

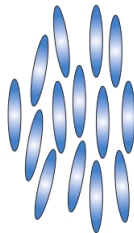
# Analysis and approximation of the nematic Helmholtz–Korteweg equation

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<sup>1</sup>University of Oxford; <sup>2</sup>University of Göttingen

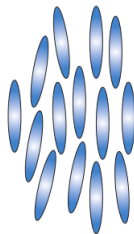
Applied Mathematics Seminar, Pavia, Dec. 10th, 2024

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W. Wang, L. Zhang, P. Zhang,  
*Modelling and computation of liquid crystals.*  
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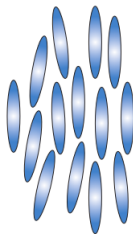
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- nematic LC can be considered as a Korteweg-fluid:

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

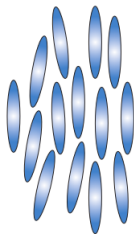


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- time harmonic acoustic waves described by the **nematic Helmholtz–Korteweg** equations!
- how does the alignment of the nematic field influence the propagation of the acoustic wave?

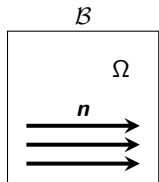


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Given  $f \in L^2(\Omega)$ , find  $u : \Omega \rightarrow \mathbb{C}$  s.t.

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

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



<sup>1</sup>P.E. Farrell, U. Zerbinati, *Time-harmonic waves in Korteweg and nematic-Korteweg fluids*. arXiv, 2024.

→ 4<sup>th</sup>-order PDE, so we need two boundary conditions

1. *sound soft*:

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

2. *sound hard*:

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

3. *impedance*:

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

→ our analysis covers all cases!

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<sup>2</sup>P.E. Farrell, U. Zerbinati, *Time-harmonic waves in Korteweg and nematic-Korteweg fluids*. arXiv, 2024.

# Abstract framework

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

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

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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- 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:

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

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

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

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

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

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## 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

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

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## Definition (T-coercivity<sup>4</sup>)

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.

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

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

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

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

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- what about boundary terms?

## 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.

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## Definition (Weak T-coercivity<sup>5</sup>)

$A \in L(X, X')$  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.

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→ i.e.  $AT = \text{bij.} + \text{comp.}$ , so  $AT$  is Fredholm with index zero!

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

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→ (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  $\alpha_*$  independent of  $h$  s.t.

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



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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

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

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

where

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

→  $K \in L(X, X')$  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*:  $X = H^2(\Omega)$

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

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

- *impedance*:

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

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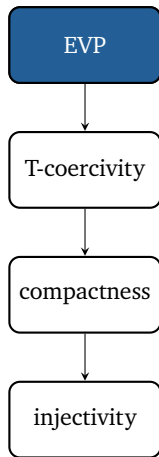
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$\Rightarrow \mathcal{A}$  is weakly T-coercive and injective, so (CP) is well-posed.

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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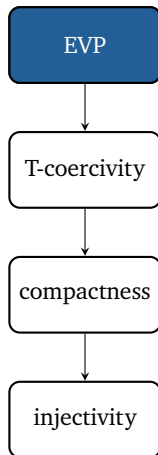


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## Lemma

*If  $\beta$  is sufficiently small, the EVP is well-posed and the solution operator is compact and self-adjoint.*



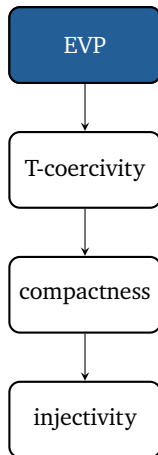
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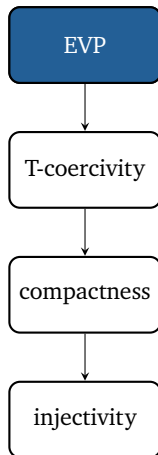
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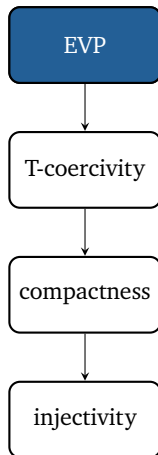
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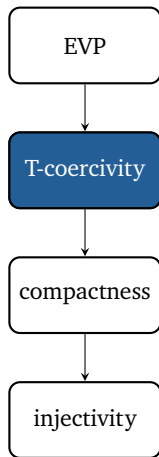
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- compactness follows from the compact emb.  $H_0^2(\Omega) \hookrightarrow L^2(\Omega)$



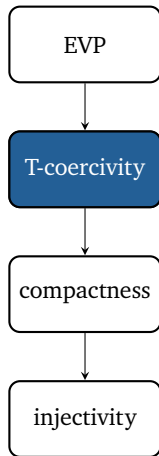
→  $\exists$  eigenpairs  $(\lambda^{(i)}, e^{(i)})_{i \in \mathbb{N}}$  of  $e(\cdot, \cdot)$  s.t.  $(e^{(i)})_{i \in \mathbb{N}}$  forms an orthonormal basis of  $X$





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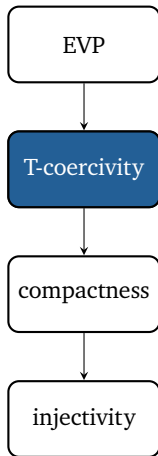
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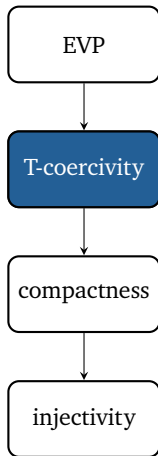


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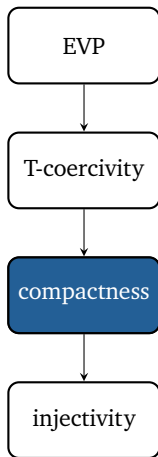
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- We have that

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



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

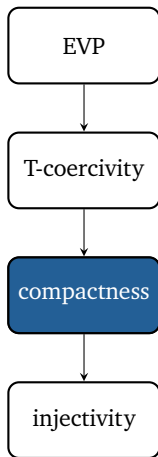
$$\begin{aligned}\|Ku\|_{X'} &= \sup_{v \in X \setminus \{0\}} \frac{|\langle Ku, v \rangle_{X', X}|}{\|v\|_{H^2(\Omega)}} \\ &\leq \sup_{v \in X \setminus \{0\}} \frac{|\alpha| \|\gamma_0 \Delta u\|_{L^2(\partial\Omega)} \|\gamma_0 \nabla v \cdot \nu\|_{L^2(\partial\Omega)}}{\|v\|_{H^2(\Omega)}} \\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



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→ last step uses continuity of normal trace operator

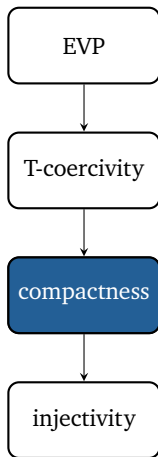


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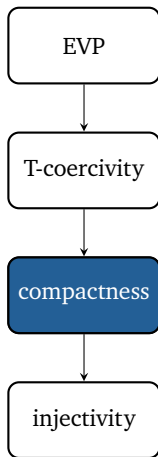
→ Thus:  $\forall (u_n)_{n \in \mathbb{N}} \subset H^2$  s.t.  $u_n \xrightarrow{H^2} u \Rightarrow Ku_n \rightarrow Ku$ , so  $K$  is compact



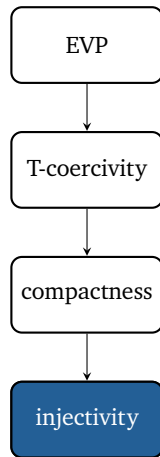
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- use similar arguments for  $\beta > 0$  & the *impedance* case



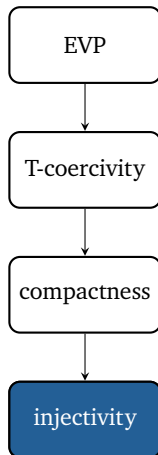
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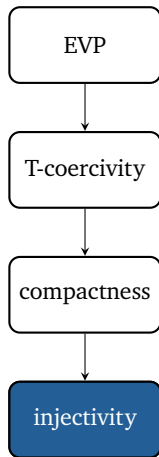
$$0 = |-\Im a(v, v)| \geq \left| \frac{\alpha\zeta}{2} \|\Delta v\|_{L^2(\partial\Omega)}^2 + \frac{\theta}{2\zeta} \|v\|_{L^2(\partial\Omega)}^2 \right|$$



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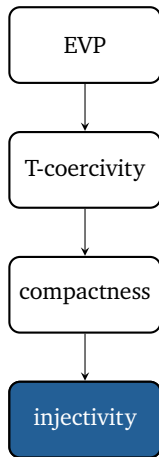
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**We have shown:**

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



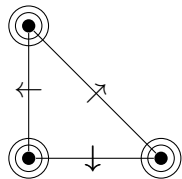
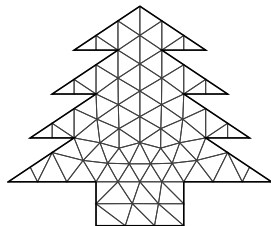
# Discrete problem

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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<sup>6</sup>;
- use Nitsche's method to impose BCs (for *sound soft* & *sound hard*, not necessary for *impedance*)



Argiris-element,  
 $p \geq 5$

<sup>6</sup>R.C. Kirby, L. Mitchell, *Code generation for generally mapped finite elements*. ACM TOMS, 2019.

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

$$\begin{aligned}\mathcal{N}_h(u_h, v_h) &:= \alpha(\nabla(\Delta u_h) \cdot \boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} - (\nabla u_h \cdot \boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} \\ &\quad + \beta(\nabla(\mathbf{n}^T(\mathcal{H}u_h)\mathbf{n}) \cdot \boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} \\ &\quad + \alpha(u_h, \nabla(\Delta v_h) \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} - (u_h, \nabla v_h \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} \\ &\quad + \beta(u_h, \nabla(\mathbf{n}^T(\mathcal{H}v_h)\mathbf{n}) \cdot \boldsymbol{\nu})_{L^2(\partial\Omega)} \\ &\quad + \alpha \frac{\eta_1}{h^3} (u_h, v_h)_{L^2(\partial\Omega)} + \frac{\eta_2}{h} (u_h, v_h)_{L^2(\partial\Omega)} \\ &\quad + \beta \frac{\eta_3}{h^3} (u_h, v_h)_{L^2(\partial\Omega)}\end{aligned}$$

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natural boundary  
terms



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} symmetry terms

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 & + \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(\mathbf{n}^T(\mathcal{H}v_h)\mathbf{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}
 \left. \begin{array}{l} \\ \\ \\ \\ \end{array} \right\} \begin{array}{l} \text{natural boundary} \\ \text{terms} \\ \\ \text{symmetry} \\ \text{terms} \\ \\ \text{penalty} \\ \text{terms} \end{array}$$

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

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

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

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## Lemma

*For  $\eta_i$ ,  $i = 1, 2, 3$ , 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  $\zeta_i$  small enough,  $\eta_i$  large enough,  $i = 1, 2, 3$ . □



→ 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

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

if  $h$  is **small enough** s.t.  $\lambda_h^{(i_*)} < k^2$ .

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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

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

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

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→ 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

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→ plane wave solution  $u(\mathbf{x}) = e^{i\mathbf{d}\cdot\mathbf{x}}$ ,  
choose  $\mathbf{d} \in \mathbb{C}^d$  s.t.  $u$  solves the  
nematic Helmholtz–Korteweg eqs.

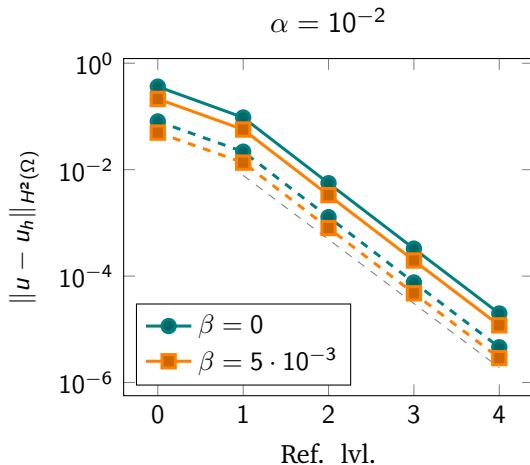
- plane wave solution  $u(\mathbf{x}) = e^{i\mathbf{d}\cdot\mathbf{x}}$ ,  
choose  $\mathbf{d} \in \mathbb{C}^d$  s.t.  $u$  solves the  
nematic Helmholtz–Korteweg eqs.
- for  $u \in H^5(\Omega)$ , we can construct  
 $I_h : u \rightarrow X_h$  s.t.

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

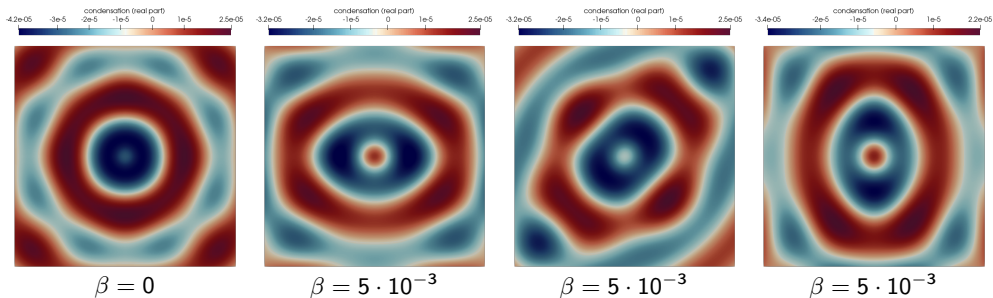
- plane wave solution  $u(\mathbf{x}) = e^{i\mathbf{d}\cdot\mathbf{x}}$ , choose  $\mathbf{d} \in \mathbb{C}^d$  s.t.  $u$  solves the nematic Helmholtz–Korteweg eqs.
- for  $u \in H^5(\Omega)$ , we can construct  $I_h : u \rightarrow X_h$  s.t.

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

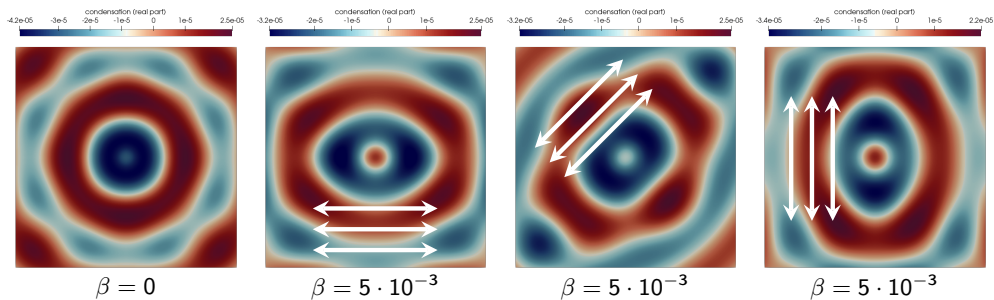
- dashed:  $k = 20$ , solid:  $k = 30$



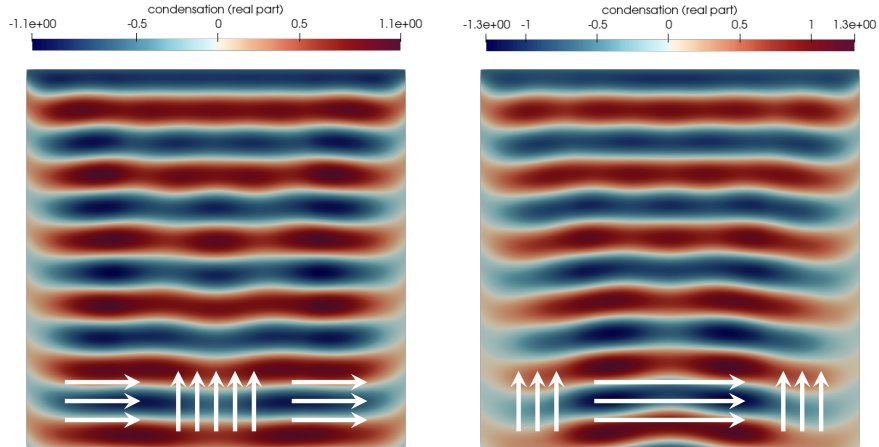
→ rhs: symmetric Gaussian pulse in  $(0, 0)$ , *impedance* BCs,  $k = 40$ ,  $\alpha = 10^{-2}$



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# Mullen-Lüthi-Stephen experiment<sup>7</sup>



<sup>6</sup>M.E. Mullen, B. Lüthi, M.J. Stephen, *Sound velocity in a nematic liquid crystal*. Physics review letters, 1972.

- we showed well-posedness of the (continuous) nematic Helmholtz–Korteweg equations
  - (weak)  $T$ -coercivity argument where  $T$  flips the sign of 'problematic' eigenfcts.
  - analysis applies to *sound soft*, *sound hard* & *impedance* BCs

- we showed well-posedness of the (continuous) nematic Helmholtz–Korteweg equations
  - (weak) T-coercivity argument where  $T$  flips the sign of 'problematic' eigenfcts.
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- we analysed the discretization with  $H^2$ -conforming FEM
  - imposition of essential BCs through Nitsche's method
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**Thank you for your attention!**