

Optimisation topologique d'interfaces microstructurées

Rémi Cornaggia,

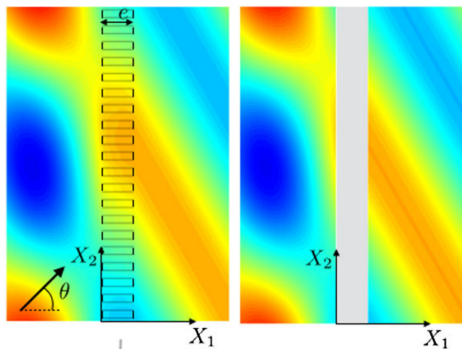
Institut d'Alembert, Sorbonne Université, Paris, France

en collaboration avec **Marie Touboul** (Imperial College) et **Cédric Bellis** (LMA, Marseille)

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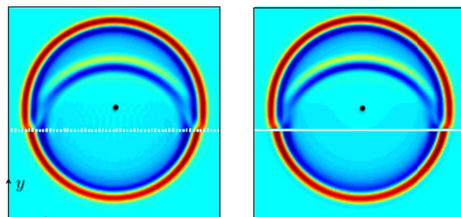


Microstructured interfaces and effective transmission conditions



Frequency domain [Marigo et al., 2017]

$$kl = 0.5 \Rightarrow \ell/\lambda \approx 0.08$$



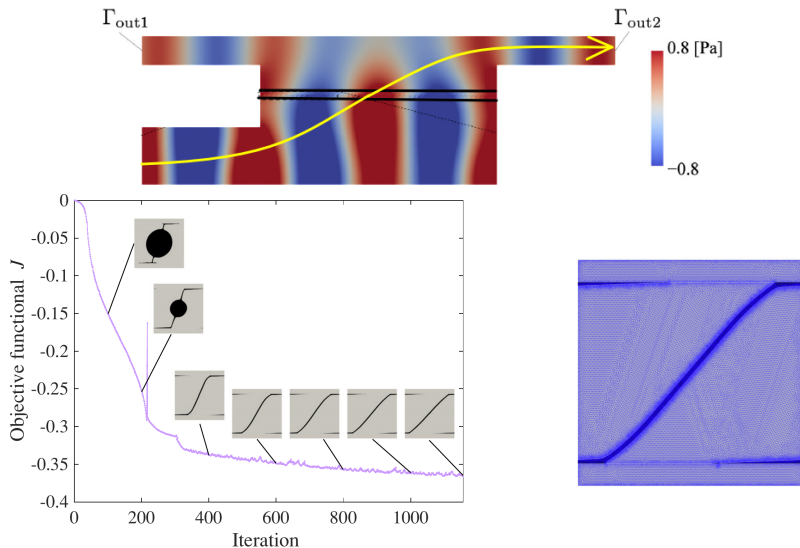
Time domain, rigid inclusions

[Lombard et al., 2017]

Multiple frequency signal $\Rightarrow \ell/\lambda \in [0.1, 0.6]$

Is it possible to *attenuate* or *enhance* the transmitted wave in some specific direction ?

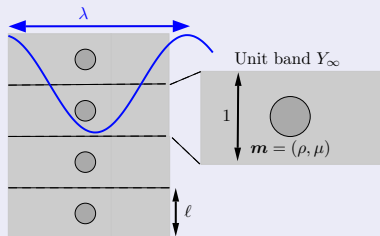
An example from [Noguchi and Yamada, 2021]



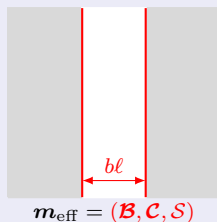
Noguchi, Y. & Yamada, T. *Topology optimization of acoustic metasurfaces by using a two-scale homogenization method* Applied Mathematical Modelling, 2021

Optimization based on an effective model

Periodic interfaces



Effective transmission conditions Optimized microstructure



(1) Homogenization process toward **effective transmission conditions**:

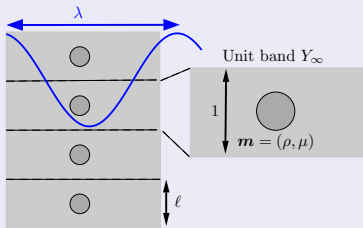
- Double-scale expansions and matched asymptotics
- **Band problems** to capture the microstructural effects
- **FFT-based solvers** to address these problems

(2) Optimization strategy:

- Cost functionals based on **effective transmission properties**
- **Topological sensitivity** to drive updating steps
- Level-set representation, **regularization** and iterative algorithm
- Initialisation with optimal elliptic inclusions.

Outline

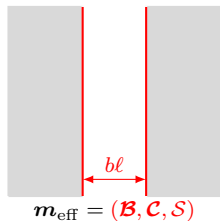
- 1 Introduction
- 2 Effective models, cell/band problems and FFT-based solvers
- 3 Optimization
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- 5 Conclusions and perspectives



- Antiplane shear waves:

$$\rho \left(\frac{\mathbf{x}}{\ell} \right) \frac{\partial^2 u_\ell(\mathbf{x}, t)}{\partial t^2} - \nabla \cdot \left[\mu \left(\frac{\mathbf{x}}{\ell} \right) \nabla u_\ell(\mathbf{x}, t) \right] = 0$$

- (ρ, μ) : density and shear modulus, **1-periodic along the interface**
- **Long-wavelength** assumption: $\ell \ll \lambda$
- Double scale dependency **and matched asymptotic expansions.**

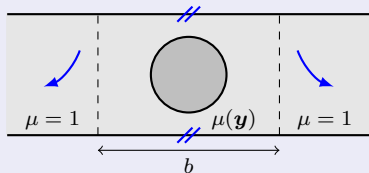


Effective model for **macroscopic fields** (V, S) :

$$\left\{ \begin{array}{l} \rho_m \frac{\partial V}{\partial t} = \nabla \cdot S \\ \frac{\partial S}{\partial t} = \mu_m \nabla V \\ [V]_{bl} = \ell \mathbf{B} \cdot \langle \nabla V \rangle_{bl} \\ [S_1]_{bl} = \ell \mathbf{S} \langle \nabla \cdot S \rangle_{bl} - \ell \mathbf{C} \cdot \langle \nabla S_2 \rangle_{bl} \end{array} \right. \quad \begin{array}{l} |x_1| > \frac{bl}{2} \\ |x_1| > \frac{bl}{2} \end{array}$$

Effective parameters computed from Φ , solution of a **band problem** on Y_∞ .

Band problem



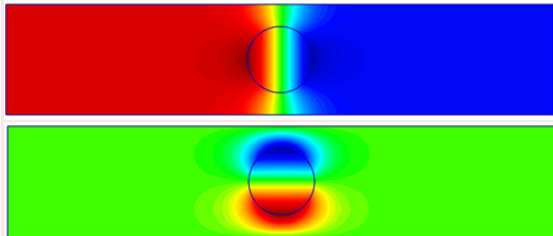
Original problem in **infinite band**:
(normalized “fast” coordinate $\mathbf{y} = \mathbf{x}/\ell$)

$$\nabla \cdot (\mu [\mathbf{I} + \nabla \Phi]) = \mathbf{0} \quad \text{in } Y_\infty$$

Φ is periodic in the y_2 variable

$$\lim_{y_1 \rightarrow \pm\infty} \nabla \Phi = \mathbf{0}$$

Computations in artificially bounded domain:

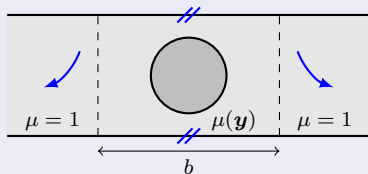


Effective coefficients [Marigo et al., 2017]

$$\mathcal{B} = \lim_{y_1 \rightarrow +\infty} \Phi - \lim_{y_1 \rightarrow -\infty} \Phi + \mathbf{f}(b)$$

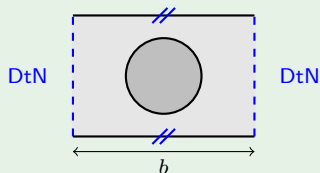
$$\mathcal{C} = \int_{Y_\infty} \mu(\mathbf{y}) \partial_2 \Phi(\mathbf{y}) \, d\mathbf{y} + \mathbf{g}(b, \mu)$$

$$\mathcal{S} = h(b, \rho)$$



Original problem in **infinite band**:

$$\begin{cases} \nabla \cdot (\mu [I + \nabla \Phi]) = 0 & \text{in } Y_\infty \\ \Phi \text{ is periodic in the } y_2 \text{ variable} \\ \lim_{y_1 \rightarrow \pm\infty} \nabla \Phi = 0 \end{cases}$$



Equivalent cell problem:

$$\begin{cases} \nabla \cdot (\mu [I + \nabla \Phi]) = 0 & \text{in } Y_b \\ \Phi \text{ is periodic in the } y_2 \text{ variable} \\ \partial_n \Phi (\pm b/2, \cdot) = \Lambda [\Phi (\pm b/2, \cdot)] \end{cases}$$

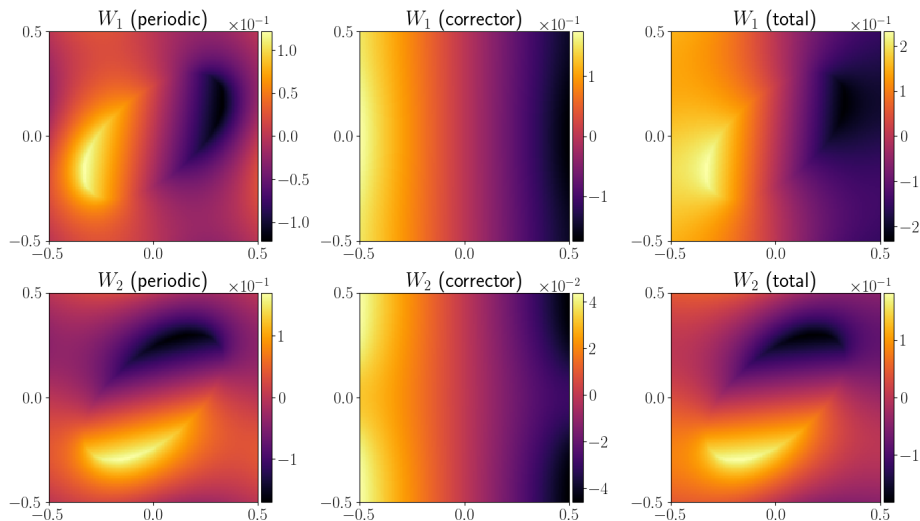
Λ : **Dirichlet-to-Neumann (DtN) operator**.
 $(\mathcal{B}, \mathcal{C})$ have expressions implying only integrals on Y_b

Numerical strategy: decomposition $\Phi = \Phi_{\text{per}} + \Phi_{\text{bound}}$ (periodic + corrector)

- Λ and Φ_{bound} have an **explicit expression** in Fourier basis.
- Φ_{per} satisfies $\nabla \cdot (\mu [I + \nabla \Phi_{\text{bound}} + \nabla \Phi_{\text{per}}]) = 0$
 \implies **iterative FFT-based solvers** [Moulinec and Suquet, 1995]

Examples for an elliptic inclusion

$\mu_{\text{inc}}/\mu_{\text{mat}} = 6$, 129×129 pixels:



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Cost functionals and optimization problem

Cost functionals: evaluate the medium performance through its **effective** properties:

$$\mathcal{J}(\mathbf{m}) = J(\mathbf{m}_{\text{eff}}) \quad \text{here: } \begin{cases} \mathbf{m} = (\rho(\mathbf{y}), \mu(\mathbf{y})), & \mathbf{y} \in Y_b \\ \mathbf{m}_{\text{eff}} = (\mathbf{B}, \mathbf{C}, \mathbf{S}) \end{cases}$$

Examples : cost functionals on **effective reflexion and transmission coefficients** for incident direction θ_I :

$$J(\mathbf{m}_{\text{eff}}) = F(\mathcal{R}(\mathbf{m}_{\text{eff}}, \theta_I), \mathcal{T}(\mathbf{m}_{\text{eff}}, \theta_I))$$

Optimization problem

Find \mathbf{m}_{opt} that minimizes $\mathcal{J}(\mathbf{m})$.

With the dependencies $\mathbf{m} \rightarrow$ cell problems $\rightarrow \mathbf{m}_{\text{eff}} \rightarrow J(\mathbf{m}_{\text{eff}}) = \mathcal{J}(\mathbf{m})$

General strategy:

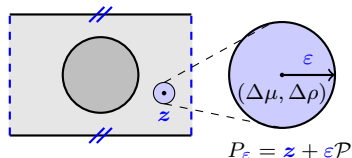
- Constraints and parametrization of \mathbf{m} , e.g. **piecewise uniform materials**
- **Iterative “material update” algorithms**

$$\mathbf{m}^{(n+1)} = \mathbf{m}^{(n)} + \Delta\mathbf{m}^{(n)} \quad \text{such that} \quad \mathcal{J}(\mathbf{m}^{(n+1)}) < \mathcal{J}(\mathbf{m}^{(n)})$$

- Main tool: **sensitivity** of \mathcal{J} to a material update $\Delta\mathbf{m}$ to choose a “good” $\Delta\mathbf{m}^{(n)}$.

Topological sensitivity of a cost functional

[Sokolowski and Zochowski, 1999, Garreau et al., 2001, Amstutz, 2011, Bonnet et al., 2018] ...



- **Localized phase change** in the cell: $\mathbf{m} \rightarrow \mathbf{m}_\epsilon = \mathbf{m} + \chi_{P_\epsilon} \Delta \mathbf{m}$

Expansion of \mathcal{J} : $\mathcal{J}(\mathbf{m}_\epsilon) = \mathcal{J}(\mathbf{m}) + \epsilon^2 \mathcal{D}\mathcal{J} + o(\epsilon^2)$ as $\epsilon \rightarrow 0$

- $\mathcal{D}\mathcal{J}(\mathbf{m}; \mathbf{z}; \mathcal{P}, \Delta\mu, \Delta\rho)$: **topological sensitivity** (or gradient, or derivative) of \mathcal{J} .

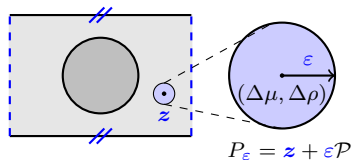
If $\mathcal{D}\mathcal{J}(\mathbf{z}) < 0$, then $\mathcal{J}(\mathbf{m}_\epsilon) < \mathcal{J}(\mathbf{m})$ and therefore \mathbf{z} is a good choice for a phase change !

- **Chain rule** for $\mathcal{J}(\mathbf{m}) = \mathcal{J}(\mathbf{m}_{\text{eff}})$:

$$\mathcal{D}\mathcal{J} = \frac{\partial \mathcal{J}}{\partial \mathbf{m}_{\text{eff}}} \mathcal{D}\mathbf{m}_{\text{eff}}$$

\Rightarrow Need to compute (**DB, DC, DS**)

Example : topological derivative of \mathcal{S}



By definition :

$$\begin{cases} \mathcal{S} = b + \frac{\rho_i - \rho_m}{\rho_m} |\Omega_i| \\ \mathcal{S}_\epsilon = b + \frac{\rho_i - \rho_m}{\rho_m} |\Omega_i| + \frac{\Delta \rho}{\rho_m} |P_\epsilon| \end{cases}$$

Exact expansion:

$$\mathcal{S}_\epsilon = \mathcal{S} + \underbrace{\epsilon^2 \frac{\Delta \rho}{\rho_m} |\mathcal{P}|}_{\mathcal{DS}}$$

Here \mathcal{DS} does not depend on z nor on the shape \mathcal{P} (*not* the general case).

Topological derivatives and polarization tensor

The topological derivatives are (see [Touboul, PhD thesis, Chap. 4, 2021]) :

$$\mathcal{DS}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta \mathbf{m}) = \frac{\Delta \rho}{\rho_{\text{m}}} |\mathcal{P}|,$$

$$\mathcal{DB}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta \mathbf{m}) = -(\nabla \Phi_1(\mathbf{z}) + \mathbf{e}_1) \cdot \mathbf{A}(\mathbf{z}) \cdot (\nabla \Phi(\mathbf{z}) + \mathbf{I}),$$

$$\mathcal{DC}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta \mathbf{m}) = (\nabla \Phi_2(\mathbf{z}) + \mathbf{e}_2) \cdot \mathbf{A}(\mathbf{z}) \cdot (\nabla \Phi(\mathbf{z}) + \mathbf{I}).$$

depend on

- the cell solution gradient at perturbation point $\nabla \Phi(\mathbf{z})$,
- the **polarization tensor** $\mathbf{A}(\mathbf{z}) = \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta \mu)$

Polarization tensor \mathbf{A} :

- used in [Cedio-Fengya et al., 1998, Ammari and Kang, 2007] in similar context,
- also called *localization* or *concentration* tensor, related to Eshelby and Hill tensors in elasticity/micromechanics [Eshelby, 1957, Parnell, 2016],
- symmetric,
- known analytically for **elliptic shapes** of semiaxes lengths $(1, \gamma)$, and directions $(\mathbf{n}_1, \mathbf{n}_2)$:

$$\mathbf{A}^{\text{ellipse}}(\mu(\mathbf{z}), \Delta \mu) = \pi \gamma (\gamma + 1) \frac{\Delta \mu}{\mu(\mathbf{z})} \left(\frac{\mathbf{n}_1 \otimes \mathbf{n}_1}{1 + \gamma + \gamma \frac{\Delta \mu}{\mu(\mathbf{z})}} + \frac{\mathbf{n}_2 \otimes \mathbf{n}_2}{1 + \gamma + \frac{\Delta \mu}{\mu(\mathbf{z})}} \right).$$

Numerical validation

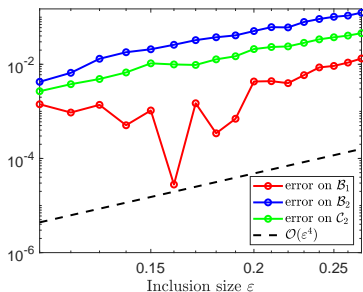
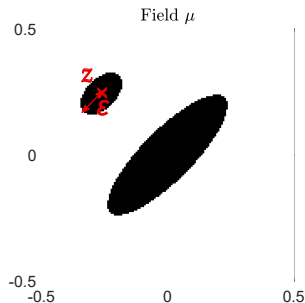
- Leading-order approximation of homogenized coefficients e.g.

$$\mathbf{B}_\varepsilon = \mathbf{B} + \varepsilon^2 \mathcal{D}\mathbf{B}(\mathbf{z}) + o(\varepsilon^2)$$

- Computation of relative error e.g. :

$$\frac{|\mathbf{B}_{1,\varepsilon} - [\mathbf{B}_1 + \varepsilon^2 \mathcal{D}\mathbf{B}_1]|}{|\mathbf{B}_{1,\varepsilon}|}$$

(should be $o(\varepsilon^2)$, expected at least $O(\varepsilon^3)$)



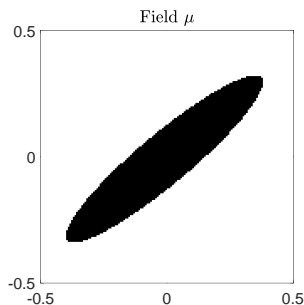
\Rightarrow Error in $O(\varepsilon^4)$ and $< 15\%$ (even for “big” perturbations $\varepsilon = 0.25$)
(term in ε^3 vanishes, should be true for *any centrally-symmetric shape* \mathcal{P} [Bonnet, 2009])

Approximative effective coefficients for elliptic inclusions

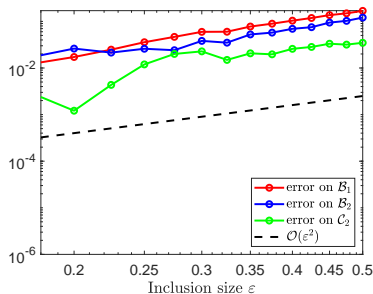
Particular case: one inclusion P_ε in an **homogeneous** cell ($\Phi = 0$)

$$\mathcal{S} = b + \varepsilon^2 \frac{\Delta \rho}{\rho_m} |\mathcal{P}|, \quad \mathcal{B}_1 = b - \varepsilon^2 A_{11} + o(\varepsilon^2), \quad \mathcal{B}_2 = -\varepsilon^2 A_{12} + o(\varepsilon^2), \quad \mathcal{C}_2 = b + \varepsilon^2 A_{22} + o(\varepsilon^2).$$

- Analytical expressions when \mathbf{A} is known
- Example : ellipse tilted at 40° , semi-axes $(\varepsilon, 0.2\varepsilon)$:



Case $\varepsilon = 0.5$



Relative error : $< 15\%$ for $\varepsilon \leq 0.5$

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Level-set representation and projection algorithm

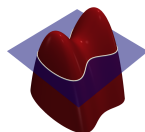
[Amstutz and André, 2006, Amstutz, 2011]

- Material distribution at iteration n represented by a **level-set function** ψ^n :

$$(*) \begin{cases} \psi^n > 0 & \text{in } Y_1 \\ \psi^n < 0 & \text{in } Y_2 \end{cases} \quad \text{and} \quad \|\psi^n\|_{L^2(Y)} = 1$$

- Signed and normalized TD $\bar{\mathcal{D}}\mathcal{J}$ (here for $\mathcal{P} = \text{disk}$):

$$\bar{\mathcal{D}}\mathcal{J} := \begin{cases} \mathcal{D}\mathcal{J}/\|\mathcal{D}\mathcal{J}\|_{L^2(Y)} & \text{in } Y_1 \\ -\mathcal{D}\mathcal{J}/\|\mathcal{D}\mathcal{J}\|_{L^2(Y)} & \text{in } Y_2 \end{cases} \quad \text{so that} \quad \|\bar{\mathcal{D}}\mathcal{J}\|_{L^2(Y)} = 1$$



(Wikipedia)

Optimality condition: If $\bar{\mathcal{D}}\mathcal{J}$ satisfies the sign condition $(*)$ then $\mathcal{D}\mathcal{J}(z) > 0 \quad \forall z \in Y$
then \mathcal{J} reached a **local minimum**

Update of ψ by **projection** onto $\bar{\mathcal{D}}\mathcal{J}$:

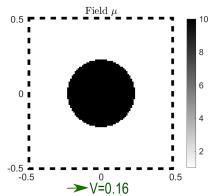
$$\psi^{n+1} = a_n \psi^n + b_n \bar{\mathcal{D}}\mathcal{J}(\psi^n)$$

(a_n, b_n) are chosen so that $\|\psi^{n+1}\|_{L^2(Y)} = 1$ and $\mathcal{J}(\psi^{n+1}) < \mathcal{J}(\psi^n)$

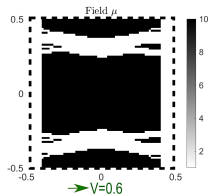
A first test [Touboul, Ph.D. Thesis, 2021 (Chap. 4)]

- **Goal** : minimization of the **effective reflexion coefficient** \mathcal{R} for an incident angle $\theta_I = \pi/4$
 - ▶ Define $\mathcal{R}(\mathbf{m}_{\text{eff}}, \theta_I)$ with $\mathbf{m}_{\text{eff}} = (\mathcal{B}, \mathcal{C}, \mathcal{S})$
 - ▶ Compute the sensibilities $(\mathcal{DB}, \mathcal{DC}, \mathcal{DS})$
- **Two-phase material**: (1) matrix and (2) inclusion.
- **Volume constraint** on inclusion phase Y_2 in the unit cell: $V_C = 0.6$
- **Perimeter penalization** following [Amstutz, 2013] to get smooth final configurations

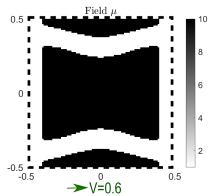
$$\mathcal{J} = |\mathcal{R}|^2 + \lambda \left(\frac{|Y_2|}{V_C} - 1 \right)^2 + \alpha_{\text{per}} \text{Per}(Y_2) \quad (\lambda: \text{iteratively chosen weight})$$



Initial unit cell



Final unit cell



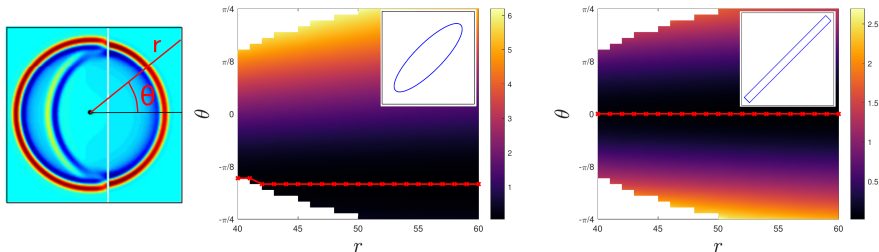
with perimeter penalization



Microstructure

Attenuated scattered field

- **Numerical experiments** : for a pulse emitted at a **source point**, measure the **energy of the scattered field** by the interface:



- “Attenuated direction” linked to the **effective transmission coefficient** \mathcal{T} computed for a plane wave with wavenumber k and incident angle θ_1 :

$$\mathcal{T}(\theta_1) = 1 + i(kl)\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_1) + O((kl)^2)$$

“Attenuated direction” at θ_{\min} when $\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_1)$ changes sign at $\theta_1 = \theta_{\min}$.

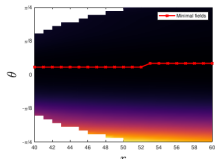
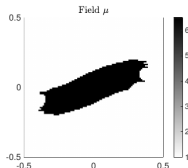
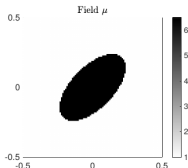
- Main cost functional:

$$\mathcal{J}_{\text{main}}(\mathbf{m}_{\text{eff}}) = \left(\frac{\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_{\min})}{\partial_{\theta} \mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_{\min})} \right)^2 \quad \text{with} \quad \partial_{\theta} \mathcal{T}_1 = \frac{\partial \mathcal{T}_1}{\partial \theta_1}$$

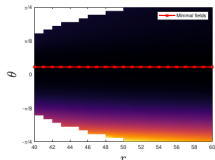
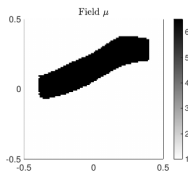
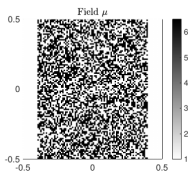
Results for $\theta_{\min} = 0$, $V_C = 0.2$, perimeter penalisation

Initialisations:

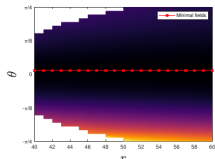
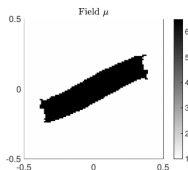
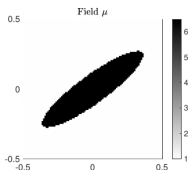
ellipse at 45°



Random distribution



“Optimal” ellipse
(almost) analytical
optimisation based on
approximative m_{eff}



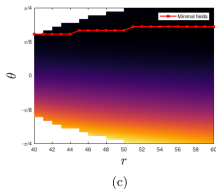
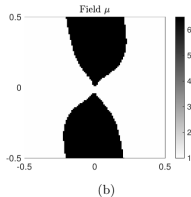
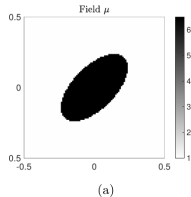
Performances for for $\theta_{\min} = 0$, $V_C = 0.2$

	N_{iter}	V end	\mathcal{J} init.	\mathcal{J} end	$\mathcal{J}_{\text{main}}$ init.	$\mathcal{J}_{\text{main}}$ end
ellipse	103	0.15	1.21	$2.24 \cdot 10^{-1}$	$9.72 \cdot 10^{-1}$	$1.4 \cdot 10^{-2}$
random	82	0.16	$5.23 \cdot 10^3$	$1.93 \cdot 10^{-1}$	$5.23 \cdot 10^3$	$7.2 \cdot 10^{-3}$
optimal ellipse	60	0.14	$1.02 \cdot 10^{-1}$	$6.76 \cdot 10^{-2}$	$3.61 \cdot 10^{-1}$	$2.1 \cdot 10^{-3}$

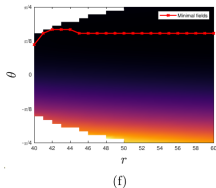
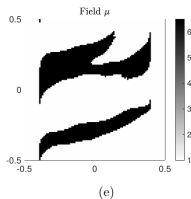
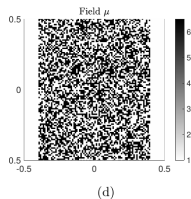
Results for $\theta_{\min} = \pi/4$, $V_C = 0.3$, perimeter penalisation

Initialisations:

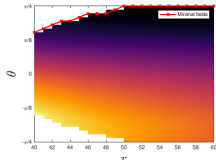
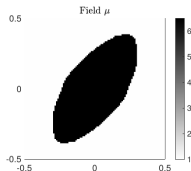
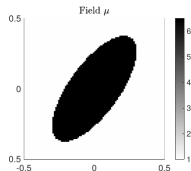
ellipse at 45°



Random distribution



“Optimal” ellipse
(almost) analytical
optimisation based on
approximative m_{eff}



Performances for $\theta_{\min} = \pi/4$, $V_C = 0.3$:

	N_{iter}	V end	\mathcal{J} init.	\mathcal{J} end	$\mathcal{J}_{\text{main}}$ init.	$\mathcal{J}_{\text{main}}$ end
ellipse	49	0.30	1.51	$2.84 \cdot 10^{-2}$	1.40	$9.72 \cdot 10^{-5}$
random	52	0.24	$2.03 \cdot 10^{-1}$	$1.35 \cdot 10^{-1}$	$2.11 \cdot 10^{-4}$	$7.99 \cdot 10^{-4}$
optimal ellipse	28	0.28	$6.27 \cdot 10^{-2}$	$2.96 \cdot 10^{-2}$	$3.30 \cdot 10^{-3}$	$8.76 \cdot 10^{-5}$

Conclusions

- A topological optimization procedure is proposed, combining
 - ▶ Effective model obtained via two-scale asymptotic homogenization
 - ▶ FFT-based algorithms to solve cell problems
 - ▶ Approximative effective coefficients (for ellipses, using topological derivatives)
⇒ Help to find specific initialisations.
 - ▶ Level-set, TD-based, projection algorithm (with volume and perimeter constraints)
- The procedure is applied to achieve
 - ▶ Minimal reflexion under volume constraint.
 - ▶ Attenuation of scattered energy in chosen direction.

Perspectives

- Time-domain simulations of waves in the designed materials
- Extensions to other other physics and regimes:
 1. Elasticity
 2. Resonant interfaces with high-contrast inclusions [Pham et al., 2017, Touboul et al., 2020] [Nicolas Lebbe, hier]
- Improve the optimization algorithm
 - ▶ Couple shape and topological derivative [Allaire et al., 2005, Amstutz et al., 2018]
 - ▶ Use optimized FFT solvers.

Merci pour votre attention !

Et à toutes les personnes qui œuvrent et ont œuvré
pour le GDR MecaWave !

- *FFT-based computation of homogenized interface parameters*

Rémi Cornaggia, Marie Touboul & Cédric Bellis

Comptes Rendus Mécanique, 2022

- Marie Touboul's Ph.D. :

Acoustic and elastic wave propagation in microstructured media with interfaces: homogenization, simulation and optimization

<https://tel.archives-ouvertes.fr/tel-03411353>

- *Topological sensitivity-based analysis and optimization of microstructured interfaces*

Marie Touboul, Rémi Cornaggia & Cédric Bellis

Hopefully on HAL before summer ...

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