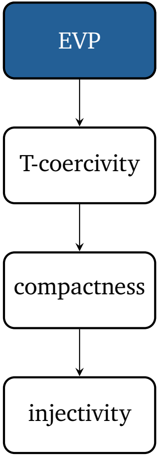

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- ➔ coercivity of $e(\cdot,\cdot)$ on $H_0^2(\Omega)$ with C. S. and Poincaré ineq.

$$\begin{array}{c} \text{EVP} \\ \downarrow \\ \text{T-coercivity} \\ \downarrow \\ \text{compactness} \\ \downarrow \\ \text{injectivity} \end{array}$$

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- ➔ coercivity of $e(\cdot, \cdot)$ on $H_0^2(\Omega)$ with C. S. and Poincaré ineq.
- ➔ compactness follows from the compact emb. $H_0^2(\Omega) \hookrightarrow L^2(\Omega)$

EVP
↓
T-coercivity
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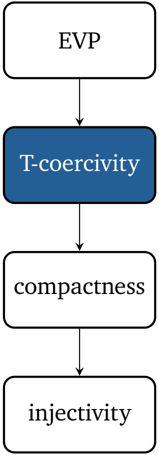
Continuous Analysis: T-coercivity

→ $\exists$ 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



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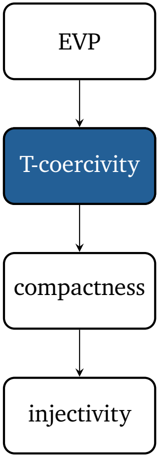

Continuous Analysis: T-coercivity

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EVP

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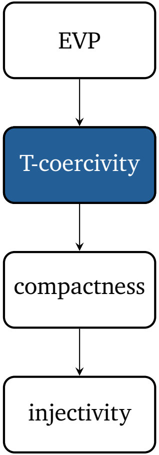
- We have that

$$\begin{aligned} &e(u, Tu) - k^2(u, Tu)_{L^2} \\ &\quad = \sum_{i\le i_*} C_\lambda(k^2 - \lambda^{(i)})(u^{(i)})^2 + \sum_{i>i_*} C_\lambda(\lambda^{(i)} - k^2)(u^{(i)})^2 \ge \gamma\|u\|_X^2 \end{aligned}$$



Continuous Analysis: compactness

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

$$
\begin{aligned}
\|Ku\|_{H^2(\Omega)} &= \sup_{v \in X \setminus \{0\}} \frac{|(Ku, v)_{H^2(\Omega)}|}{\|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)}
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EVP → T-coercivity → **compactness** → injectivity

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→ last step uses continuity of normal trace operator

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➔ 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

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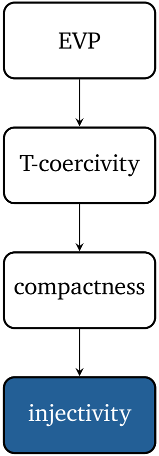
- ➔ Thus: $\forall (u_n)_{n\in\mathbb{N}} \subset H^2$ s.t. $u_n \overset{H^2}{\rightharpoonup} u \Rightarrow Ku_n \to Ku$, so K is compact
- ➔ use similar arguments for $\beta > 0$ & the *impedance* case

EVP → T-coercivity → **compactness** → injectivity

Continuous Analysis: injectivity

➔ need to assume that $k^2 \notin \{\lambda^{(i)}\}_{i\in\mathbb{N}}$



Continuous Analysis: injectivity

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

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

EVP → T-coercivity → compactness → **injectivity**

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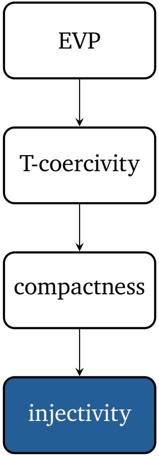
- $\gamma_0 v = 0$ and $\gamma_0 \Delta v = 0$ on $\partial\Omega$, use unique continuation principle to conclude that $v = 0$ in Ω



Continuous Analysis: injectivity

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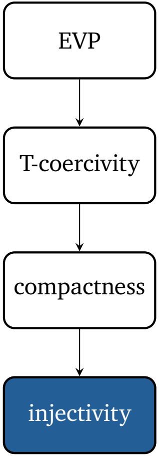
- $\gamma_0 v = 0$ and $\gamma_0 \Delta v = 0$ on $\partial\Omega$, use unique continuation principle to conclude that $v = 0$ in Ω

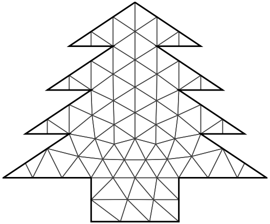
We have shown:

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



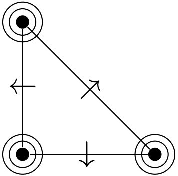
Discrete problem

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, $p > 4$:

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



Argyris-element, $p \geq 5$

- imposing essential BCs for $\mathcal{C}^1$-conf. FEM challenging[5];
- use Nitsche's method to impose BCs (for *sound soft* & *sound hard*, not necessary for *impedance*)

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

Discrete problem

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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)} \\
&+\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)} \\
&+\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}
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\end{aligned}\right\}\text{natural boundary terms}\\
&+\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)}\\
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Nitsche terms

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

Discrete EVP

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

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

Discrete EVP

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

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➔ $\tilde{X}_h = X_h$ 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 $\epsilon = 0$

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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. $\|\cdot\|_\epsilon$.

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

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- as in the continuous case, we have that

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& e_h(u_h, T_h u_h) - k^2(u_h, T_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,
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- (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:

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

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- 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.

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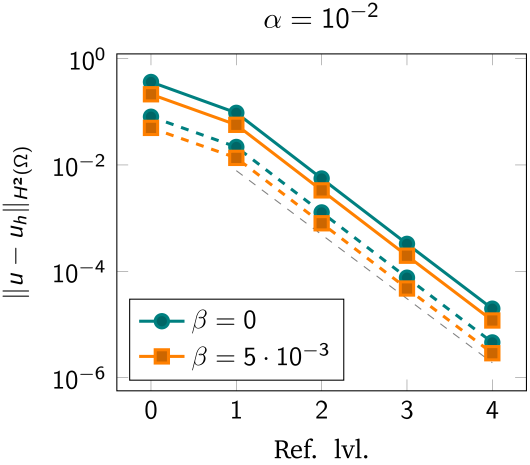
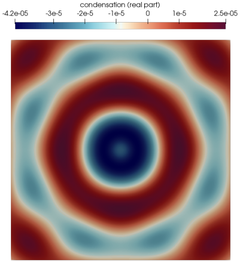
- dashed: $k = 20$, solid: $k = 30$



Gaussian pulse

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



$\beta = 0$

Gaussian pulse

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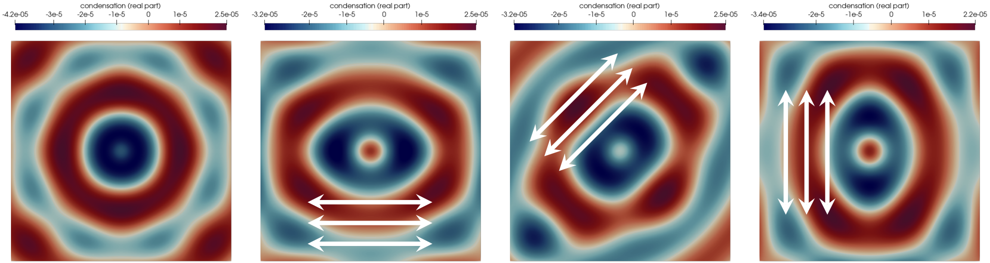
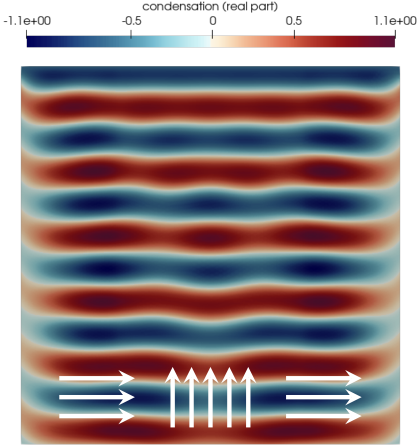
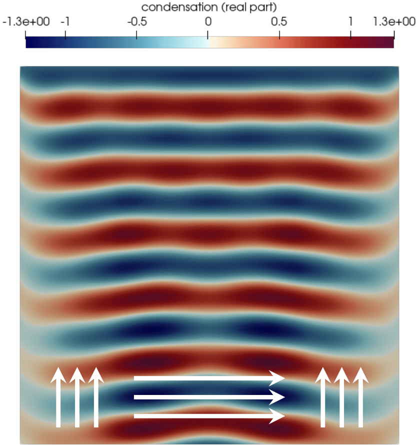


$\beta = 0$ $\quad$ $\beta = 5 \cdot 10^{-3}$ $\quad$ $\beta = 5 \cdot 10^{-3}$ $\quad$ $\beta = 5 \cdot 10^{-3}$

Mullen-Lüthi-Stephen experiment[6]





[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

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Thank you for your attention!