Derivation, Analysis and Numerical Analysis of the Helmholtz–Korteweg equation

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UNIVERSITY OF OXFORD

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Oxford Mathematics

L. S. Hirst, G. Charras, *Liquid crystals in living tissue*, Nature, 2017.

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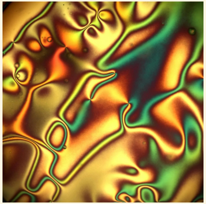
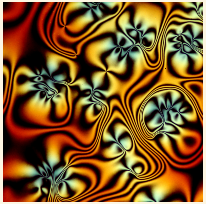
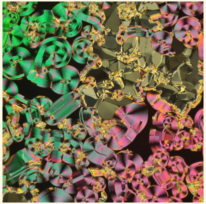

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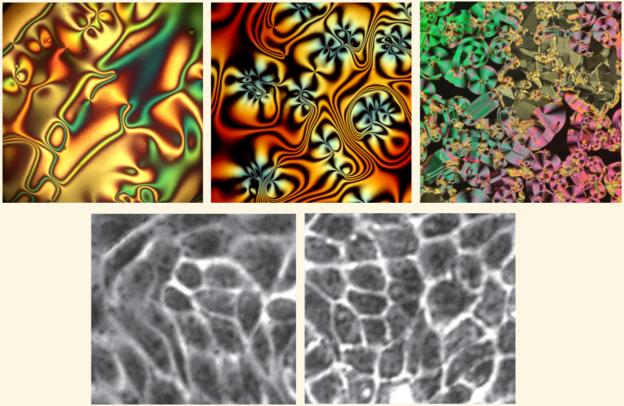

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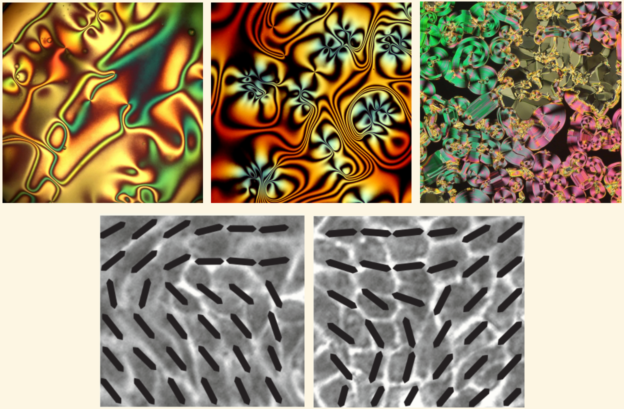

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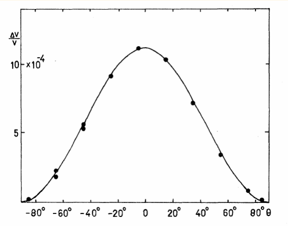

Figure: Angular dependence of sound velocity. $T = 21$ C, $v = 10$ MHz, and $H = 5$ kOe. θ is the angle between the field direction and propagation direction. Solid line is $12.5 \cdot 10^{-4} \cos(\theta)^2$.

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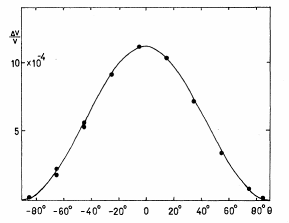

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- Historically the interaction of acoustic waves with the nematic director field was first explained by means of the minimal entropy production principle, i.e. the acoustic anisotropy is assumed to be the result of calamitic molecules reorienting in order to minimize the propagation losses.
- We here assume the aligning torque acting on the nematic director field is of elastic nature, rather than of a dissipative viscous one. This idea was already proposed, and validated experimentally, by Mullen, Lüthi, and Stephen.

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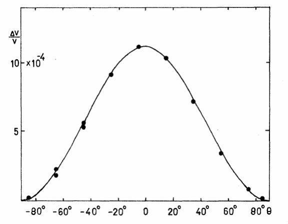

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THE HELMHOLTZ–KORTEWEG EQUATION

1

TIME-HARMONIC CONDENSATION WAVES

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Let us consider the continuity equation and the balance law of linear momentum in the absence of external body forces, i.e.

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0, \qquad \rho \left[\partial_t \boldsymbol{v} + (\underline{\underline{\nabla \boldsymbol{v}}}) \boldsymbol{v} \right] = -(\nabla \cdot \underline{\underline{\sigma}}) \,, \tag{1}$$

where $\boldsymbol{v}(\boldsymbol{x}, t)$ is the fluid velocity and $\underline{\underline{\sigma}}$ is the Cauchy stress tensor.

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where $\boldsymbol{v}(\boldsymbol{x}, t)$ is the fluid velocity and $\underline{\underline{\sigma}}$ is the Cauchy stress tensor.
We are interested in disturbances in the density field of the form $\rho(\boldsymbol{x}, t) = \rho_0 \left(1 + s(\boldsymbol{x}, t)\right)$, where $s(\boldsymbol{x}, t)$ is a time-harmonic condensation, i.e.

$$s(\boldsymbol{x}, t) = \Re\left[S(\boldsymbol{x})e^{-i\omega t}\right] \,,$$

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$$s(\boldsymbol{x}, t) = \Re\left[S(\boldsymbol{x})e^{-i\omega t}\right],$$

with ω being the frequency of the disturbances. Furthermore, we will assume that the condensation is a small perturbation of the density field, i.e. $|s(\boldsymbol{x}, t)| = \mathcal{O}(\varepsilon)$, with $\varepsilon \ll 1$. Lastly, we will assume that the velocity field is a small perturbation around the stationary regime, i.e. $\|\boldsymbol{v}(\boldsymbol{x}, t)\| = \mathcal{O}(\varepsilon)$.

A GENERALIZED HELMHOLTZ EQUATION

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Under these assumptions, we can rewrite (1) as

$$\rho_0\left[\partial_t \boldsymbol{s} + \nabla\cdot\boldsymbol{v} + \mathcal{O}(\varepsilon^2)\right] = 0, \qquad \partial_t \boldsymbol{v} + \mathcal{O}(\varepsilon^2) = -\rho^{-1}(\nabla\cdot\underline{\underline{\sigma}})\,.$$

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Neglecting terms of order $\mathcal{O}(\varepsilon^2)$, since $|s(\boldsymbol{x},t)| \ll 1$ we have $\rho^{-1}\approx\rho_0^{-1}$, thus

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Substituting the time-harmonic ansatz (2) in the general wave equation (1) yields

$$\Re\left[-\rho_0 \omega^2 S(\boldsymbol{x}) e^{-i\omega t}\right] = -\Re\left[\nabla \cdot \left(\nabla \cdot \underline{\underline{\sigma}}\right)\right].$$

STRESS TENSOR: SPHERICAL RESPONSE

The Cauchy stress tensor $\underline{\underline{\sigma}}$ encodes the elastic response of the liquid crystal to any defromation.

Spherical response

The isotropic response of a compressible fluid is usually modeled as a spherical stress tensor, i.e. the stress tensor is given by

$$\underline{\underline{\sigma}}^{(I)} = -p\underline{\underline{\mathrm{Id}}}$$

where p is the fluid pressure, which we assume is of the form $p = \rho c_0^2$, with c_0 being the speed of sound in the isotropic phase and ρ the density of the liquid crystal.

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STRESS TENSOR: TRANSVERSALLY ISOTROPIC RESPONSE

P. Biscari, A. DiCarlo, S. S. Turzi *Anisotropic wave propagation in nematic liquid crystals*, Soft Matter, 2014.

Transversally isotropic response

Originally Ericksen modeled the elastic response of the liquid crystal as a transversally isotropic material, i.e. the stress tensor is given by

$$\underline{\underline{\sigma}}^{(T)} = -p\underline{\underline{\mathsf{Id}}} + \mu\left(\boldsymbol{n}\otimes\boldsymbol{n}\right)$$

where $\boldsymbol{n}$ is the nematic director field and μ is a fixed constant.

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- The transversally isotropic stress tensor, is incompatible with an hyperelastic formulation.

STRESS TENSOR: NEMATIC–KORTEWEG RESPONSE

E. Virga *Variational theory for nematoacoustics*, Physics Review E (2009).

Nematic–Korteweg response

Virga proposed a different model for the elastic response of the liquid crystal, which is compatible with an hyperelastic formulation. The stress tensor is given by

$$\underline{\underline{\sigma}}^{(V)} = p\underline{\underline{I}} - \alpha\rho\left(\nabla\rho\otimes\nabla\rho\right) - \beta\left(\nabla\rho\cdot\boldsymbol{n}\right)\nabla\rho\otimes\boldsymbol{n},$$

where the coefficients α and β are positive constants and the pressure is given by

$$p = \rho c_0^2 - \rho\nabla\cdot\left[\rho\left(\alpha\nabla\rho + \beta(\nabla\rho\cdot\boldsymbol{n})\boldsymbol{n}\right)\right].$$

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- It can be proven that this stress tensor is compatible with an hyperelastic formulation, i.e. it can be derived from the free energy functional

$$W(\rho, \nabla\rho, \boldsymbol{n}) = c_0^2\rho + \frac{1}{2}\alpha\|\nabla\rho\|^2 + \frac{1}{2}\beta(\nabla\rho \cdot \boldsymbol{n})^2.$$

THE NEMATIC HELMHOLTZ–KORTEWEG EQUATION

Consider the nematic Korteweg stress tensor and the time-harmonic ansatz we can rewrite the right-hand side of the generalised wave equation (1) as

$$\nabla \cdot \underline{\underline{\sigma}} \approx \Re\Big[-\rho_0 c_0^2 \nabla S(\boldsymbol{x}) + \alpha \rho_0^3 \nabla(\Delta S(\boldsymbol{x})) + \rho_0^3 u_2 \nabla\left((\nabla S \cdot \boldsymbol{n})\boldsymbol{n}\right)\Big].$$

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Dividing by $\rho_0 e^{-\omega t}$ the generalised wave equation (1) yields

$$-\omega^2 S(\boldsymbol{x}) - c_0^2 \Delta S(\boldsymbol{x}) + \rho_0^2 \alpha \Delta^2 S(\boldsymbol{x}) + \rho_0^2 u_2 \nabla \cdot \nabla \Big[\underline{\underline{\mathcal{H}S}}\boldsymbol{n} \cdot \boldsymbol{n} + \underline{\underline{\nabla \boldsymbol{n}}}\nabla S \cdot \boldsymbol{n} + (\nabla S \cdot \boldsymbol{n})(\nabla \cdot \boldsymbol{n})\Big] = 0.$$

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A reasonable assumption is that the nematic director field $\boldsymbol{n}$ is regarded as undistorted at the acoustic length scale, so that we can assume $\underline{\underline{\nabla \boldsymbol{n}}} = 0$.

Under this hypothesis we obtain the **nematic Helmholtz–Korteweg equation**, i.e.

$$-\omega^2 S(\boldsymbol{x}) - c_0^2 \Delta S(\boldsymbol{x}) + \rho_0^2 \alpha \Delta^2 S(\boldsymbol{x}) + \rho_0^2 u_2 \nabla \cdot \nabla \left[\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right] = 0.$$

BOUNDARY CONDITIONS

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Sound-soft boundary conditions

Sound-soft boundary conditions impose that the excess-pressure defined as

$$c_0^2\rho_0 S(\boldsymbol{x}) - \rho_0^3\alpha\Delta S(\boldsymbol{x}) - u_2\rho_0^3\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right) = 0.$$

vanish along the boundary. Sound-soft boundary conditions thus correspond to imposing homogeneous Dirichlet boundary conditions on $S(\boldsymbol{x})$ and

$$\Delta S(\boldsymbol{x}) = -\frac{u_2}{\alpha}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

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Sound-hard boundary conditions

Sound-hard boundary conditions also change since the normal derivative of the fluid velocity $\partial_{\boldsymbol{\nu}} \boldsymbol{v}$ now satisfies the equation

$$i\omega\rho_0(\boldsymbol{n}\cdot\boldsymbol{\nu}) = c_0^2\partial_{\boldsymbol{\nu}} S(\boldsymbol{x}) - \rho_0^2\alpha\partial_{\boldsymbol{\nu}}\Delta S(\boldsymbol{x}) - \rho_0^2 u_2 \partial_{\boldsymbol{\nu}}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

Sound-hard boundary conditions thus correspond to imposing homogeneous Neumann boundary conditions on $S(\boldsymbol{x})$ and

$$\partial_{\boldsymbol{\nu}}\Delta S(\boldsymbol{x}) = -\frac{u_2}{\alpha}\partial_{\boldsymbol{\nu}}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

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Impedance boundary conditions

Some computation shows that the impedance boundary conditions for the nematic Helmholtz–Korteweg equation are equivalent to imposing Robin boundary conditions on $S(\boldsymbol{x})$ and

$$\partial_{\boldsymbol{\nu}} \Delta S(\boldsymbol{x}) = i\zeta \Delta S(\boldsymbol{x}) + i\zeta \frac{u_2}{\alpha} \left(\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right) - \frac{u_2}{\alpha} \partial_{\boldsymbol{\nu}} \left(\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right),$$

where ζ is the impedance of the boundary.

ANALYSIS

2

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 the bilinear form associated to the eigenvalue problem: find $u \in X$, $\lambda \in \mathbb{C}$ such that

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

We will assume this eigenvalue problem is well-posed and the associated solution operator is compact and self-adjoint.

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

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

T-COERCIVITY

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

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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

CONSTRUCTION OF T – EXAMPLE

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

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

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

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

WEAK FORMULATION

We want to find $u \in X$ such that

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

where

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

We will only consider sound-soft boundary conditions for which $X = H^2_0(\Omega) := H^2(\Omega) \cap H^1_0(\Omega)$

CONTINUOUS ANALYSIS: THE EIGENVALUE PROBLEM

Find $u \in H^2_0(\Omega)$, $\lambda \in \mathbb{C}$ s.t. $e(u,v) = \lambda(u,v)_{L^2(\Omega)}$ for all $v \in H^2_0(\Omega)$,

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

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- coercivity of $e(\cdot,\cdot)$ on $H_0^2(\Omega)$ can be proven using Poincaré inequality.
- compactness follows from the compact embedding $H_0^2(\Omega) \hookrightarrow L^2(\Omega)$.

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

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- We have that

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

NUMERICAL SIMULATIONS

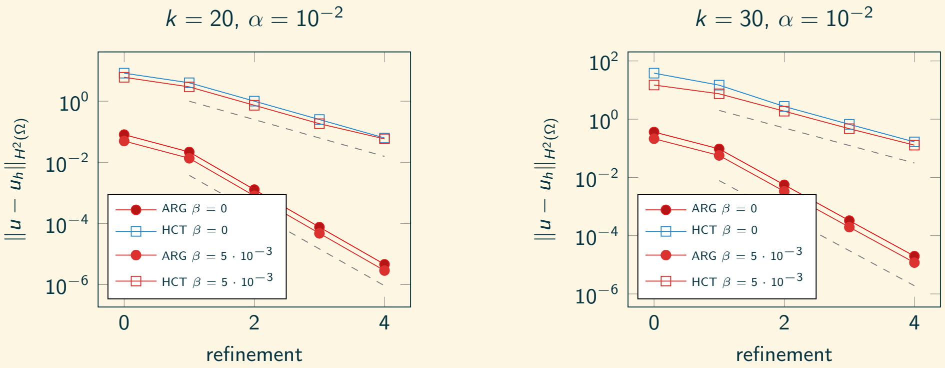


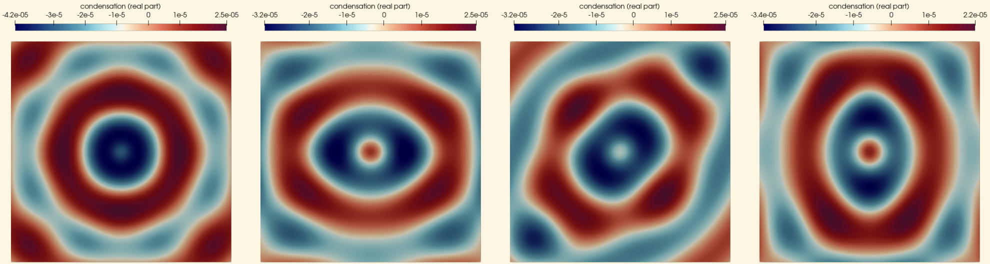
Figure: The convergence of the H^2-norm of the error for the Helmholtz–Korteweg equation for different values of k (top row) and the corresponding manufactured solution (bottom row).

FEATURES OF THE MODEL

3

ANISOTROPIC SPEED OF SOUND

We demonstrate the anisotropic speed of sound considering as right-hand side asymmetric Gaussian pulse in $(0,0)$, *impedance* BCs, $k = 40$, $\alpha = 10^{-2}$



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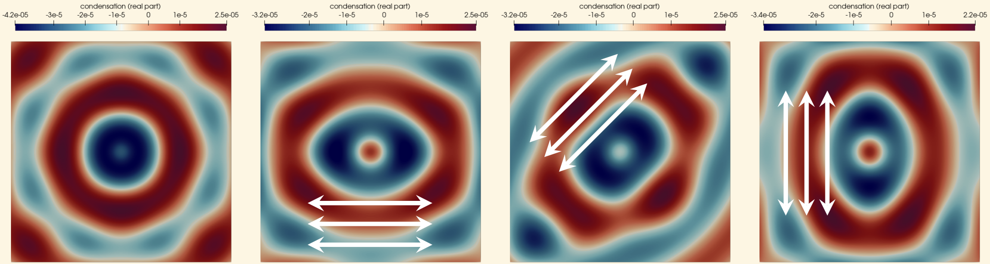

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TOTAL INTERNAL REFLECTION

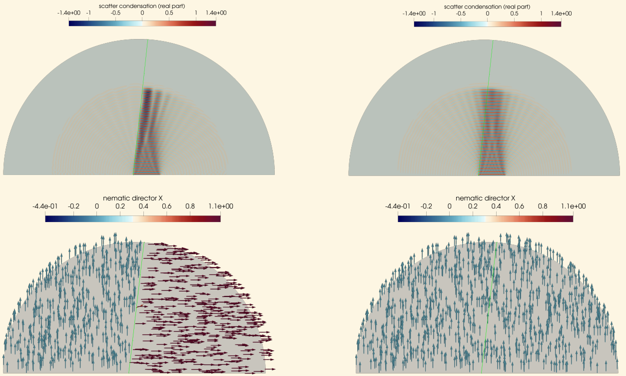

Figure: An acoustic reflection phenomenon in a nematic Korteweg fluid can be caused by a discontinuity in the nematic director field. We consider a Gaussian beam travelling upwards in a semicircular domain, with two different nematic director fields.

SCATTERING BY A CIRCULAR OBSTACLE

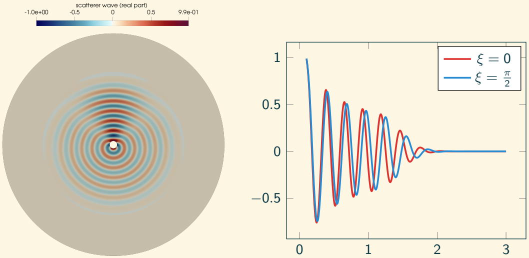

Figure: The scattered wave produced by a circular obstacle in a nematic Korteweg fluid with $\alpha = 10^{-3}$ and $u_2 = 5 \cdot 10^{-4}$, has a greater amplitude when the incoming plane wave is orthogonal to the nematic director field. Recall that ξ is the angle between $\boldsymbol{d}$ and $\boldsymbol{n}$. We simulated a plane wave propagating parallel to the y-axis and impinging on a circular obstacle, centered at the origin (left). The amplitude of the scattered wave, for different values of ξ, is measured along the y-axis (right). An adiabatic layer has been used to implement the Sommerfeld radiation condition on the outer bounday.

THANK YOU!

Derivation, Analysis and Numerical Analysis of the Helmholtz–Korteweg equation

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