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Topological optimization of microstructures in 2D

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► **To cite this version:**

Rémi Cornaggia. Topological optimization of microstructures in 2D. Doctoral. C2305: Wave Motion in Heterogeneous Media: Analysis, Modeling and Design, CISM, Udine, Italy. 2023. hal-04186515

HAL Id: hal-04186515

<https://hal.science/hal-04186515v1>

Submitted on 23 Aug 2023

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Theme 2 : Topological optimization of microstructures in 2D

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Joint work with Bojan B. Guzina², Marc Bonnet³, Cédric Bellis⁴ and Marie Touboul⁵

CISM Course C2305: *Wave Motion in Heterogeneous Media: Analysis, Modeling and Design*
June 19-23, 2023



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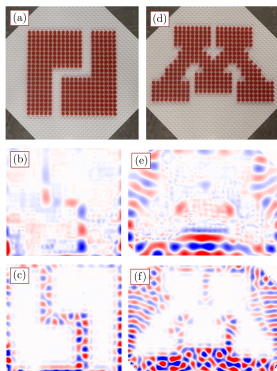
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Control of wave propagation using periodic structures

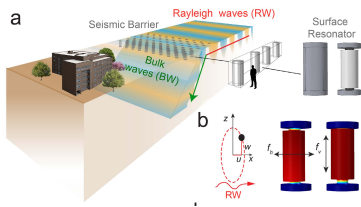


[Celli and Gonella, 2015]

... to design waveguides

- with resonators for long wavelengths / low frequencies
- with Bragg effects for medium wavelengths / frequencies

... to design seismic protections (with resonators)



[Palermo et al., 2016]

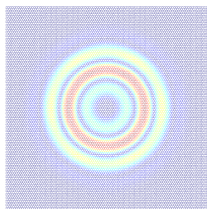
... and more (negative effective properties, cloaking ...)

How to obtain desired properties ?

- Known design (cylinders, spheres, cones, LEGO bricks ...) \implies **parameter optimization**
[Huang et al., 2016, Palermo et al., 2016] ...
- Given materials, unknown design \implies **topological optimization**
[Vondřejc et al., 2017, Kook and Jensen, 2017, Allaire and Yamada, 2018] ...

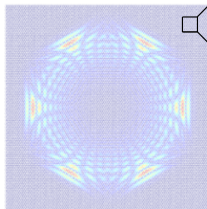
This work: long wavelengths, no resonances, “toolbox” to address topological optimization of periodic materials.

A motivation : dispersion and anisotropy in 2D elasticity [Rosi and Auffray, 2019]

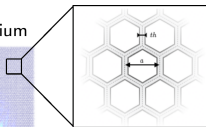


$$\frac{\ell}{\lambda_c} \ll 1$$

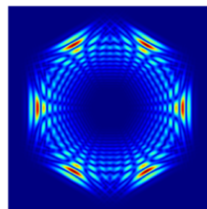
Microstructured medium



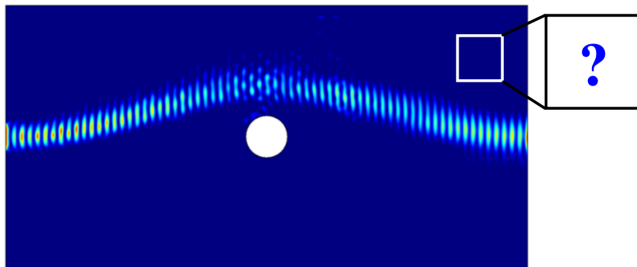
$$\frac{\ell}{\lambda_c} \approx \frac{1}{6}$$



Continuum model



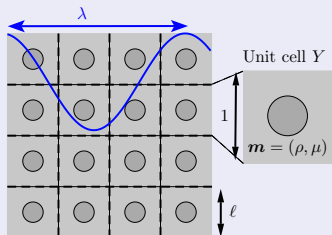
Effective (strain-gradient) model.



Optimized effective model \Rightarrow "de-homogenization" ?

Strategy : optimization using an intermediate effective model

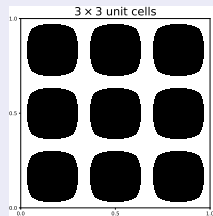
Microstructured medium



(1) Effective model

$$m_{\text{eff}} = (\rho_0, \mu_0, \rho_2, \mu_2)$$

(2) Optimized microstructure



(1) Homogenization process:

- Double-scale expansions
- Cell problems to capture the microstructural effects
- FFT-based solvers to address these problems

(2) Optimization tools:

- Cost functionals based on effective properties
- Topological sensitivity to drive updating steps
- Level-set representation and iterative algorithm

Outline

1 Introduction

2 Optimization for scalar waves in bi-periodic media

- Second-order homogenization, cell problems, FFT-based solver
- Optimization problem, cost functional, topological sensitivity
- Level-set algorithm on a first example
- Examples : anisotropic dispersion optimization and data fitting

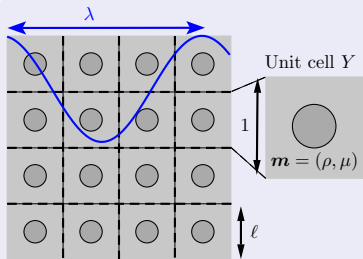
3 Microstructured interface optimization

- Effective model, cell/band problems and FFT-based solver
- Optimization problem, topological sensitivity
- Examples

4 Key ideas and perspectives

Second-order homogenization: two-scale expansion

[Sanchez-Palencia, 1974, Bensoussan et al., 1978, Cioranescu and Donato, 1999] ...



- 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) : Y -periodic density and shear modulus
- **Long-wavelength** assumption: $\varepsilon = \ell/\lambda \ll 1$
- “Slow” and “fast” variable: $\mathbf{x} = \mathbf{X}/\lambda$ and $\mathbf{y} = \mathbf{X}/\ell = \mathbf{x}/\varepsilon$
- **Double scale dependency**: $u_\ell(\mathbf{X}, t) \rightarrow \hat{u}(\mathbf{x}, \mathbf{y}; t)$ (Y -periodic in \mathbf{y})

Differential operator split:

$$\nabla_{\mathbf{X}} \rightarrow \lambda^{-1}(\nabla_{\mathbf{x}} + \varepsilon^{-1} \nabla_{\mathbf{y}})$$

Ansatz: $\hat{u}(\mathbf{x}, \mathbf{y}; t) = \sum_{j \geq 0} \varepsilon^j u_j(\mathbf{x}, \mathbf{y}; t)$

Cascade of equations for the u_j , separated variables solution:

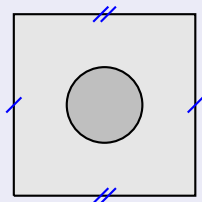
$$u_0(\mathbf{x}, \mathbf{y}; t) = U_0(\mathbf{x}; t),$$

$$u_1(\mathbf{x}, \mathbf{y}; t) = U_1(\mathbf{x}; t) + \mathbf{P}_1(\mathbf{y}) \cdot \nabla U_0(\mathbf{x}; t),$$

$$u_2(\mathbf{x}, \mathbf{y}; t) = U_2(\mathbf{x}; t) + \mathbf{P}_1(\mathbf{y}) \cdot \nabla U_1(\mathbf{x}; t) + \mathbf{P}_2(\mathbf{y}) : \nabla^2 U_0(\mathbf{x}; t),$$

- **Macroscopic fields** U_j
- **Cell functions**:
 $\mathbf{P}_1 = (P_1^{(1)}, P_1^{(2)})$
 $\mathbf{P}_2 = (P_2^{(11)}, P_2^{(12)}, P_2^{(22)})$

Cell problems and FFT-based algorithms



Classical RVE problem for P_1 : Second cell problem for P_2 :

$$\begin{cases} \nabla \cdot S_0 = \mathbf{0} \text{ in } Y, \\ S_0 = \mu(\nabla P_1 + \mathbf{I}) \\ P_1 \text{ is } Y\text{-periodic,} \\ \langle P_1 \rangle = 0, \end{cases}$$

$$\begin{cases} \nabla \cdot S_1 + [S_0 - (\rho/\varrho_0)\boldsymbol{\mu}_0] = 0 \text{ in } Y, \\ S_1 = \mu(\nabla P_2 + \mathbf{I} \otimes P_1) \\ P_2 \text{ is } Y\text{-periodic,} \\ \langle P_2 \rangle = 0, \end{cases}$$

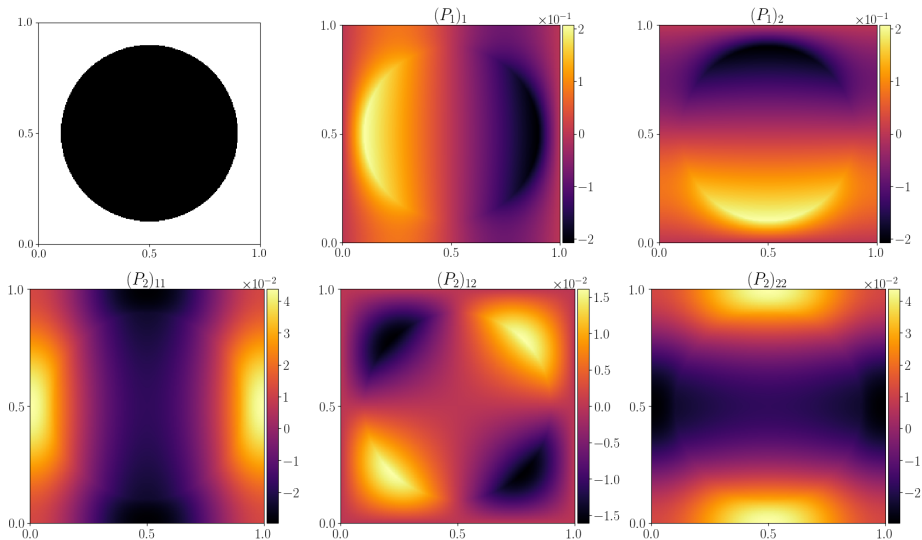
$$\text{With: } \begin{cases} \varrho_0 = \langle \rho \rangle = \text{mean of } \rho \text{ on } Y \\ \boldsymbol{\mu}_0 = \langle S_0 \rangle = \langle \mu(\mathbf{I} + \nabla P_1) \rangle_{\text{sym}} \end{cases}$$

Numerical strategy: **Fourier-based approach**

- Regular grid of **pixels** for the discretisation of (ρ, μ) .
- (P_1, P_2) discretised on a Fourier basis.
- **Iterative solvers** relying on **Fast Fourier Transforms (FFT)** to go back and forth between space and wavenumbers domains.
- Original “basic scheme” by [Moulinec and Suquet, 1995], many other schemes since then [Schneider, 2021].

Examples for a circular inclusion

$$\mu_{\text{inc}}/\mu_{\text{mat}} = 6, \quad \rho_{\text{inc}}/\rho_{\text{mat}} = 1.5, \quad 256 \times 256 \text{ pixels}$$



Second-order homogenization: effective wave equation

[Andrianov et al., 2008, Wautier and Guzina, 2015, Bonnet et al., 2018]

Mean field equations:

$$\begin{array}{l} O(1) : \varrho_0 \partial_{tt} U_0 - \nabla \cdot (\boldsymbol{\mu}_0 \cdot \nabla U_0) = 0, \\ O(\varepsilon) : \varrho_0 \partial_{tt} U_1 - \nabla \cdot (\boldsymbol{\mu}_0 \cdot \nabla U_1) = 0, \\ O(\varepsilon^2) : \varrho_0 \partial_{tt} U_2 - \nabla \cdot (\boldsymbol{\mu}_0 \cdot \nabla U_2) \\ \quad + \boldsymbol{\varrho}_2 : \nabla^2 \partial_{tt} U_0 - \boldsymbol{\mu}_2 :: \nabla^4 U_0 = 0, \end{array} \quad \left| \begin{array}{l} \varrho_0 = \langle \rho \rangle \\ \boldsymbol{\mu}_0 = \langle \boldsymbol{\mu} (\nabla \mathbf{P}_1 + \mathbf{I}) \rangle_{\text{sym}} \\ \text{Vanishing first-order} \\ \text{contribution (for 1D and antiplane 2D)} \\ \boldsymbol{\varrho}_2 = \langle \rho \mathbf{P}_2 \rangle \\ \boldsymbol{\mu}_2 = \left[\begin{array}{l} \boldsymbol{\varrho}_2 \\ \boldsymbol{\varrho}_0 \end{array} \otimes \boldsymbol{\mu}_0 \right]_{\text{sym}} + \mathbf{M}(\mathbf{P}_1, \mathbf{P}_2) \end{array} \right.$$

Effective wave equation for the macroscopic field $U = U_0 + \varepsilon U_1 + \varepsilon^2 U_2$:

$$\left[\varrho_0 + \varepsilon^2 \boldsymbol{\varrho}_2 : \nabla^2 \right] \frac{\partial^2 U}{\partial t^2} - \nabla \cdot \left[\left[\boldsymbol{\mu}_0 + \varepsilon^2 \boldsymbol{\mu}_2 : \nabla^2 \right] \cdot \nabla U \right] = 0$$

Second-order displacement approximation: (coming back to $\mathbf{y} = \mathbf{x}/\varepsilon$)

$$u_\ell(\mathbf{x}, t) \approx U(\mathbf{x}, t) + \varepsilon \mathbf{P}_1 \left(\frac{\mathbf{x}}{\varepsilon} \right) \cdot \nabla U(\mathbf{x}, t) + \varepsilon^2 \mathbf{P}_2 \left(\frac{\mathbf{x}}{\varepsilon} \right) : \nabla^2 U(\mathbf{x}, t)$$

For elastodynamics: C. Boutin, J.L. Auriault. *Rayleigh scattering in elastic composite materials*. International Journal of Engineering Science, Elsevier, 1993

Effective dispersion (and anisotropy)

- Plane wave mean field $U(x, t) = \exp[i(k\mathbf{d} \cdot \mathbf{x} - \omega t)] \implies$ **dispersion relation** $\omega = \omega(k, \mathbf{d})$.
- Phase velocity** for the second-order homogenized model:

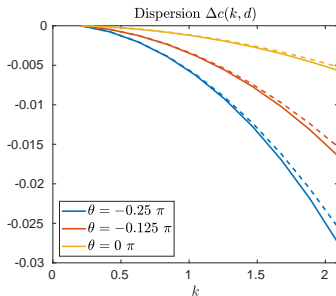
$$c(k, \mathbf{d}) = \frac{\omega(k, \mathbf{d})}{k} = \underbrace{c_0(\mathbf{d})}_{\text{limit velocity}} + \underbrace{\Delta c(k, \mathbf{d})}_{\text{dispersion}}$$

$$= c_0(\mathbf{d}) + \frac{1}{2} \frac{\gamma(\mathbf{d})}{c_0(\mathbf{d})} (k\varepsilon)^2 + o((k\varepsilon)^2) \quad \text{as } k\varepsilon \rightarrow 0$$

$$c_0(\mathbf{d}) = \sqrt{\frac{\mu_0}{\rho_0} : (\mathbf{d} \otimes \mathbf{d})} \quad \text{and} \quad \gamma(\mathbf{d}) = \left[\frac{\rho_2 \otimes \mu_0 - \rho_0 \mu_2}{(\rho_0)^2} \right] :: (\mathbf{d} \otimes \mathbf{d} \otimes \mathbf{d} \otimes \mathbf{d})$$

$\mu = 7$ $\rho = 1.2$	$\mu = 1$ $\rho = 1$
$\mu = 1$ $\rho = 1$	$\mu = 7$ $\rho = 1.2$

$c_0(\mathbf{d}) \approx 1.55$ (isotropic)



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3 Microstructured interface optimization

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4 Key ideas and perspectives

Cost functionals and optimization problem

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

$$\mathcal{J}(\mathbf{m}) = J(\mathbf{m}_{\text{eff}}) \quad \text{here: } \begin{cases} \mathbf{m} = (\rho(\mathbf{y}), \mu(\mathbf{y})), & \mathbf{y} \in Y \\ \mathbf{m}_{\text{eff}} = (\varrho_0, \boldsymbol{\mu}_0, \varrho_2, \boldsymbol{\mu}_2) & (\text{or } c_0(\mathbf{d}), \gamma(\mathbf{d})) \end{cases}$$

Optimization problem

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

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

Extremal effective properties:

$$\mathcal{J}(\mathbf{m}) = \frac{1}{2} [\gamma(\mathbf{d}^+)]^{-2}$$

(to **maximize** the dispersion in direction \mathbf{d}^+)

Fitting “target” data: (e.g. phase velocity)

$$\mathcal{J}(\mathbf{m}) = \frac{1}{2} \sum_{i=1}^{N_k} \sum_{j=1}^{N_d} |c^{\text{eff}}(k_i, \mathbf{d}_j) - c_{ij}^{\text{target}}|^2$$

General strategy:

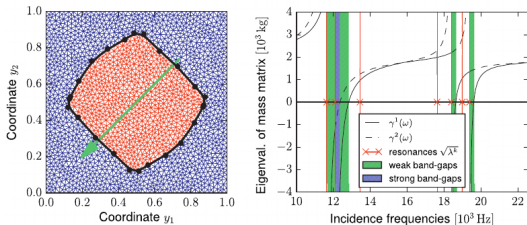
- Constraints and parametrization of \mathbf{m} , e.g. **piecewise uniform materials**
- **Iterative “material update” algorithms**

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

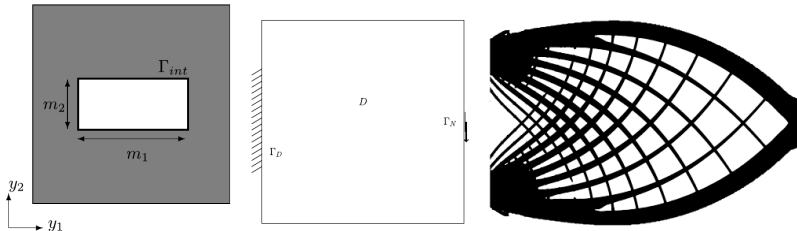
- Main tool: **sensitivity** of \mathcal{J} to a material update $\Delta\mathbf{m}$ to choose a “good” $\Delta\mathbf{m}^{(n)}$.

Parameter and shape sensitivities – Examples

[Vondřejc et al., 2017]: High-contrast bulk periodic medium, band-gap optimization, B-spline parametrization of inclusion boundary
⇒ **Parameters:** positions of control points.

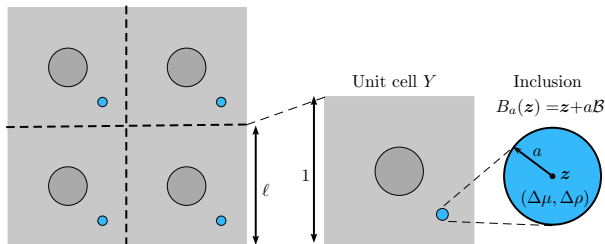


[Allaire et al., 2019] (P. Geoffroy-Donders): Elastic media, static optimization, chosen unit cell
⇒ **Parameters (fields):** geometrical parameters (m_1, m_2), cell orientation α



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 unit cell: $\mathbf{m} \rightarrow \mathbf{m}_a = \mathbf{m} + \chi_{B_a} \Delta \mathbf{m}$

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

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

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

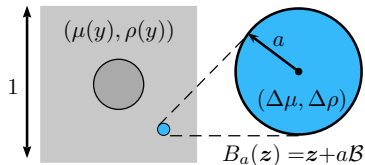
- **Chain rule** for $\mathcal{J}(\mathbf{m}) = J(\mathbf{m}_{\text{eff}})$:

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

For $\mathbf{m}_{\text{eff}} = (\varrho_0, \boldsymbol{\mu}_0, \varrho_2, \boldsymbol{\mu}_2)$, $\mathcal{D}\mathbf{m}_{\text{eff}}$ computed in [Bonnet et al., 2018].

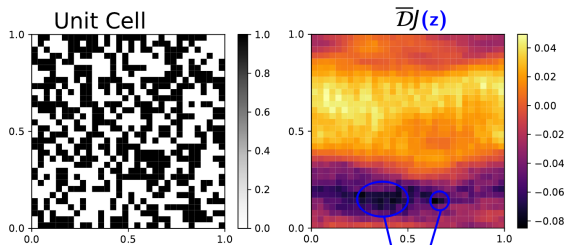
One tools, two functionalities

- Asymptotic approximations of perturbed quantities:



$$f(m_a) \approx f(m) + a^2 \mathcal{D}f(m; z, B, \Delta m) \text{ for any function } f \text{ of } m$$

- Indicator function / "map" to find interesting points z :



"Interesting" z

Also used as an *imaging function* in *qualitative inverse scattering* e.g. [Tokmashev et al., 2013]

Topological derivatives of effective properties, polarization tensor

The topological derivatives are [Bonnet et al., 2018, Cornaggia and Bellis, 2020] :

$$\begin{aligned}\varrho_0 &= \langle \rho \rangle & \Rightarrow & \mathcal{D}\varrho_0 = |\mathcal{B}|\Delta\rho, \\ \mu_0 &= \langle \mathbf{S}_0 \rangle = \langle \mu(\mathbf{I} + \nabla \mathbf{P}_1) \rangle & \Rightarrow & \mathcal{D}\mu_0 = (\mathbf{I} + \nabla \mathbf{P}_1(\mathbf{z})) \cdot \mathbf{A} \cdot (\mathbf{I} + \nabla \mathbf{P}_1(\mathbf{z})), \\ & & & = \frac{1}{\mu^2(\mathbf{z})} \mathbf{S}_0(\mathbf{z}) \cdot \mathbf{A} \cdot \mathbf{S}_0(\mathbf{z}) \\ \mathcal{D}\varrho_2 &= \text{(ugly)} & & \mathcal{D}\mu_2 = \text{(even uglier)}\end{aligned}$$

All depend on (i) the cell solutions at perturbation point $\mathbf{P}_j(\mathbf{z})$ (or $\mathbf{S}_j(\mathbf{z})$),
(ii) the **polarization tensor** $\mathbf{A}(\mathbf{z}) = \mathbf{A}(\mathcal{B}, \mu(\mathbf{z}), \Delta\mu)$

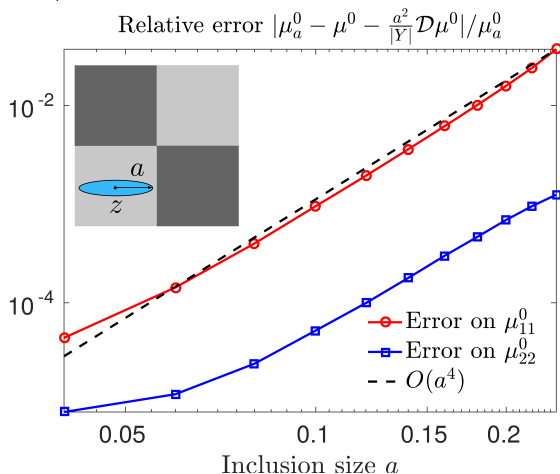
Polarization tensor \mathbf{A} :

- 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 $(\mathbf{n}_1, \mathbf{n}_2)$:

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

Fast computation of approximate homogenized coefficients

- Reference “chessboard” unit cell with $\mu \in [1, 2]$.
- Ellipsoidal inclusion with
 - ▶ center $z = (0.25, 0.25)$
 - ▶ axes $(a, 0.2a)$, with $a < 0.25$
 - ▶ stiffness contrast $\Delta\mu = 1$



- Error in $O(a^4)$ instead of *a priori* expected $O(a^3)$: it should be the case for any *centrally symmetric* inclusion [Bonnet, 2008].

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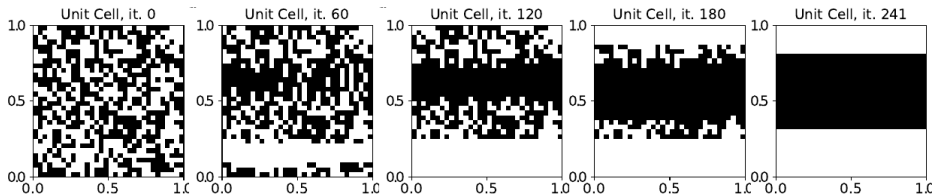
Pixel-by-pixel two-directions optimization

- Directions of interest $\mathbf{d}^- = \mathbf{e}_1$ (horizontal), $\mathbf{d}^+ = \mathbf{e}_2$ (vertical).

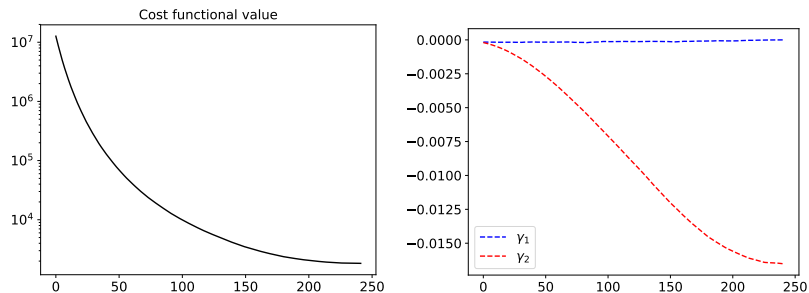
$$\mathcal{J}(\rho, \mu) = \frac{1}{2} \left[[\gamma(\mathbf{d}^-)]^2 + \frac{1}{[\gamma(\mathbf{d}^+)]^2} \right]$$

- Two-phase unit cell: $Y = Y_1 \cup Y_2$, with:
 - ▶ material ratios $\rho_2 = 2\rho_1$ and $\mu_2 = 2\mu_1 \Rightarrow$ uniform wavespeed
 - ▶ equal phase ratio: $|Y_1| = |Y_2|$
- Pixel-by-pixel update step:

While $(\min_{Y_1} D\mathcal{J} + \min_{Y_2} D\mathcal{J}) < 0$, exchange the two pixels where the minima are reached



Pixel-by-pixel two-directions optimization - cost functional and dispersions



Computational remarks:

- 241 iterations
- 1205 cell and adjoint cell problems i.e. **2892 scalar cell problems** on a 32×32 grid
- Moulinec-Suquet FFT method (tolerance on relative residual error: 10^{-8}) implemented using Python.

⇒ \approx 15-20s on a (good) laptop.

Level-set representation and projection algorithm

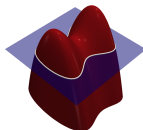
[Amstutz and Andrä, 2006, Amstutz, 2011]

- 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 $\bar{\mathcal{D}}\mathcal{J}$:

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



(Wikipedia)

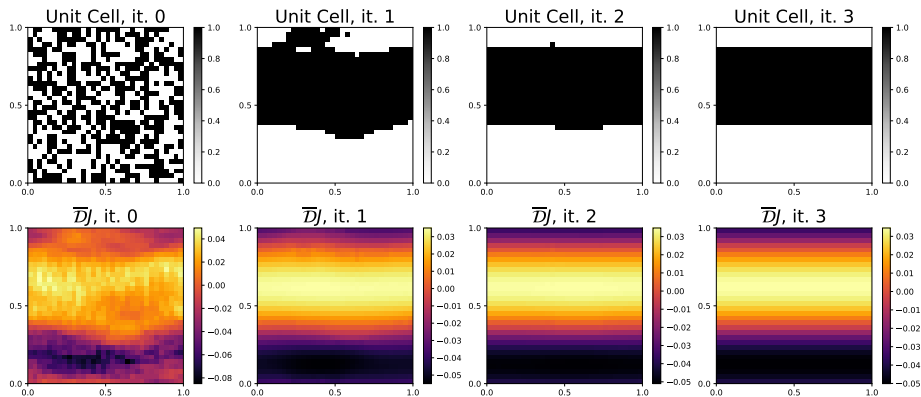
Optimality condition: If $\bar{\mathcal{D}}\mathcal{J}$ satisfies the sign condition $(*)$ then $\mathcal{D}\mathcal{J}(z) > 0 \quad \forall z \in Y$
then \mathcal{J} reached a **local minimum**

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

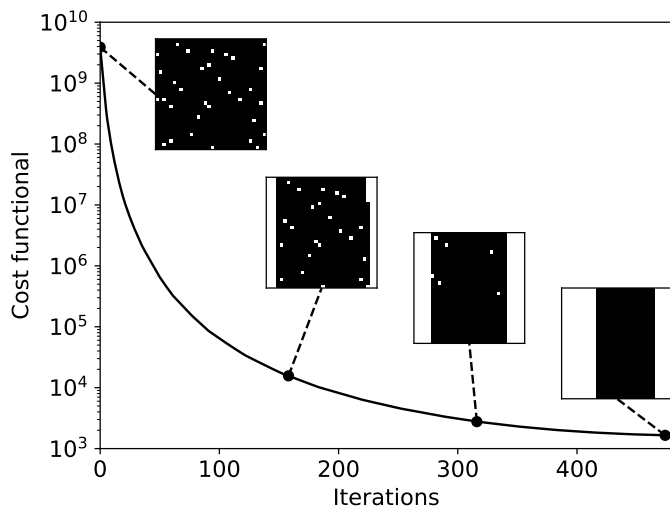
$$\psi^{n+1} = a_n \psi^n + b_n \bar{\mathcal{D}}\mathcal{J}(\psi^n)$$

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

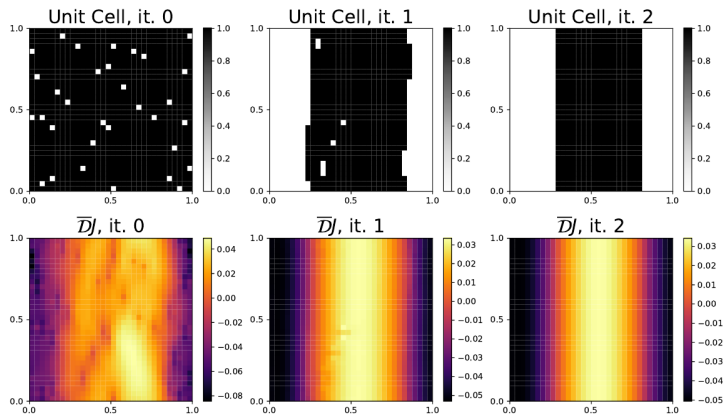
Two-directions optimization by projection algorithm (with phase ratio constraint $|Y_1| = |Y_2|$)



One-by-one pixels vs level-set



One-by-one pixels vs level-set



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- Level-set algorithm on a first example
- **Examples : anisotropic dispersion optimization and data fitting**

3 Microstructured interface optimization

- Effective model, cell/band problems and FFT-based solver
- Optimization problem, topological sensitivity
- Examples

4 Key ideas and perspectives

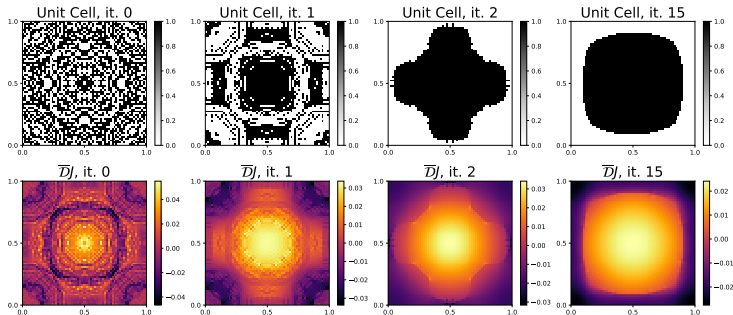
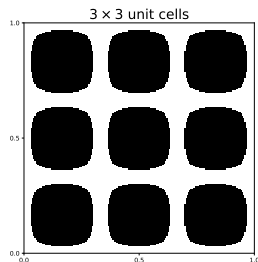
Maximizing horizontal and vertical and minimizing diagonal dispersions

- Recall : $c(k, \mathbf{d}) = c_0(\mathbf{d}) + \frac{1}{2}(k\ell)^2 \frac{\gamma(\mathbf{d})}{c_0(\mathbf{d})} + o((k\ell)^2)$
- Cost functional:

$$J_{4d} = \frac{1}{2} \sum_{j=1}^2 \left(\frac{\gamma(\mathbf{d}_j)}{c_0(\mathbf{d}_j)} \right)^{-2} + \frac{1}{2} \sum_{j=3}^4 10 \left(\frac{\gamma(\mathbf{d}_j)}{c_0(\mathbf{d}_j)} \right)^2$$

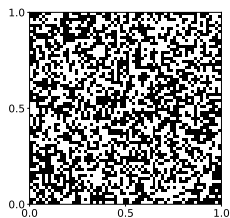
$$\mathbf{d}_j = (\cos \theta_j, \sin \theta_j), \quad \theta_{1,2} = 0, 90^\circ, \quad \theta_{3,4} = \pm 45^\circ$$

- Material ratios: $\mu_2/\mu_1 = 6$ and $\rho_2/\rho_1 = 1.5$

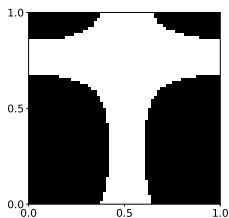


Other initializations with the same result

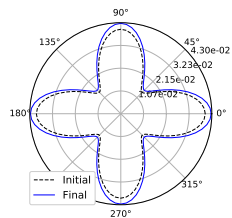
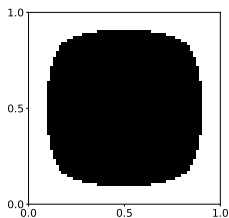
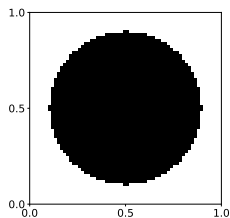
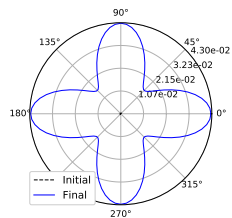
Initial cell



Final cell

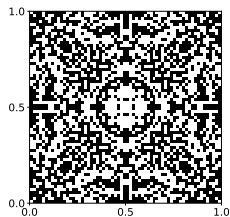


Dispersion indicator $\frac{\gamma(\mathbf{d})}{c_0(\mathbf{d})}$

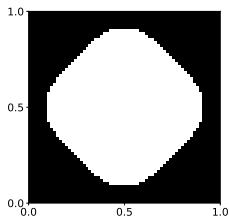


Initializations leading to sub-optimal results

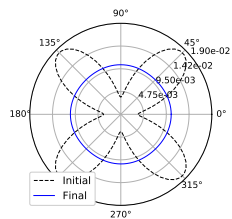
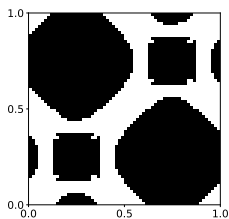
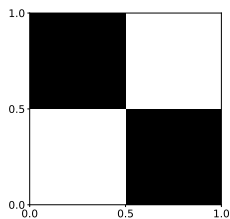
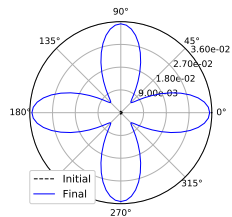
Initial cell



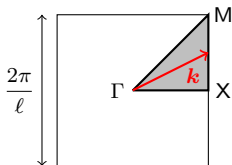
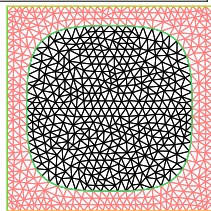
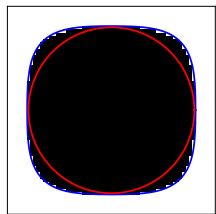
Final cell



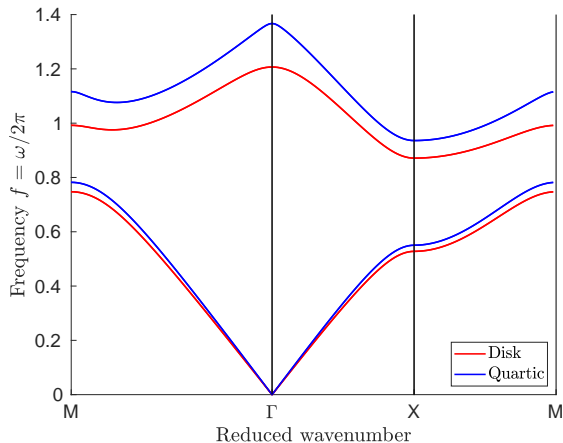
Dispersion indicator $\frac{\gamma(\mathbf{d})}{c_0(\mathbf{d})}$



Bloch-Floquet analysis of the optimal unit cell



- Fit of the optimal inclusion by a quartic curve.
- Finite element meshing using `FREEFEM++` [Hecht, 2012, Laude, 2015]
- Computation of the first two Bloch frequencies in the reduced Brillouin zone.



Fitting an objective anisotropic phase velocity c^{obj}

- **Goal:** fitting phase velocity:

$$c^{\text{obj}}(k_p, \mathbf{d}_j) = c_0^{\text{obj}}(\mathbf{d}_j) + \Delta c^{\text{obj}}(k_p, \mathbf{d}_j), \quad p = 1..N_k, \quad j = 1..N_\theta$$

- Quasistatic and dispersive least-square cost functionals:

$$\mathcal{J}^{\text{stat}} = \frac{1}{2} \sum_{j=1}^{N_\theta} \left[c_0(\mathbf{d}_j) - c_0^{\text{obj}}(\mathbf{d}_j) \right]^2, \quad \mathcal{J}^{\text{dyn}} = \frac{1}{2} \sum_{j=1}^{N_\theta} \sum_{p=1}^{N_k} \left[\Delta c(k_p, \mathbf{d}_j) - \Delta c^{\text{obj}}(k_p, \mathbf{d}_j) \right]^2$$

- Weighted total cost functional:

$$\mathcal{J} = \alpha \mathcal{J}^{\text{stat}} + \mathcal{J}^{\text{dyn}}$$

Example: chessboard reconstruction

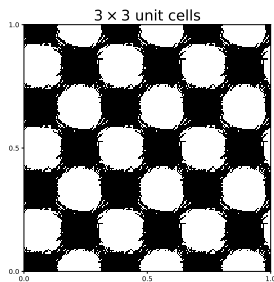
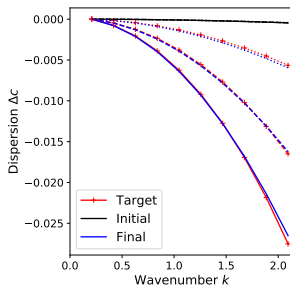
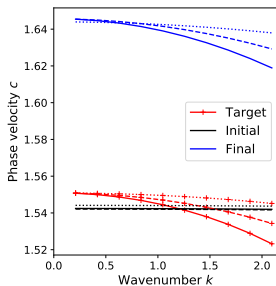
$\mu = 7$ $\rho = 1.2$	$\mu = 1$ $\rho = 1$
$\mu = 1$ $\rho = 1$	$\mu = 7$ $\rho = 1.2$

Data and constraints:

- $c^{\text{obj}} = c^{\text{chess}}$ (Floquet-Bloch, $N_\theta = 7$, $N_k = 10$)
- Exact material ratios
- Exact phase ratio $|Y_1| = |Y_2| = 1/2$

Chessboard reconstruction from phase velocity data

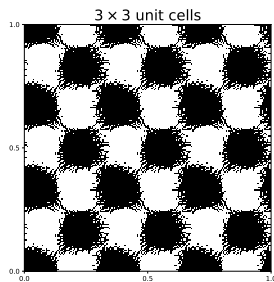
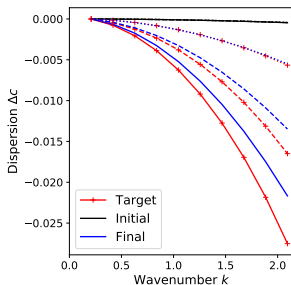
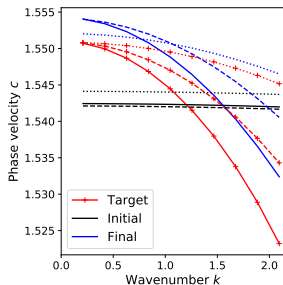
$$\alpha = 0 \quad (\mathcal{J} = \mathcal{J}^{\text{dyn}})$$



- : $\theta = -\pi/4$
- - - : $\theta = -\pi/8$
- ⋯ : $\theta = 0$

Chessboard reconstruction from phase velocity data

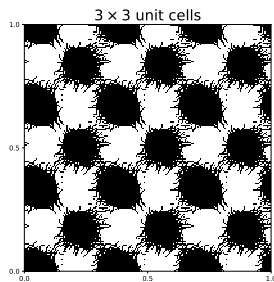
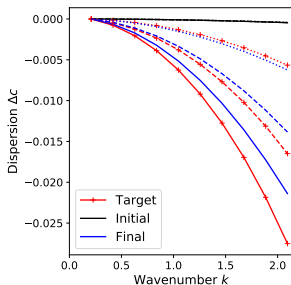
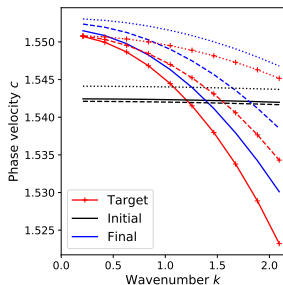
$$\alpha = 0.1$$



- : $\theta = -\pi/4$
- - - : $\theta = -\pi/8$
- ⋯ : $\theta = 0$

Chessboard reconstruction from phase velocity data

$$\alpha = 0.2$$



- : $\theta = -\pi/4$
- - - : $\theta = -\pi/8$
- ⋯ : $\theta = 0$

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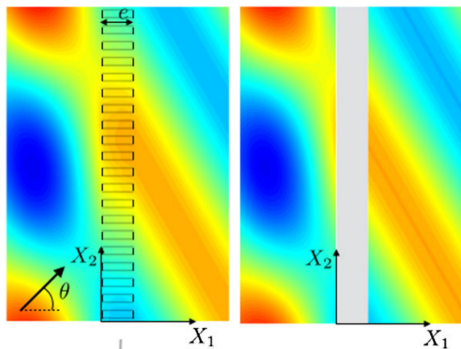
- Second-order homogenization, cell problems, FFT-based solver
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- Examples : anisotropic dispersion optimization and data fitting

3 Microstructured interface optimization

- Effective model, cell/band problems and FFT-based solver
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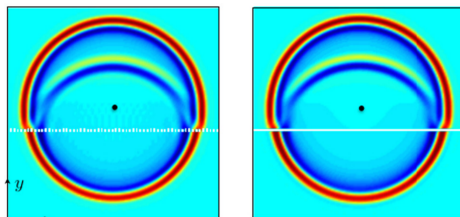
4 Key ideas and perspectives

Microstructured interfaces and effective transmission conditions



Frequency domain [Marigo et al., 2017]

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



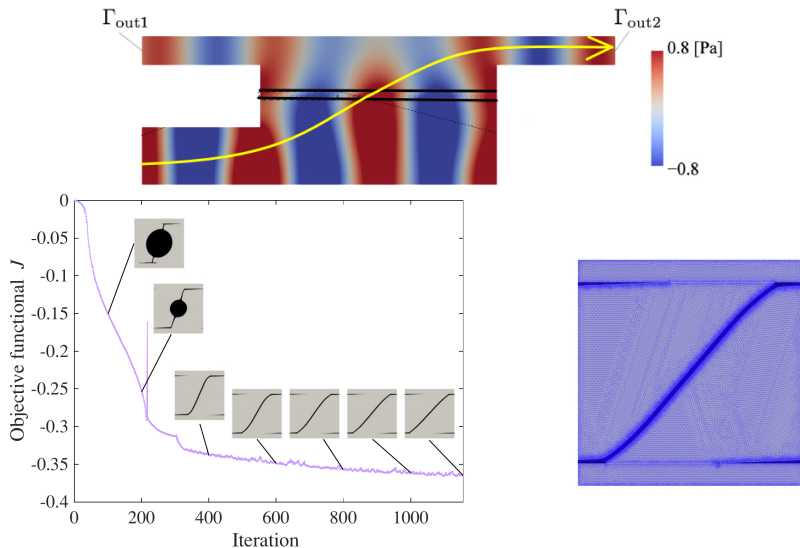
Time domain, rigid inclusions

[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 ?

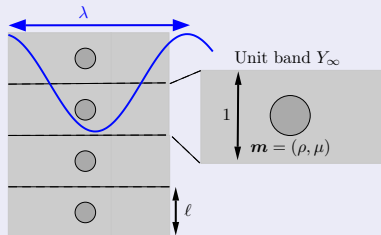
An example from [Noguchi and Yamada, 2021b]



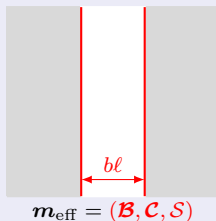
Noguchi, Y. & Yamada, T. *Topology optimization of acoustic metasurfaces by using a two-scale homogenization method* Applied Mathematical Modelling, 2021

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

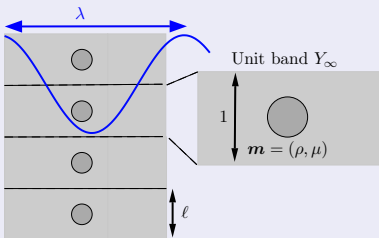
2 Optimization for scalar waves in bi-periodic media

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- **Effective model, cell/band problems and FFT-based solver**
- Optimization problem, topological sensitivity
- Examples

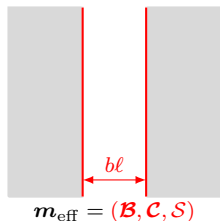
4 Key ideas and perspectives



- 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: $\varepsilon = \ell/\lambda \ll 1$
- Double scale dependency **and matched asymptotic expansions.**

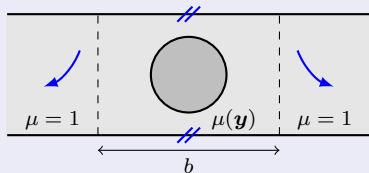


Effective model for **macroscopic fields** (V, S) :

$$\left\{ \begin{array}{l} \rho_m \frac{\partial V}{\partial t} = \nabla \cdot S \\ \frac{\partial S}{\partial t} = \mu_m \nabla V \\ [V]_{bl} = \ell \mathbf{B} \cdot \langle \nabla V \rangle_{bl} \\ [S_1]_{bl} = \ell \mathbf{S} \cdot \langle \nabla \cdot S \rangle_{bl} - \ell \mathbf{C} \cdot \langle \nabla S_2 \rangle_{bl} \end{array} \right. \quad \begin{array}{l} |X_1| > \frac{bl}{2} \\ |X_1| > \frac{bl}{2} \end{array}$$

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

Band problem



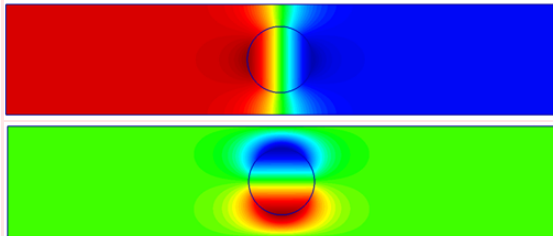
Original problem in **infinite band**:
(normalized “fast” coordinate $\mathbf{y} = \mathbf{x}/\ell$)

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

Φ is periodic in the y_2 variable

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

Computations in artificially bounded domain:

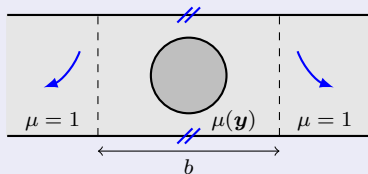


Effective coefficients [Marigo et al., 2017]

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

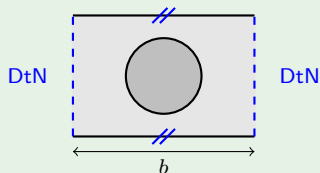
$$\mathcal{C} = \int_{Y_\infty} \mu(\mathbf{y}) \partial_2 \Phi(\mathbf{y}) \, d\mathbf{y} + \mathbf{g}(b, \mu)$$

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



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:

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

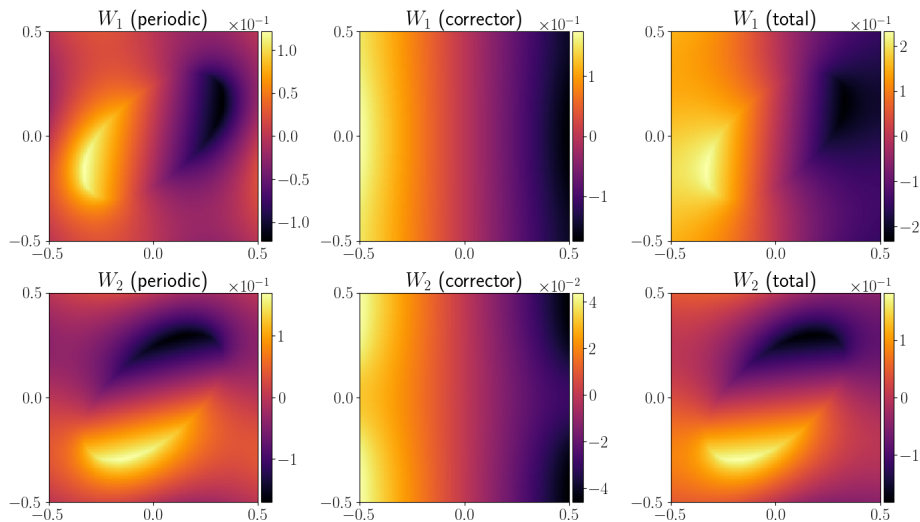
Λ : **Dirichlet-to-Neumann (DtN) operator**.
 $(\mathcal{B}, \mathcal{C})$ have expressions implying only integrals on Y_b

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:

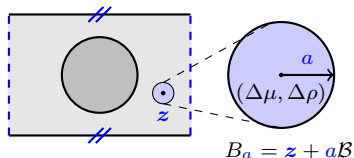
- Constraints and parametrization of \mathbf{m} , e.g. **piecewise uniform materials**
- **Iterative “material update” algorithms**

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

- 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: $m \rightarrow m_a = m + \chi_{B_a} \Delta m$

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

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

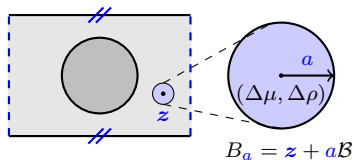
If $\mathcal{D}\mathcal{J}(z) < 0$, then $\mathcal{J}(m_a) < \mathcal{J}(m)$ and therefore z is a good choice for a phase change !

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

$$\mathcal{D}\mathcal{J} = \frac{\partial J}{\partial m_{\text{eff}}} \mathcal{D}m_{\text{eff}}$$

\Rightarrow Need to compute ($\mathcal{D}B, \mathcal{D}C, \mathcal{D}S$)

Example : topological derivative of \mathcal{S}



By definition :

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

Exact expansion:

$$\mathcal{S}_a = \mathcal{S} + a^2 \underbrace{\frac{\Delta\rho}{\rho_m} |\mathcal{B}|}_{\mathcal{DS}}$$

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

Topological derivatives

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

$$\mathcal{D}S(\mathbf{m}, \mathbf{z}, \mathcal{B}, \Delta\mathbf{m}) = \frac{\Delta\rho}{\rho_{\mathbf{m}}} |\mathcal{B}|,$$

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

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

depend on

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

Numerical validation

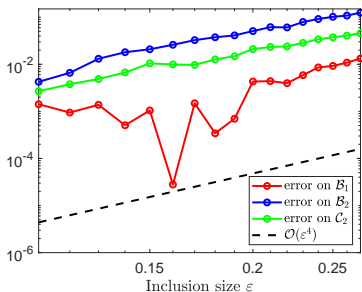
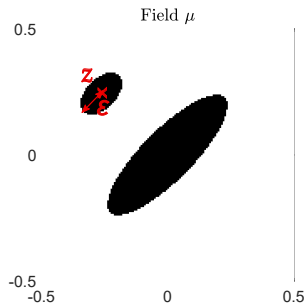
- Leading-order approximation of homogenized coefficients e.g.

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

- Computation of relative error e.g. :

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

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



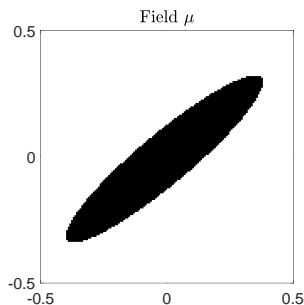
\Rightarrow Error in $O(a^4)$ and $< 15\%$ (even for "big" perturbations $a = 0.25$)
(term in a^3 vanishes, should be true for *any centrally-symmetric shape* \mathcal{B} [Bonnet, 2009])

Approximative effective coefficients for elliptic inclusions

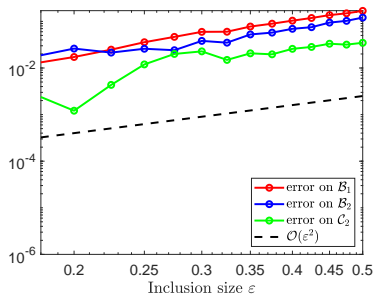
Particular case: one inclusion B_a in an **homogeneous** cell ($\Phi = 0$)

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

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



Case $a = 0.5$



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

Outline

1 Introduction

2 Optimization for scalar waves in bi-periodic media

- Second-order homogenization, cell problems, FFT-based solver
- Optimization problem, cost functional, topological sensitivity
- Level-set algorithm on a first example
- Examples : anisotropic dispersion optimization and data fitting

3 Microstructured interface optimization

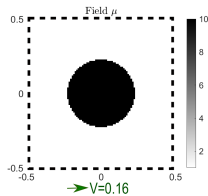
- Effective model, cell/band problems and FFT-based solver
- Optimization problem, topological sensitivity
- Examples

4 Key ideas and perspectives

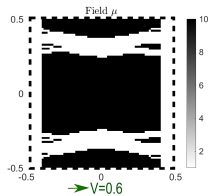
A first test [Touboul, Ph.D. Thesis, 2021 (Chap. 4)]

- **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

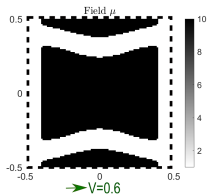
$$\mathcal{J} = |\mathcal{R}|^2 + \lambda \left(\frac{|Y_2|}{V_C} - 1 \right)^2 + \alpha_{\text{per}} \text{Per}(Y_2) \quad (\lambda: \text{iteratively chosen weight})$$



Initial unit cell



Final unit cell



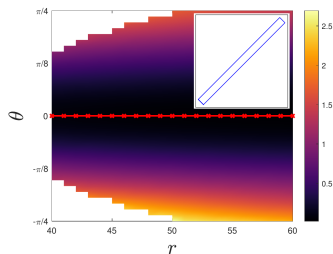
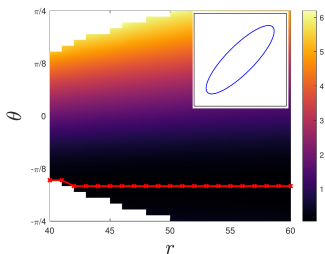
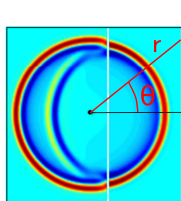
with **perimeter penalization**



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 $\theta_1 = \theta_{\min}$.

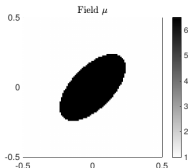
- Main cost functional:

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

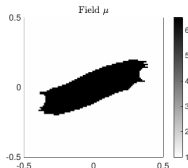
Results for $\theta_{\min} = 0$, $V_C = 0.2$, perimeter penalisation

Initialisations:

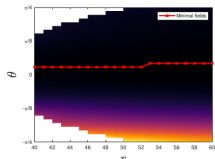
ellipse at 45°



(d)

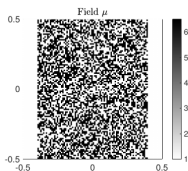


(e)

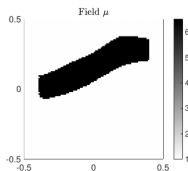


(f)

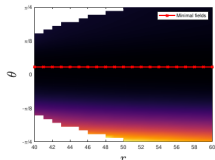
Random distribution



(g)

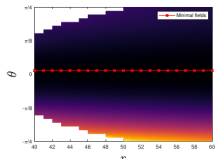
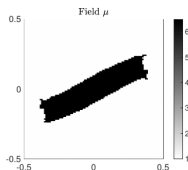
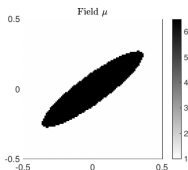


(h)



(i)

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



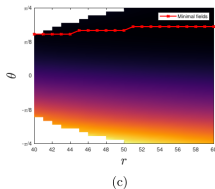
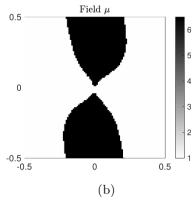
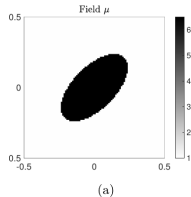
Performances for for $\theta_{\min} = 0$, $V_C = 0.2$

	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	$1.02 \cdot 10^{-1}$	$6.76 \cdot 10^{-2}$	$3.61 \cdot 10^{-1}$	$2.1 \cdot 10^{-3}$

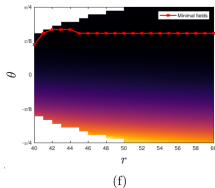
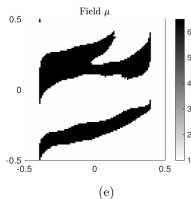
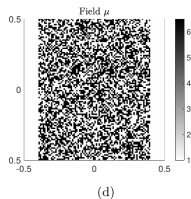
Results for $\theta_{\min} = \pi/4$, $V_C = 0.3$, perimeter penalisation

Initialisations:

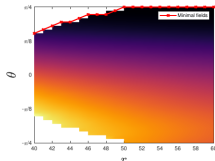
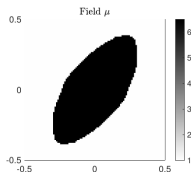
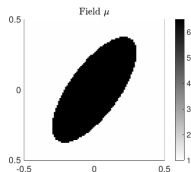
ellipse at 45°



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	$6.27 \cdot 10^{-2}$	$2.96 \cdot 10^{-2}$	$3.30 \cdot 10^{-3}$	$8.76 \cdot 10^{-5}$

Key ideas

- A topological optimization procedure is proposed, combining
 - ▶ **Effective models** obtained via two-scale asymptotic homogenization
 - ▶ **FFT-based algorithms** to solve cell problems
 - ▶ **Topological derivatives** to **propose initialisations** and guide the updating steps
 - ▶ **Level-set projection algorithm** (with **volume** and **perimeter** constraints)
- The procedure is applied to various cost functionals to achieve
 - ▶ Maximization of dispersion in given directions
 - ▶ “De-homogenization” of a chessboard from phase velocity data.
 - ▶ Attenuation of scattered energy in chosen direction.

Perspectives / ongoing

- Time-domain simulations of waves in the designed materials
- Extensions to other other physics and regimes:
 1. **Elasticity**: links with **strain/stress gradient models** [Auffray et al., 2015, Rosi and Auffray, 2019].
 2. **High frequencies** [Craster et al., 2010, Guzina et al., 2019] to optimize **band-gaps** ...
 3. **Resonant interfaces** with high-contrast inclusions [Pham et al., 2017, Touboul et al., 2020]
 4. **Graded / quasi-periodic** interfaces [Noguchi and Yamada, 2021a, Pham et al., 2023]
- Improve the optimization algorithm
 - ▶ Couple shape and topological derivative [Allaire et al., 2005, Amstutz et al., 2018]
 - ▶ Use optimized FFT solvers ⇒ **go to 3D**

Thank you for your attention !
And thanks to Bruno, Bojan, all lecturers and CISM for this fantastic school !

- *Microstructural topological sensitivities of the second-order macroscopic model for waves in periodic media.*
Marc Bonnet, Rémi Cornaggia, Bojan B. Guzina,
SIAM Journal on Applied Mathematics, 2018
- *Tuning effective dynamical properties of periodic media by FFT-accelerated topological optimization*
Rémi Cornaggia, Cédric Bellis
International Journal for Numerical Methods in Engineering, 2020
- *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
Preprint on HAL: <https://hal.science/hal-04180360>

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