Modeling and controlling dispersive waves in architected materials : second-order homogenization and topological optimization

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joint work with Bojan B. Guzina, Marc Bonnet, Cédric Bellis and Bruno Lombard

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SORBONNE UNIVERSITÉ

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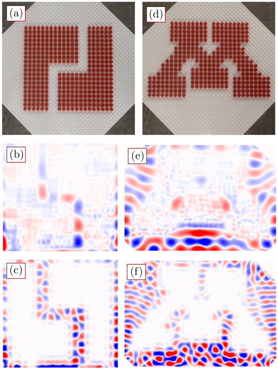
Control of wave propagation using periodic structures



[Celli and Gonella, 2015]

... to design waveguides

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

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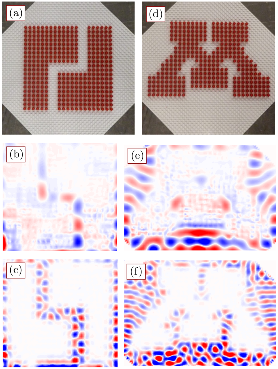

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... to design waveguides

- with resonators for long wavelengths / low frequencies
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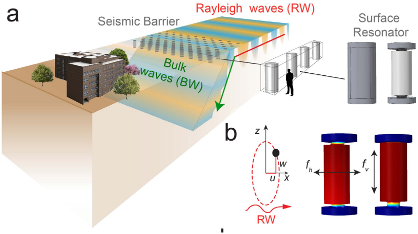
... to design seismic protections (with resonators)



[Palermo et al., 2016]

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

Modeling and optimisation

How to model the wave propagation in periodic structures ?

- Accounting for all interactions $\rightarrow$ costly
- *Floquet-Bloch* theory
- *Homogenization* (/averaging/effective) methods and models
- **This work:** *asymptotic double-scale homogenization*
  - Formal procedure to obtain effective models
  - Accuracy can be improved by pushing the expansion to higher orders
  - Extensions to *high frequencies* [Craster et al., 2010, Guzina et al., 2019]

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How to obtain desired properties ?

- Known design (cylinders, spheres, cones, LEGO bricks ...) $\Longrightarrow$ *parameter optimization* [Huang et al., 2016, Palermo et al., 2016] ...
- Given materials, unknown design $\Longrightarrow$ *topological optimization* [Vondřejc et al., 2017, Kook and Jensen, 2017, Allaire and Yamada, 2018] ...
- **This work:** topological optimization of *dispersive properties* (long wavelengths, no resonances)

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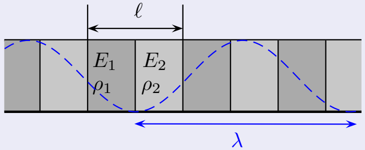
Two-scale asymptotic homogenization in a 1D periodic medium



- Wave equation in a ℓ-periodic medium

$$\rho\left(\frac{X}{\ell}\right)\frac{\partial^2 u_\ell}{\partial t^2} - \frac{\partial}{\partial X}\left[E\left(\frac{X}{\ell}\right)\frac{\partial u_\ell}{\partial X}\right] = 0$$

- *Reference wavelength* λ

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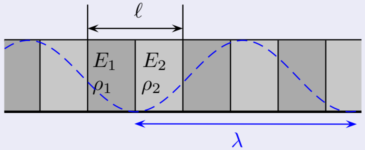

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[Sanchez-Palencia, 1974, Bensoussan et al., 1978, Cioranescu and Donato, 1999] ...

- **Scale separation** $\varepsilon = \ell/\lambda \ll 1$
- **Slow variable** $x = X/\lambda$ and **fast variable** $y = X/\ell = x/\varepsilon$
- Look for u_ℓ as a **function of both variables**: $u_\ell(X;t) = \hat{u}(x,y;t)$, **1-periodic in** y

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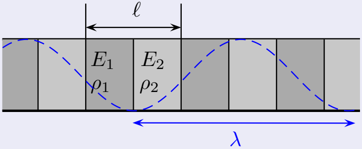

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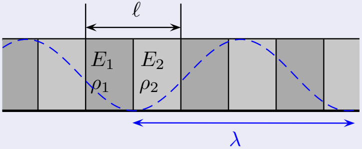

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- **Separated variable solution** featuring mean fields $U_j(x;t)$ and cell functions $P_j(y)$:

$$\begin{aligned}
u_0(x,y;t) &= U_0(x;t)\\
u_1(x,y;t) &= U_1(x;t) + U_{0,x}(x;t)P_1(y)\\
u_2(x,y;t) &= U_2(x;t) + U_{1,x}(x;t)P_1(y) + U_{0,xx}(x;t)P_2(y)
\end{aligned}$$

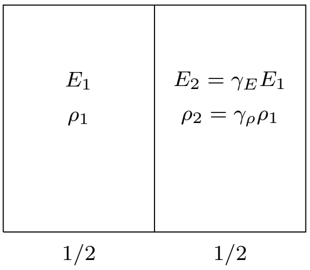
Cell functions

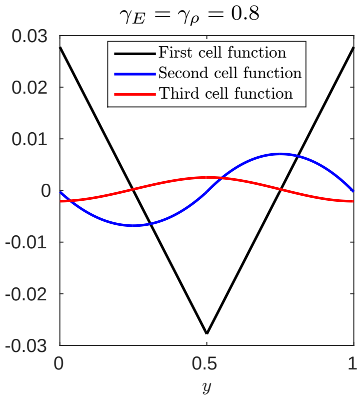
(P_1, P_2, P_3): *static* equilibrium problems posed in the unit cell $Y = [0,1]$

$$[E(1+P_{1,y})]_{,y} = 0 \quad \text{in } Y, \quad P_1 \text{ is } Y\text{-periodic}, \quad \langle P_1 \rangle = 0$$

$$[E(P_1+P_{2,y})]_{,y} = \mathcal{E}_0 \frac{\rho}{\varrho_0} - E(1+P_{1,y}) \quad \text{in } Y, \quad P_2 \text{ is } Y\text{-periodic}, \quad \langle P_2 \rangle = 0$$

$$[E(P_2+P_{3,y})]_{,y} = \mathcal{E}_0 \frac{\rho}{\varrho_0} P_1 - E(P_1+P_{2,y}) \quad \text{in } Y, \quad P_3 \text{ is } Y\text{-periodic}, \quad \langle P_3 \rangle = 0$$





Mean fields equations

- Equations satisfied by the mean fields:

$$\varrho_0 U_{0,tt} - \mathcal{E}_0 U_{0,xx} = 0 \qquad \left| \begin{aligned} \varrho_0 &= \langle \rho \rangle \\ \mathcal{E}_0 &= \langle E(1 + P_{1,y}) \rangle \end{aligned} \right.$$

$$\varrho_0 U_{1,tt} - \mathcal{E}_0 U_{1,xx} = 0 \qquad \mathcal{E}_1 = \frac{\varrho_1}{\varrho_0} \mathcal{E}_0 \Rightarrow \text{no first-order contribution}$$

$$\varrho_0 U_{2,tt} - \mathcal{E}_0 U_{2,xx} + \varrho_2 U_{0,xxtt} - \mathcal{E}_2 U_{0,xxxx} = 0 \qquad \left| \begin{aligned} \varrho_2 &= \langle \rho P_2 \rangle \\ \mathcal{E}_2 &= \langle E(1 + P_{3,y}) \rangle \end{aligned} \right.$$

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- Second-order **total mean field** $U = U_0 + \varepsilon U_1 + \varepsilon^2 U_2$:

$$\varrho_0 U_{,tt} - \mathcal{E}_0 U_{,xx} + \varepsilon^2 \left(\varrho_2 U_{0,xxtt} - \mathcal{E}_2 U_{0,xxxx} \right) = 0$$

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- Using (i) $\varrho_0 U_{0,tt} = \mathcal{E}_0 U_{0,xx}$ and (ii) $U_0 = U + o(1)$ [Wautier and Guzina, 2015] :

$$\frac{1}{c_0^2} U_{,tt} - U_{,xx} - \varepsilon^2 \left(\beta_x U_{,xxxx} - \frac{\beta_m}{c_0^2} U_{,xxtt} - \frac{\beta_t}{c_0^4} U_{,tttt} \right) = 0 \qquad \text{at order } O(\varepsilon^2)$$

with $c_0^2 = \dfrac{\mathcal{E}_0}{\varrho_0}$ and $\beta_x - \beta_m - \beta_t = \beta := \left[\dfrac{\mathcal{E}_2}{\mathcal{E}_0} - \dfrac{\varrho_2}{\varrho_0} \right]$

Link with gradient elasticity models

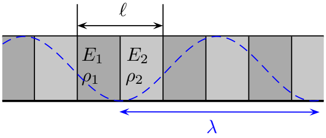
$$\frac{1}{c_0^2}\left[1+\varepsilon^2\beta_m\partial_{xx}+\varepsilon^2\frac{\beta_t}{c_0^2}\partial_{tt}\right]U_{,tt}=\left[1+\varepsilon^2\beta_x\partial_{xx}\right]U_{,xx},\quad \text{with}\quad \beta_x-\beta_m-\beta_t=\beta>0$$

	Gradient elasticity (see [Askes and Aifantis, 2011])	Two-scale homogenization	
(x)	[Mindlin, 1964]	"natural" result when $\rho = 1$ [Fish and Chen, 2001]	unstable if $\beta_x > 0$ [Allaire et al., 2016]
(m)		[Fish et al., 2002, Lamacz, 2011]	stable if $\beta_m < 0$
(t)	?	?	?
(xm)	[Mindlin, 1964]	"natural" result for $\rho \neq 1$ Used to stabilize (x)	
(mt)	[Pichugin et al., 2008] [Forest and Sab, 2017]	[Cornaggia and Guzina, 2020]	
(xmt)	[Dontsov et al., 2013]	[Wautier and Guzina, 2015]	

$\beta_x \neq 0 \Longrightarrow$ *additional boundary conditions* for bounded domains

- Some attempts for *well-posed* gradient elasticity models [Askes et al., 2008, Kaplunov and Pichugin, 2009]
- Difficult to deal with in homogenization theory (proofs when $\varepsilon \to 0$?)

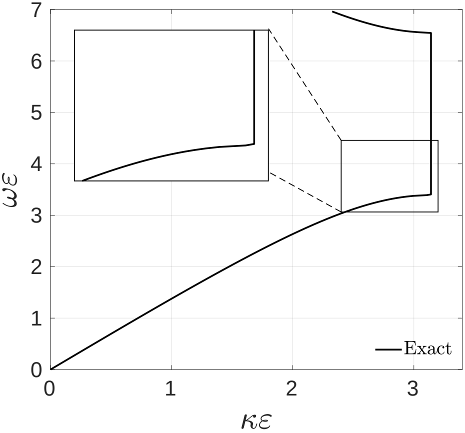
Choosing a model by fitting dispersion curves



Material contrasts: $\dfrac{E_2}{E_1} = 6, \quad \dfrac{\rho_2}{\rho_1} = 1.5$

Phase ratio: $\dfrac{\ell_2}{\ell_1} = 3$

(≈ maximal dispersion [Santosa and Symes, 1991])



- Bloch wave: $u(x, y; t) = \phi(y)e^{\mathrm{i}(\kappa x - \omega t)}$
  $\Longrightarrow$ *Dispersion relation* $\kappa = f(\omega)$

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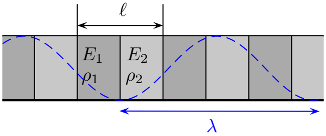

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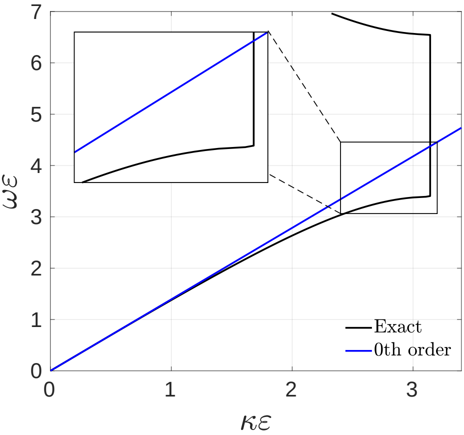

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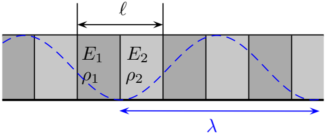

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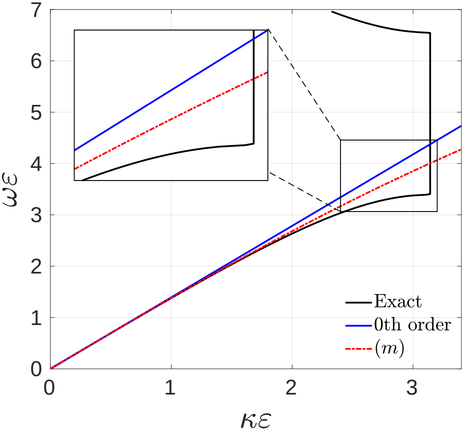

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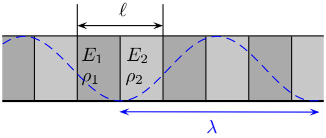

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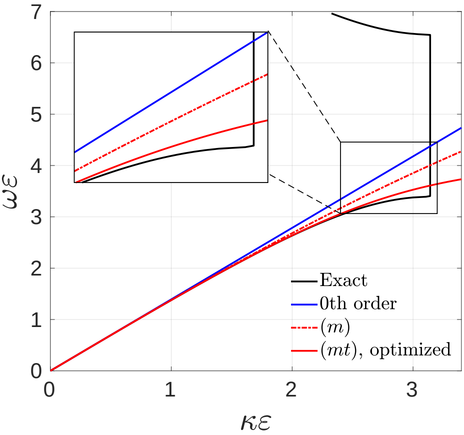

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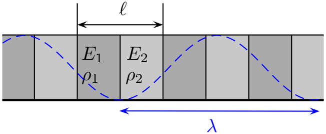

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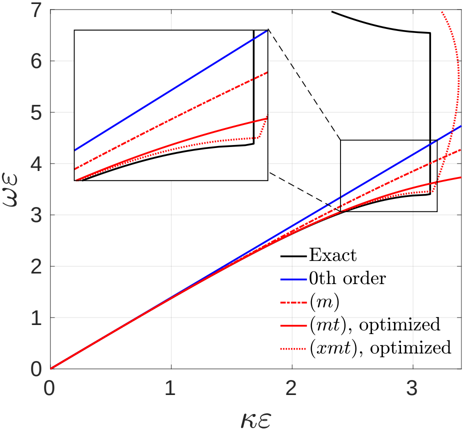

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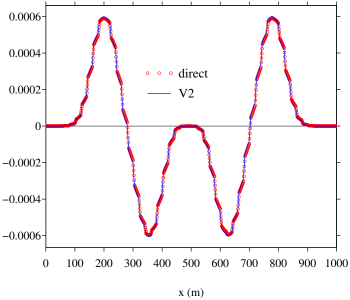
- Optimized (xmt) model, up to the *first band-gap* [Wautier and Guzina, 2015]

$\beta_x \neq 0 \implies$ *additional boundary conditions.*

Wave propagation in an infinite bilayered material
Fixed ℓ, increasing frequency (Numerics by B. Lombard)



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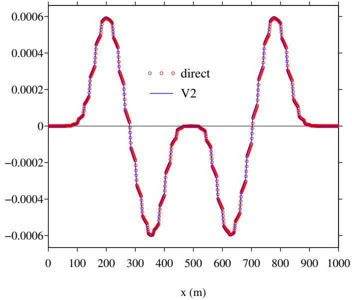

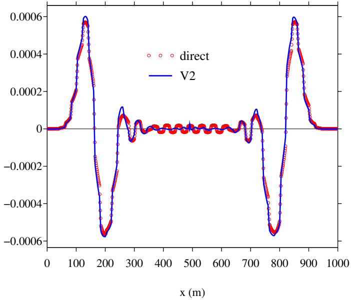

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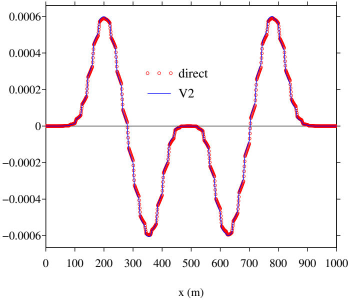

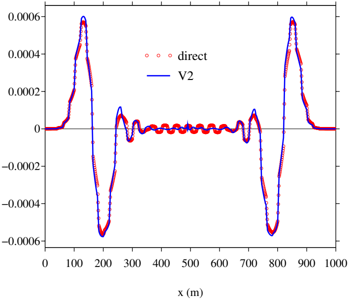

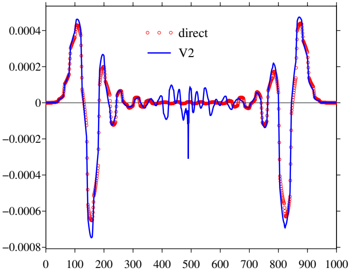

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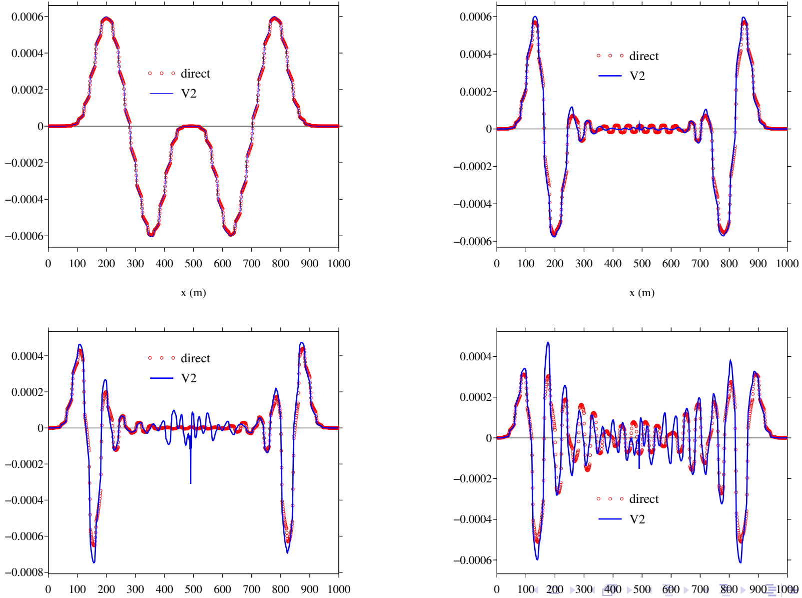

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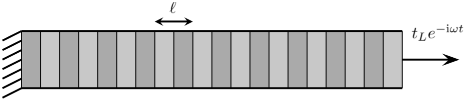
Model problem and leading-order approximation



- Time-harmonic model problem:

$$\left|\begin{array}{ll} \left[E(x/\varepsilon)u_{,x}\right]_{,x} + \rho(x/\varepsilon)\,\omega^2 u = 0 & x \in Y_L :=]0, L[\\ u = 0 & x = 0 \\ \sigma = E(x)u_{,x} = \sigma_L & x = L \end{array}\right.$$

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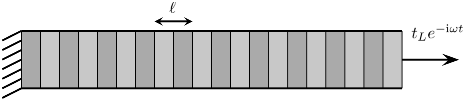

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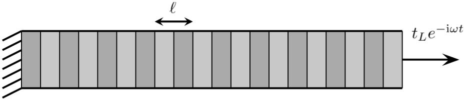
$$

- Leading-order homogenization: $(u, \sigma) \to (U, \mathcal{E}_0 U_{,x})$ with $U = U_0$

$$
\left|\begin{array}{lll}
U_{,xx} + k_0^2\, U = 0 & x \in Y_L, & k_0 := \omega / c_0 \\
U = 0 & x = 0 & \\
U_{,x} = \sigma_L / \mathcal{E}_0 & x = L &
\end{array}\right.
$$

Model problem and leading-order approximation



- Time-harmonic model problem:

$$\begin{vmatrix} \left[E(x/\varepsilon)u_{,x}\right]_{,x} + \rho(x/\varepsilon)\,\omega^2 u = 0 & x \in Y_L :=]0, L[\\ u = 0 & x = 0 \\ \sigma = E(x)u_{,x} = \sigma_L & x = L \end{vmatrix}$$

- Leading-order homogenization: $(u, \sigma) \to (U, \mathcal{E}_0 U_{,x})$ with $U = U_0$

$$\begin{vmatrix} U_{,xx} + k_0^2\, U = 0 & x \in Y_L, & k_0 := \omega / c_0 \\ U = 0 & x = 0 & \\ U_{,x} = \sigma_L / \mathcal{E}_0 & x = L & \end{vmatrix}$$

- In 2-3D, *boundary layers* must be accounted for at boundaries and interfaces [Dumontet, 1986, Moskow and Vogelius, 1997, Allaire and Amar, 1999, Gérard-Varet and Masmoudi, 2012, Armstrong et al., 2017]
- *Equivalent boundary or transmission conditions* preserving the asymptotics are difficult to build [Vinoles, 2016, Marigo and Maurel, 2017, Maurel and Marigo, 2018]
- In 1D, “boundaries” are *points* and simple conditions are available ...

First-order approximation

- First-order approximations of the displacement and stress (u, σ):

$$\left.\begin{aligned} \tilde{u}^{(1)}(x) &= U(x) + \varepsilon P_1\left(\frac{x}{\varepsilon}\right)U_{,x}(x) \\ \tilde{\sigma}^{(1)}(x) &= \mathcal{E}_0\left[U_{,x}(x) + \varepsilon\Sigma_1\left(\frac{x}{\varepsilon}\right)U_{,xx}(x)\right] \end{aligned}\right\} U = U_0 + \varepsilon U_1$$

Cell stress functions: $\Sigma_j := (E/\mathcal{E}_0)\left[P_j + P_{j+1,y}\right]$

- Boundary-value problem for the first-order mean field U:

$$\left|\begin{aligned} &U_{,xx} + k_0^2\,U = 0 && x \in Y_L \\ &\tilde{u}^{(1)} = 0 && x = 0 \\ &\tilde{\sigma}^{(1)} = \sigma_L && x = L \end{aligned}\right.$$

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$$\left|\begin{array}{ll} U_{,xx} + k_0^2\, U = 0 & x \in Y_L \\ U + \varepsilon P_1(0) U_{,x} = 0 & x = 0 \\ U_{,x} + \varepsilon\Sigma_1(0) U_{,xx} = \sigma_L/\mathcal{E}_0 & x = L \end{array}\right.$$

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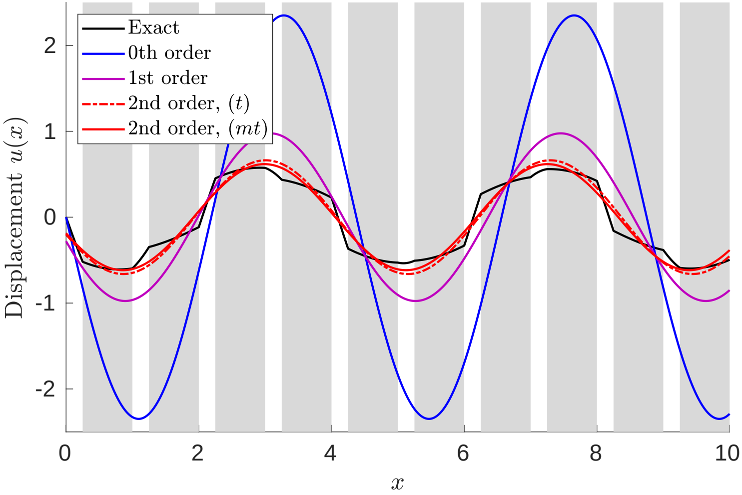
$$\left|\begin{array}{ll} U_{,xx} + k_0^2\, U = 0 & x \in Y_L \\ U + \varepsilon P_1(0) U_{,x} = 0 & x = 0 \\ U_{,x} - \varepsilon\Sigma_1(0) k_0^2\, U = \sigma_L/\mathcal{E}_0 & x = L \end{array}\right.$$

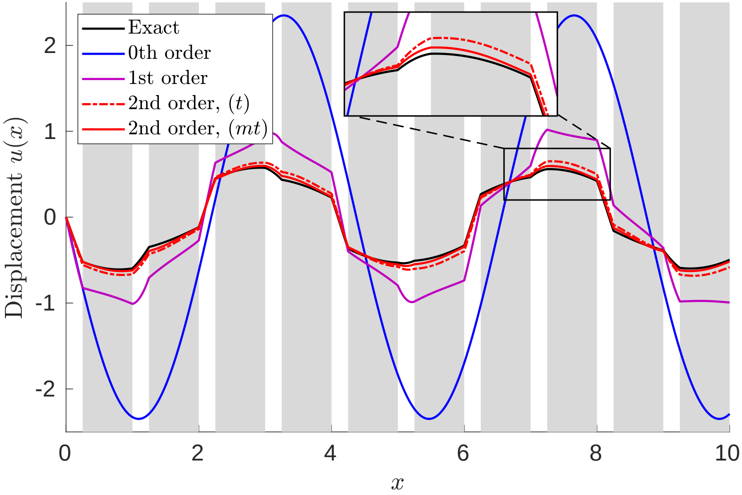
Example for a layered material - mean fields U

$$\varepsilon = \ell/\lambda_0 \approx 0.3$$



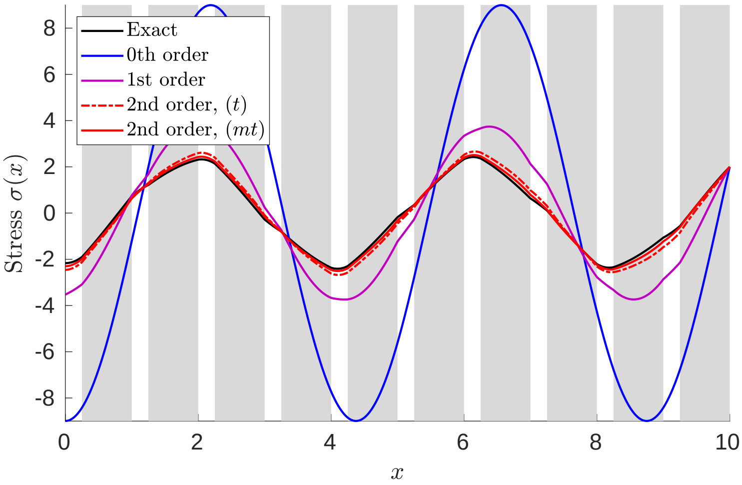
Example for a layered material - total displacement u

$$\varepsilon = \ell/\lambda_0 \approx 0.3$$

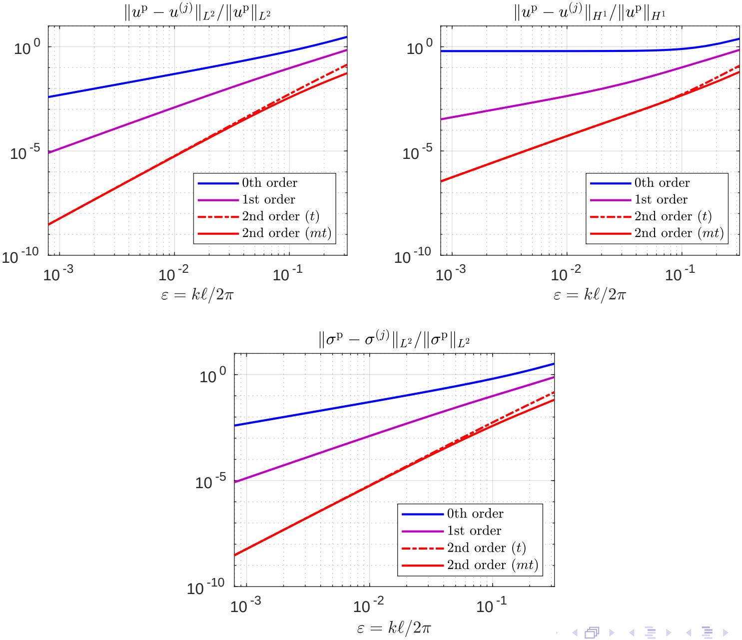


Example for a layered material - axial stress σ

$$\varepsilon = \ell/\lambda_0 \approx 0.3$$

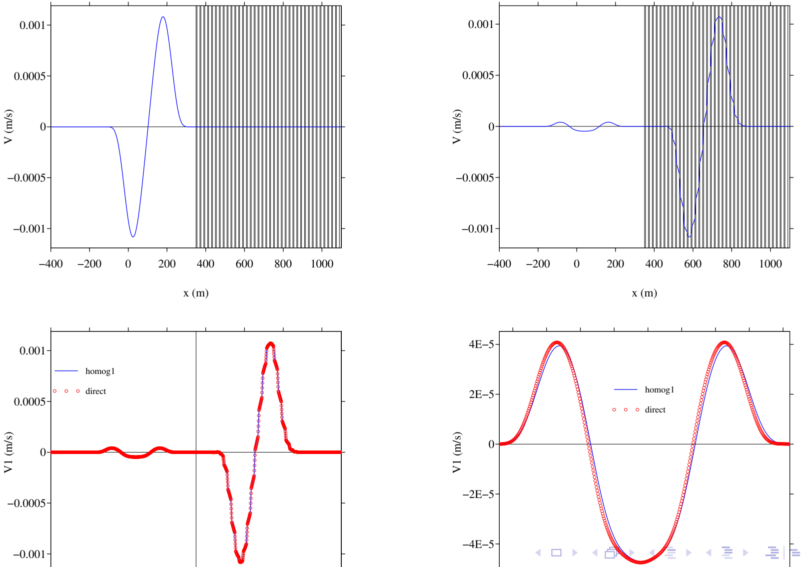


Errors for fixed ω and $\ell \to 0$ (proofs of convergence in [Cornaggia and Guzina, 2020])

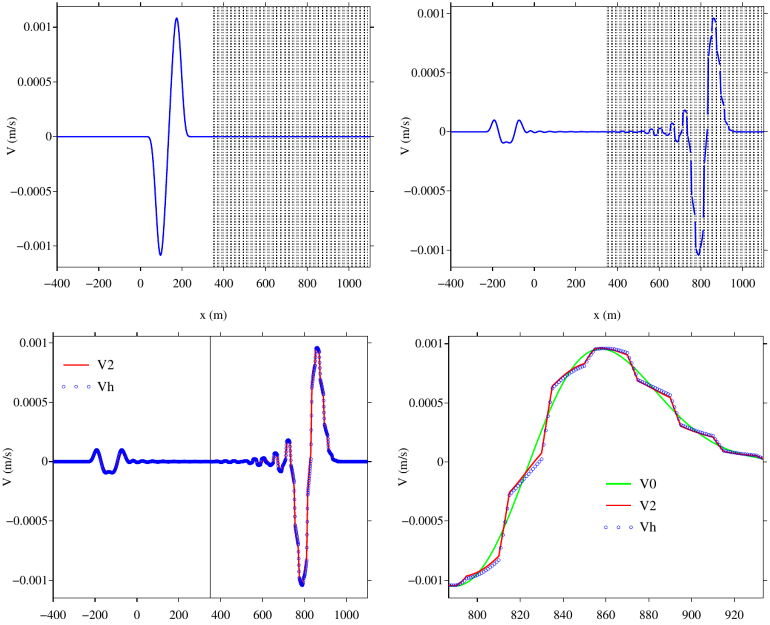


Transmission conditions in the time domain (Numerics by B. Lombard)

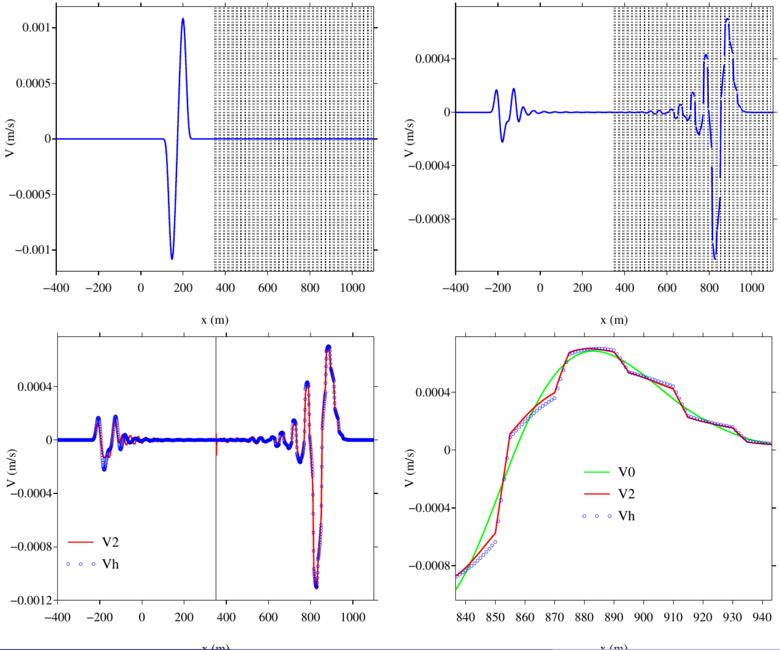
$E_{-}\rho_{-} = \mathcal{E}_0 \varrho_0 \Longrightarrow$ reflected wave due to 1st-order effects ($\varepsilon = \ell/\lambda_c \approx 0.04$)



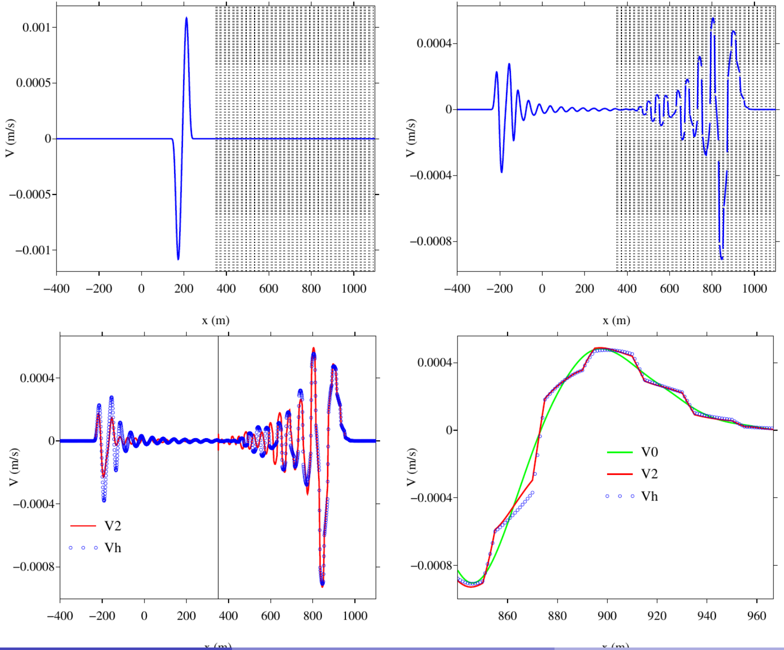
Transmission conditions, increasing central frequency, $\varepsilon \approx 0.09$



Transmission conditions, increasing central frequency, $\varepsilon \approx 0.13$



Transmission conditions, increasing central frequency, $\varepsilon \approx 0.17$

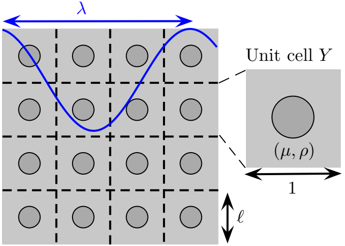


Outline

1. Introduction
2. Second-order asymptotic homogenization for waves in 1D bounded domains
   - Second-order models
   - Boundary and transmission conditions
3. Topological optimization in 2D: modeling tools
   - Dispersive model obtained by second-order homogenization
   - Optimization problem
   - Topological derivatives
   - Cell problems and FFT-based methods
4. Optimization algorithm and examples
   - Pixel-by-pixel approach
   - Level-set representation of the unit cell and projection algorithm
   - Fitting an objective phase velocity
5. Conclusions and perspectives

Second-order homogenization for waves in a periodic medium

[Bensoussan et al., 1978, Boutin and Auriault, 1993, Andrianov et al., 2008, Wautier and Guzina, 2015] ...



- Antiplane shear waves in the time-harmonic regime:

$$\text{div}\left[\mu\left(\frac{\boldsymbol{x}}{\ell}\right)\boldsymbol{\nabla}u_\ell\right] + \rho\left(\frac{\boldsymbol{x}}{\ell}\right)\omega^2 u_\ell = 0$$

- (μ, ρ): Y-periodic shear modulus and density
- Two-scale expansion for *long wavelengths* $\lambda > \ell$:

$$u_\ell(\boldsymbol{x}) = \underbrace{U(\boldsymbol{x})}_{\text{mean field}} + \underbrace{\ell\boldsymbol{\nabla}U(\boldsymbol{x})\cdot\boldsymbol{P}_1(\boldsymbol{x}/\ell) + \ldots}_{\text{oscillatory correctors}}$$

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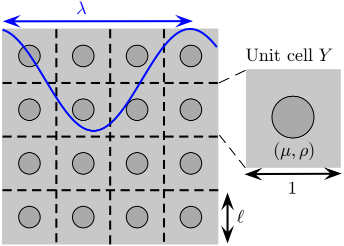

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Second-order homogenized equation for the mean field U:

$$\left[\boldsymbol{\mu}_0 + \ell^2 \boldsymbol{\mu}_2 : \boldsymbol{\nabla}^2\right] : \boldsymbol{\nabla}^2 U + \omega^2\left[\varrho_0 + \ell^2 \boldsymbol{\varrho}_2 : \boldsymbol{\nabla}^2\right] U = 0$$

$(\boldsymbol{\mu}_0, \varrho_0, \boldsymbol{\mu}_2, \boldsymbol{\varrho}_2)$: constant *tensors* obtained from *cell solutions* $(\boldsymbol{P}_1, \boldsymbol{P}_2, \boldsymbol{P}_3)$:

$$(Y, \mu, \rho) \implies \begin{cases} \boldsymbol{P}_1 = (P_1^1, P_1^2) \\ \boldsymbol{P}_2 = (P_2^{11}, P_2^{12}, P_2^{22}) \\ \boldsymbol{P}_3 = (P_3^{111}, P_3^{112}, P_3^{122}, P_3^{222}) \end{cases} \implies \begin{cases} \varrho_0 = \langle \rho \rangle = \text{mean of } \rho \text{ on } Y \\ \boldsymbol{\mu}_0 = \langle \mu(\boldsymbol{I} + \boldsymbol{\nabla} \boldsymbol{P}_1) \rangle \\ \boldsymbol{\varrho}_2 = \langle \rho \boldsymbol{P}_2 \rangle \\ \boldsymbol{\mu}_2 = \langle \mu(\boldsymbol{I} \otimes \boldsymbol{P}_2 + \boldsymbol{\nabla} \boldsymbol{P}_3) \rangle \end{cases}$$

Approximation of dispersion

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

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

$$= c_0(\boldsymbol{d}) + \frac{1}{2}\frac{\gamma(\boldsymbol{d})}{c_0(\boldsymbol{d})}(k\ell)^2 + o\left((k\ell)^2\right) \quad \text{as } k\ell \sim \frac{\ell}{\lambda} \to 0$$

$$c_0(\boldsymbol{d}) = \sqrt{\frac{\boldsymbol{\mu}_0}{\varrho_0} : (\boldsymbol{d}\otimes\boldsymbol{d})} \quad \text{and} \quad \gamma(\boldsymbol{d}) = \left[\frac{\boldsymbol{\varrho}_2 \otimes \boldsymbol{\mu}_0 - \varrho_0\boldsymbol{\mu}_2}{(\varrho_0)^2}\right] :: (\boldsymbol{d}\otimes\boldsymbol{d}\otimes\boldsymbol{d}\otimes\boldsymbol{d})$$

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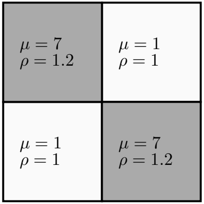
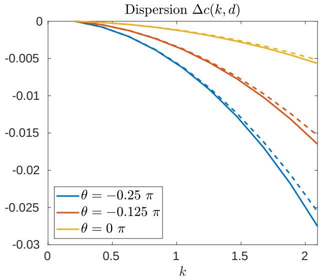


$c_0(\boldsymbol{d}) \approx 1.55$ (isotropic)



— : Bloch-Floquet
- - - : Homogenization

$\ell = 1 \ : \ \frac{\ell}{\lambda} \in \left[0, \frac{1}{3}\right]$

Cost functionals and optimization problem

- Given given N_θ directions $(\boldsymbol{d}_1, \ldots, \boldsymbol{d}_{N_\theta})$ of interest, a *cost functional* $\mathcal{J}$ can be defined as:

$$\mathcal{J}(\mu, \rho) = J\left(c_0(\boldsymbol{d}_1), \ldots, c_0(\boldsymbol{d}_{N_\theta}); \gamma(\boldsymbol{d}_1), \ldots, \gamma(\boldsymbol{d}_{N_\theta})\right)$$

- **Example:** to minimize $|\gamma(\boldsymbol{d}^-)|$ and maximize $|\gamma(\boldsymbol{d}^+)|$:

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

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Topological optimization problem

Find the distribution of (μ, ρ) in Y that minimizes $\mathcal{J}(\mu, \rho)$, with

- the dependencies
$(\mu, \rho) \to (\boldsymbol{P}_1, \boldsymbol{P}_2, \boldsymbol{P}_3) \to (\varrho_0, \boldsymbol{\mu}_0, \boldsymbol{\varrho}_2, \boldsymbol{\mu}_2) \to \{c_0(\boldsymbol{d}_j), \gamma(\boldsymbol{d}_j)\}_{j=1..N_\theta} \to \mathcal{J}$
- Constraints / parametrization of (μ, ρ) (to simplify the problem)

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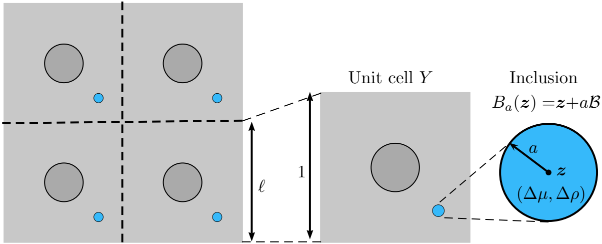
- Constraints / parametrization of (μ,ρ) (to simplify the problem)

- Matrix and inclusions, inclusion shape parametrization and shape sensitivity [Vondřejc et al., 2017]
- Two-phase material, *level-set* description of the interface and shape sensitivity [Allaire and Yamada, 2018]
- Two-phase material and **topological derivative** to quantify the effects of a phase change [Amstutz, 2011, Oliver et al., 2018] (optimization of *static* properties of microstructures)

Topological derivative of a cost functional



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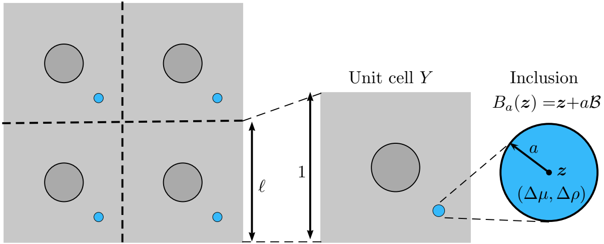
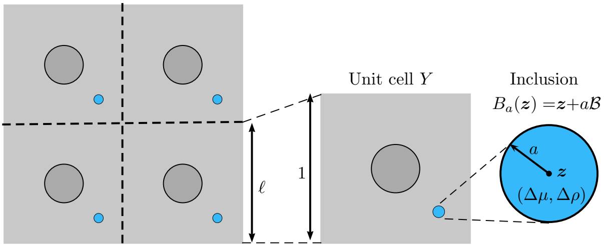


- Phase change in the unit cell: $(\mu, \rho) \to (\mu_a, \rho_a) = (\mu, \rho) + \chi_{B_a}(\Delta\mu, \Delta\rho)$
- Expansion of $\mathcal{J}$:

$$\mathcal{J}(\mu_a, \rho_a) \;=\; \mathcal{J}(\mu, \rho) + a^2\, \mathcal{D}\mathcal{J} + o(a^2) \quad \text{as} \quad a \to 0$$

- $\mathcal{D}\mathcal{J}(\mu, \rho; \boldsymbol{z}, \mathcal{B}, \Delta\mu, \Delta\rho)$ is the *topological derivative* (or gradient, or sensitivity) of $\mathcal{J}$.
[Sokolowski and Zochowski, 1999, Garreau et al., 2001, Amstutz, 2011, Bonnet et al., 2018] ...

Topological derivative of a cost functional



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- Chain rule when $\mathcal{J}(\mu, \rho) = J(\varrho_0, \boldsymbol{\mu}_0, \boldsymbol{\varrho}_2, \boldsymbol{\mu}_2)$:

$$\mathcal{D}\mathcal{J} = \frac{\partial J}{\partial \varrho_0}\mathcal{D}\varrho_0 + \frac{\partial J}{\partial \boldsymbol{\mu}_0} : \mathcal{D}\boldsymbol{\mu}_0 + \frac{\partial J}{\partial \boldsymbol{\varrho}_2} : \mathcal{D}\boldsymbol{\varrho}_2 + \frac{\partial J}{\partial \boldsymbol{\mu}_2} :: \mathcal{D}\boldsymbol{\mu}_2.$$

Cell problems and FFT-based algorithm

Computing $(\mathcal{D}\varrho_0, \mathcal{D}\boldsymbol{\mu}_0, \mathcal{D}\boldsymbol{\varrho}_2, \mathcal{D}\boldsymbol{\mu}_2)$ requires the resolution of:

$$\left.\begin{array}{l} \text{3 cell problems } \boldsymbol{P}_1,\ \boldsymbol{P}_2,\ \boldsymbol{P}_3 \\ \text{2 adjoint cell problems } \beta_0 \text{ and } \boldsymbol{\beta}_1 \end{array}\right\} \text{12 scalar cell problems}$$

[Bonnet, Cornaggia, Guzina, SIAP 2018]

All cell problems are *static equilibrium problems*: for $\boldsymbol{\chi} = \boldsymbol{P}_1,\ \boldsymbol{P}_2,\ \boldsymbol{P}_3,\ \beta_0$ or $\boldsymbol{\beta}_1$,

$$\left|\begin{array}{l} \boldsymbol{\nabla} \cdot \big[\mu(\boldsymbol{E} + \boldsymbol{\nabla}\boldsymbol{\chi})\big] + \boldsymbol{f} = \boldsymbol{0} \quad \text{in } Y, \\ \boldsymbol{\chi} \text{ is } Y\text{-periodic}, \\ \langle\boldsymbol{\chi}\rangle = 0, \end{array}\right.$$

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Numerical resolution:

- Finite elements (FreeFem++, Comsol, Fenics, Xlife++ . . .)
- FFT-based methods [Moulinec and Suquet, 1998, Moulinec et al., 2018]
  - Problem reformulation: Lippmann-Schwinger integral equation involving a *reference material*
  - Fixed-point algorithm
  - Extensive use of FFT to compute convolution products
  - Discretisation of the cell on *pixels*

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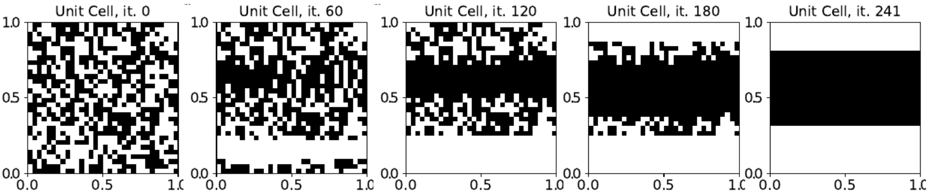
Pixel-by-pixel two-directions optimization

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

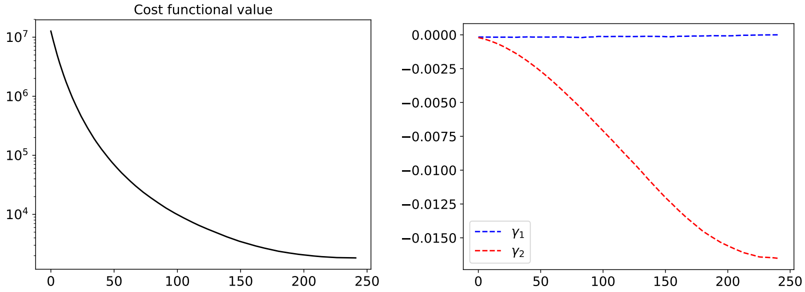
$$\mathcal{J}(\mu, \rho) = \frac{1}{2}\left[\left[\gamma(\boldsymbol{d}^-)\right]^2 + \frac{1}{\left[\gamma(\boldsymbol{d}^+)\right]^2}\right]$$

- 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 algorithm:
  - Initialize material repartition (Y_1, Y_2) with $|Y_1| = |Y_2|$
  - While $(\min_{Y_1} \mathcal{DJ} + \min_{Y_2} \mathcal{DJ}) < 0$, exchange the two pixels where the minima are reached
  - $|Y_1| = |Y_2|$ is automatically respected



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.

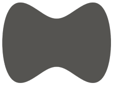
$\Longrightarrow \approx$ 15-20s on a (good) laptop.

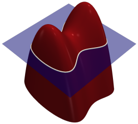
Level-set representation and projection algorithm

[Amstutz and Andrä, 2006, Amstutz, 2011]

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

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





(Wikipedia)

- Signed and normalized TD $\overline{\mathcal{D}}\mathcal{J}$:

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

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

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:

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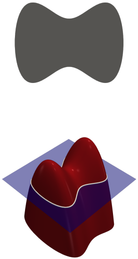


(Wikipedia)

Optimality condition: If $\overline{\mathcal{D}}\mathcal{J}$ satisfies the sign condition $(\star)$ then $\mathcal{D}\mathcal{J}(\boldsymbol{z}) > 0 \quad \forall \boldsymbol{z} \in Y$

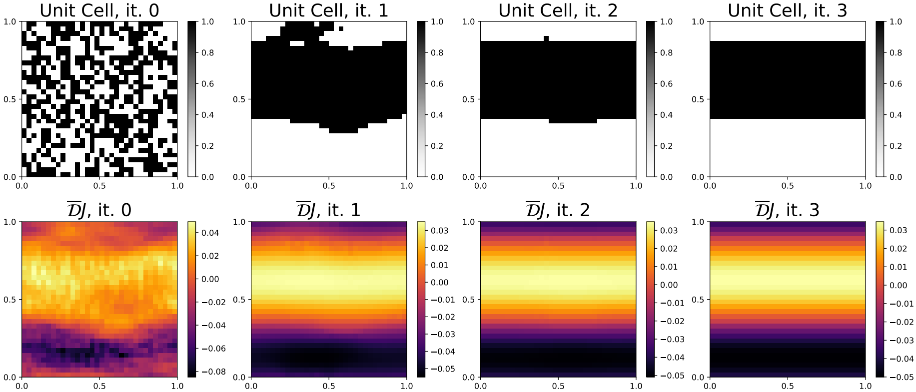
then $\mathcal{J}$ reached a *local minimum*

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

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

(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 $|Y_1| = |Y_2|$)

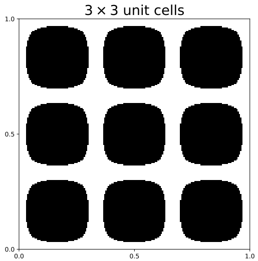


Maximizing horizontal and vertical and minimizing diagonal dispersions

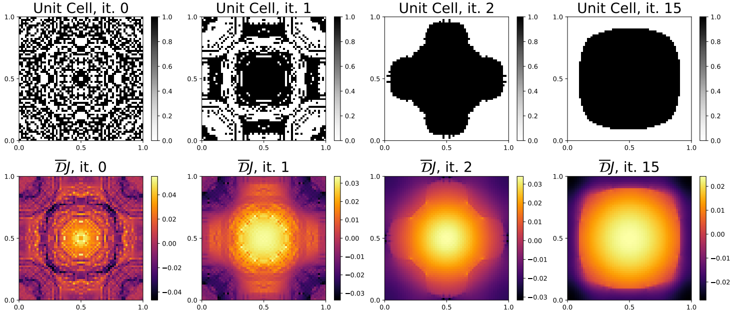
- Recall : $c(k, \boldsymbol{d}) = c_0(\boldsymbol{d}) + \frac{1}{2}(k\ell)^2 \frac{\gamma(\boldsymbol{d})}{c_0(\boldsymbol{d})} + o\left((k\ell)^2\right)$
- Cost functional:

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

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

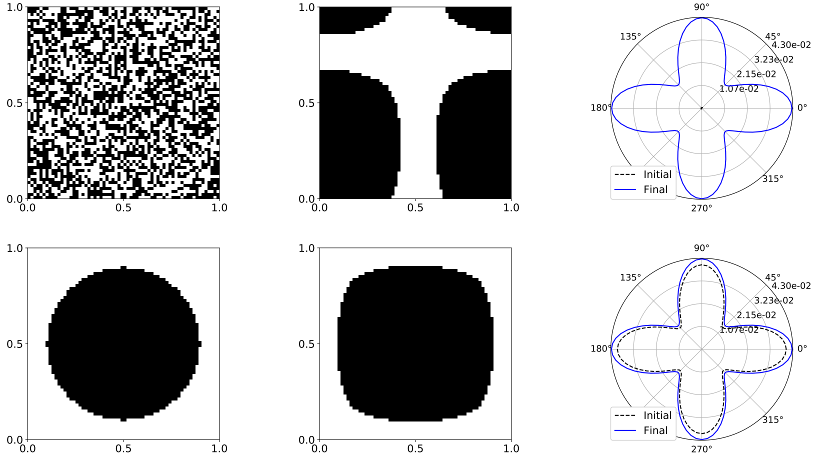


- Material ratios: $\mu_2/\mu_1 = 6$ and $\rho_2/\rho_1 = 1.5$



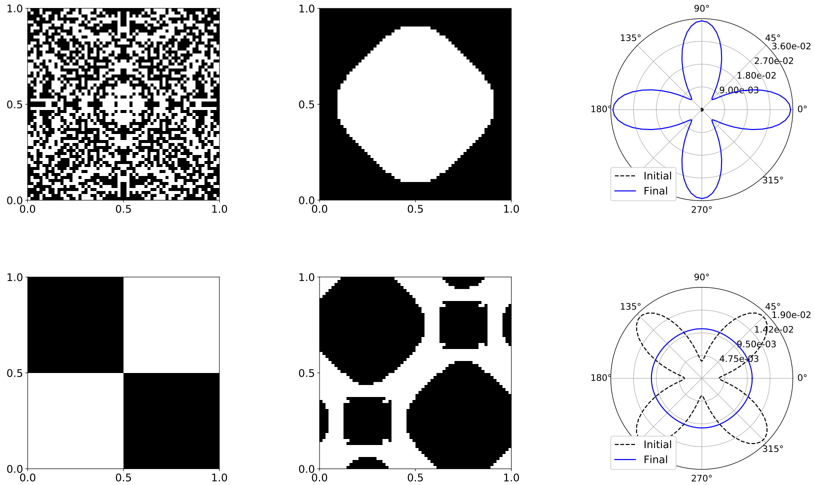
Other initializations with the same result

Initial cell | Final cell | Dispersion indicator $\dfrac{\gamma(\boldsymbol{d})}{c_0(\boldsymbol{d})}$

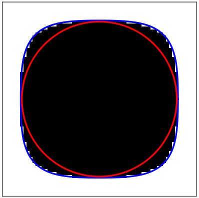


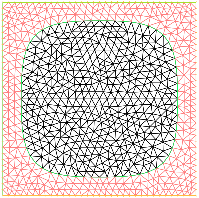
Initializations leading to sub-optimal results

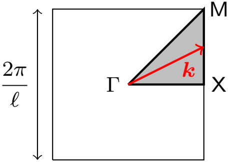
Initial cell | Final cell | Dispersion indicator $\dfrac{\gamma(\boldsymbol{d})}{c_0(\boldsymbol{d})}$



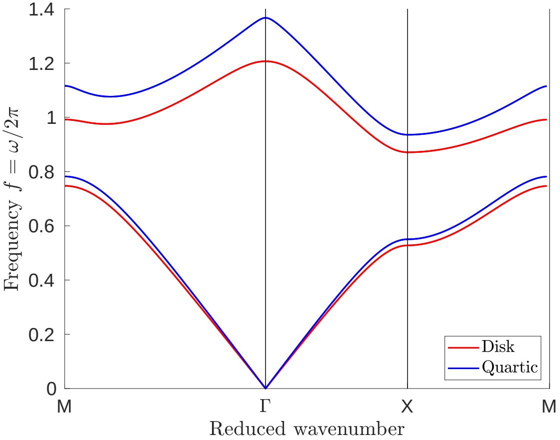
Bloch-Floquet analysis of the optimal unit cell







- 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:

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

- Quasistatic and dispersive least-square cost functionals:

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

- Weighted total cost functional:

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

Fitting an objective anisotropic phase velocity c^{obj}

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- Weighted total cost functional:

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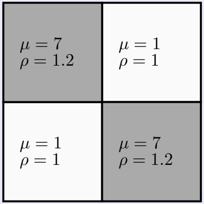
Example: chessboard reconstruction

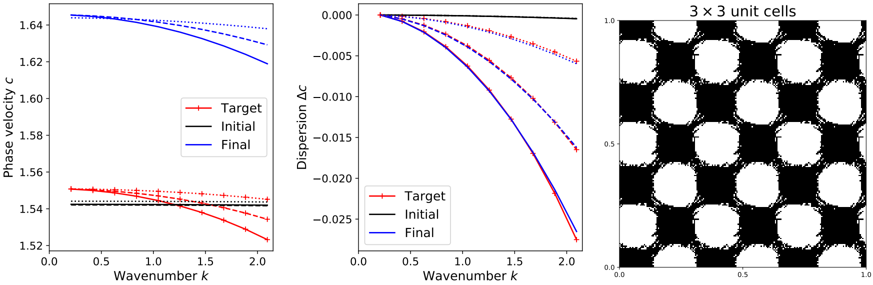


Data and constraints:

- $c^{\mathrm{obj}} = c^{\mathrm{chess}}$ (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

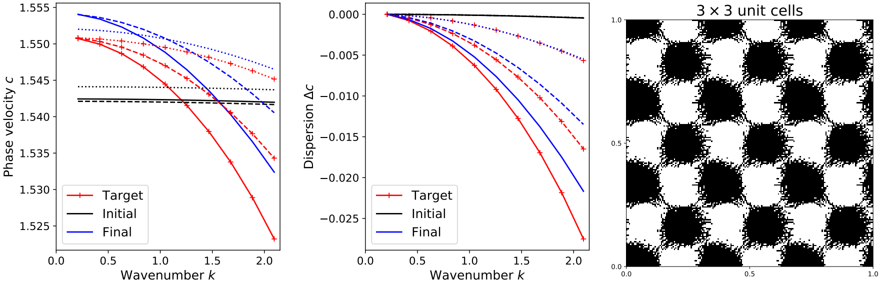
$$\color{red}{\alpha = 0} \qquad (\mathcal{J} = \mathcal{J}^{\text{dyn}})$$



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

Chessboard reconstruction from phase velocity data

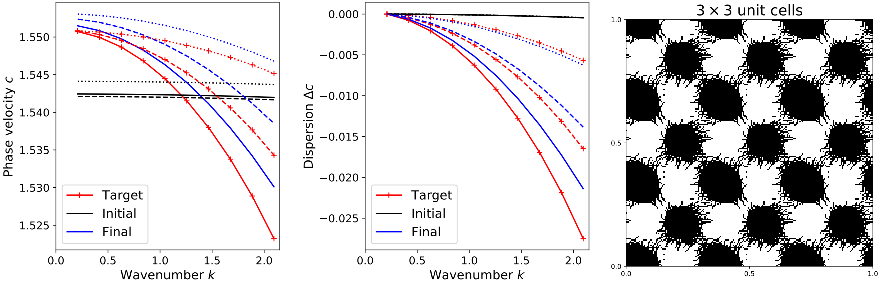
$\alpha = 0.1$



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

Chessboard reconstruction from phase velocity data

$\alpha = 0.2$



- $\cdots\cdots$: $\theta = 0$
- $- - -$: $\theta = -\pi/8$
- —— : $\theta = -\pi/4$

Key ideas

- The second-order asymptotic homogenization accounts for dispersive effects.
- Boundary and transmission conditions can be designed to complement the inner expansion. (including in 2-3D [Vinoles, 2016, Maurel and Marigo, 2018, Cakoni et al., 2019] ...)
- In 2D, a topological optimization procedure is proposed and applied to various cost functionals.

Key ideas

- The second-order asymptotic homogenization accounts for dispersive effects.
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- In 2D, a topological optimization procedure is proposed and applied to various cost functionals.

Perspectives

- In 1D, pursue the extension to time-domain simulations.
- Extend the optimization method to other geometrical and physical frameworks:
  1. **Periodic interfaces**: optimize *effective transmission conditions* [Marigo et al., 2017] (Marie Touboul's Ph.D. thesis).
  2. **Elasticity**: links with *strain/stress gradient models* [Auffray et al., 2015, Rosi and Auffray, 2019].
  3. **High contrasts** (inner resonances) [Auriault and Bonnet, 1985, Vondřejc et al., 2017] and **high frequencies** [Craster et al., 2010, Guzina et al., 2019] to optimize *band-gaps*, *memory effects* ...
- Improve the optimization algorithm
  - Compute a *pixel derivative* to work at a discrete level
  - Couple shape and topological derivative [Allaire et al., 2005, Amstutz et al., 2018]
  - Address *multiphasic* materials [Gangl, 2020]

Merci pour votre attention !

Second-order homogenization of boundary and transmission conditions for one-dimensional waves in periodic media
Rémi Cornaggia, Bojan B. Guzina
International Journal of Solids and Structures, 2020

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

https://cv.archives-ouvertes.fr/remi-cornaggia

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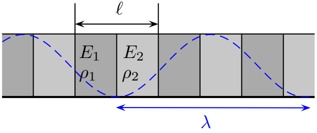
Journal of the Mechanics and Physics of Solids, 78:382 – 414.

Choosing a (mt) model from dispersion relations in layered media



- *Bloch wave* $u_\ell(X,t) = \tilde{u}(x)e^{\mathrm{i}(\kappa x - \omega t)} \implies$ *dispersion relation* $\omega = f(\kappa)$.
  About $(\omega, \kappa) = (0,0)$ (on the *acoustic branch*):

$$\frac{\omega}{c_0} = \kappa \left[1 - \frac{\beta}{2}(\kappa\varepsilon)^2 + \frac{\beta\left(2 - 27\beta - 8\overline{\beta}\right)}{40}(\kappa\varepsilon)^4 + O(\varepsilon^6) \right],$$

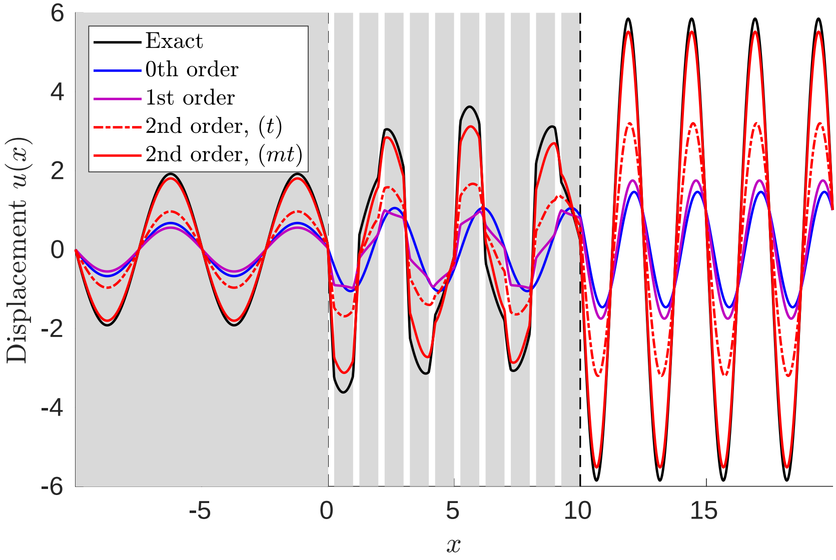
  ($\overline{\beta}$ known for layered media)

- *Plane wave* $U(x,t) = \tilde{U}e^{\mathrm{i}(\kappa x - \omega t)}$ in the second-order (mt) homogenized model:

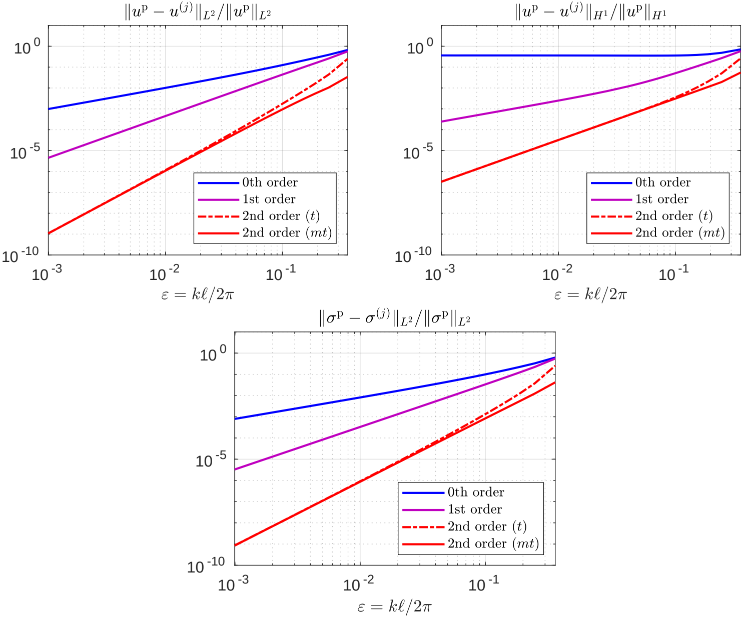
$$\frac{\omega}{c_0} = \kappa \left[1 + \frac{\beta_m + \beta_t}{2}(\kappa\varepsilon)^2 + \frac{(\beta_m + \beta_t)(3\beta_m + 7\beta_t)}{8}(\kappa\varepsilon)^4 + O(\varepsilon^6) \right].$$

- *Second-order* approximation of ω/c_0 obtained for any (β_m, β_t) satisfying $-\beta_m - \beta_t = \beta$.
  Also true in 2-3D [Allaire et al., 2016].
- *Fourth-order* approximation for $\beta_m = \dfrac{-1 - 4\beta + 4\overline{\beta}}{10}$ and $\beta_t = \dfrac{1 - 6\beta - 4\overline{\beta}}{10}$
  Similar approximation for spring-mass lattice in [Pichugin et al., 2008]

Application to a transmission problem ($\varepsilon \approx 0.3$)



Application to a transmission problem - errors



Second-order time-domain homogenization with the (mt) model

$$\partial_{tt}\left[U + \frac{\beta_t \ell^2}{{c_0}^2}\partial_{tt}U\right] - {c_0}^2\partial_{xx}\left[U - \frac{\beta_m \ell^2}{{c_0}^2}\partial_{tt}U\right] = \frac{f^{(2)}}{\varrho_0}, \quad \text{with} \quad -\beta_m - \beta_t = \beta > 0$$

- Velocity $V = \partial_t U$, stress $S = \mathcal{E}_0 \partial_x U$ and "augmented" velocity and stress:

$$V^{(t)} := \partial_t\left[U + \frac{\beta_t \ell^2}{{c_0}^2}\partial_{tt}U\right] = V + \frac{\beta_t \ell^2}{{c_0}^2}\partial_{tt}V$$

$$S^{(m)} := \mathcal{E}_0\partial_x\left[U - \frac{\beta_m \ell^2}{{c_0}^2}\partial_{tt}U\right] = S - \frac{\beta_m \ell^2}{{c_0}^2}\partial_{tt}S$$

- Equivalent first-order system:

$$\begin{cases} \partial_t V^{(t)} - \dfrac{1}{\varrho_0}\partial_x S^{(m)} = \dfrac{f^{(2)}}{\varrho_0} \\ \partial_t S^{(m)} + \mathcal{E}_0\left[\dfrac{\beta_m}{\beta_t}\partial_x V^{(t)} - \left(1 + \dfrac{\beta_m}{\beta_t}\right)\partial_x V\right] = 0 \\ \partial_t V = A \\ \partial_t A = \dfrac{(c_0)^2}{\beta_t \ell^2}\left[V^{(t)} - V\right] \end{cases}$$

- Hyperbolicity and stability for:

$$\beta_m < 0 \quad \text{and} \quad \beta_t > 0$$

First-order transmission conditions - regularization

- Stress-velocity formulation: $S = \mathcal{E}_0{}^{\pm} U_{,x}$ and $V = U_{,t}$

$$\left| \begin{aligned} & V_{,t} - \frac{1}{\varrho_0{}^{\pm}} S_{,x} = 0 \\ & S_{,t} - \mathcal{E}_0{}^{\pm} V_{,x} = 0, \end{aligned} \right.$$

- Conditions from time-harmonic study:

$$\begin{cases} [\![V]\!](0) + \varepsilon P_1(0) V_{,x}(0^+) = 0 \\ [\![S]\!](0) + \varepsilon \Sigma_1(0) S_{,x}(0^+) = 0 \end{cases}$$

  - *Assymetric* jump conditions
  - Sometimes *unstable*

- Regularization adding a *thin interphase* $I_\delta = [-\delta\varepsilon, \delta\varepsilon]$:

$$\begin{cases} [\![V]\!]_{I_\delta} = 2\varepsilon \dfrac{\delta \mathcal{E}_0 + (\delta - P_1(0)) E_-}{E_- + \mathcal{E}_0} \langle V_{,x} \rangle_{I_\delta} \\ [\![S]\!]_{I_\delta} = 2\varepsilon \dfrac{\delta \rho_- + (\delta - \Sigma_1(0)) \varrho_0}{\rho_- + \varrho_0} \langle S_{,x} \rangle_{I_\delta} \end{cases}$$

$\Longrightarrow$ Symmetric and stable transmission conditions, with $o(\varepsilon)$ additional error for:

$$\delta = \delta^{opt} := \max \left(\frac{E_- P_1(0)}{E_- + \mathcal{E}_0}, \ \frac{\varrho_0 \Sigma_1(0)}{\rho_- + \varrho_0}, \ 0 \right)$$

Topological derivatives of homogenized coefficients

[Bonnet, Cornaggia, Guzina, SIAP, 2018]

$$\varrho_0 = \langle \rho \rangle \quad \Rightarrow \quad \mathcal{D}\varrho_0 = |\mathcal{B}|\Delta\rho,$$

$$\boldsymbol{\mu}_0 = \langle \mu \left(\boldsymbol{\nabla P}_1 + \boldsymbol{I} \right) \rangle \quad \Rightarrow \quad \mathcal{D}\boldsymbol{\mu}_0(\boldsymbol{z}) = \Big\{ (\boldsymbol{\nabla P}_1 + \boldsymbol{I})^{\mathsf{T}} \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla P}_1 + \boldsymbol{I}) \Big\}(\boldsymbol{z}),$$

$\boldsymbol{A}$ is the *polarization tensor* of the inclusion: $\boldsymbol{A} = \boldsymbol{A}(\mathcal{B}, \mu(\boldsymbol{z}), \Delta\mu)$ [Ammari and Kang, 2007].

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$\boldsymbol{A}$ is the *polarization tensor* of the inclusion: $\boldsymbol{A} = \boldsymbol{A}(\mathcal{B}, \mu(\boldsymbol{z}), \Delta\mu)$ [Ammari and Kang, 2007].

$$\mathcal{D}\boldsymbol{\varrho}_2(\boldsymbol{z}) = \varrho_0 \Big\{ (\boldsymbol{\nabla}\boldsymbol{\beta}_1 + \beta_0 \boldsymbol{I}) \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla}\boldsymbol{P}_1 + \boldsymbol{I}) - \boldsymbol{\nabla}\beta_0 \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla}\boldsymbol{P}_2 + \boldsymbol{I} \otimes \boldsymbol{P}_1) \Big\}_{\text{sym}}(\boldsymbol{z})$$
$$+ \Big\{ \mathcal{D}\varrho_0 \Big[\boldsymbol{P}_2 - \beta_0 \boldsymbol{\mu}_0 \Big] - \langle \rho\beta_0 \rangle \Big[\mathcal{D}\boldsymbol{\mu}_0 - \mathcal{D}\varrho_0 \frac{\boldsymbol{\mu}_0}{\varrho_0} \Big] \Big\}_{\text{sym}}(\boldsymbol{z}),$$

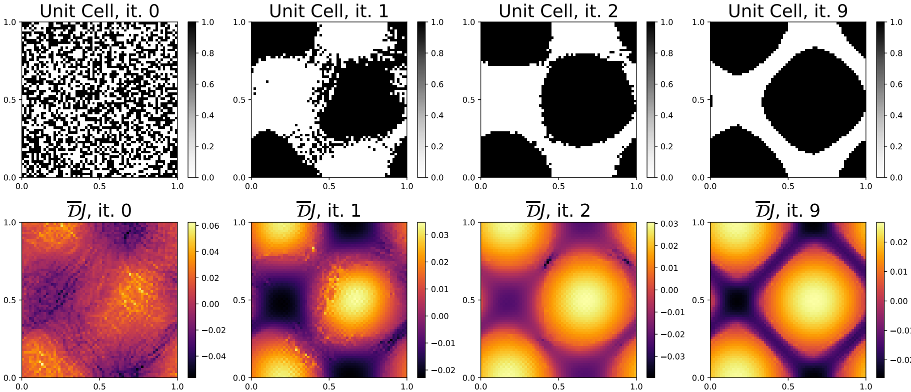
$$\mathcal{D}\boldsymbol{\mu}_2(\boldsymbol{z}) = \Big\{ 2\,(\boldsymbol{\nabla}\boldsymbol{P}_1 + \boldsymbol{I})^{\mathsf{T}} \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla}\boldsymbol{P}_3 + \boldsymbol{I} \otimes \boldsymbol{P}_2) - (\boldsymbol{\nabla}\boldsymbol{P}_2 + \boldsymbol{I} \otimes \boldsymbol{P}_1)^{\mathsf{T}} \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla}\boldsymbol{P}_2 + \boldsymbol{I} \otimes \boldsymbol{P}_1) \Big\}_{\text{sym}}(\boldsymbol{z})$$
$$+ \Big\{ \big[\mathcal{D}\boldsymbol{\varrho}_2 + \mathcal{D}\varrho_0\,(\boldsymbol{P}_1 \otimes \boldsymbol{P}_1 - 2\boldsymbol{P}_2) \big] \otimes \frac{\boldsymbol{\mu}_0}{\varrho_0} + \frac{1}{\varrho_0} (\langle \rho \boldsymbol{P}_1 \otimes \boldsymbol{P}_1 \rangle - \boldsymbol{\varrho}_2) \otimes \Big[\mathcal{D}\boldsymbol{\mu}_0 - \mathcal{D}\varrho_0 \frac{\boldsymbol{\mu}_0}{\varrho_0} \Big] \Big\}_{\text{sym}}(\boldsymbol{z}$$

Computing $(\mathcal{D}\varrho_0, \mathcal{D}\boldsymbol{\mu}_0, \mathcal{D}\boldsymbol{\varrho}_2, \mathcal{D}\boldsymbol{\mu}_2)$ requires the resolution of:

3 cell problems $\boldsymbol{P}_1$, $\boldsymbol{P}_2$, $\boldsymbol{P}_3$
2 adjoint cell problems β_0 and $\boldsymbol{\beta}_1$
} 12 scalar cell problems

Minimizing horizontal and vertical and maximizing diagonal dispersions

- Cost functional: $J_{4d} = \frac{1}{2}\left(\lambda(\gamma_1^2 + \gamma_3^2) + \frac{1}{\gamma_2^2} + \frac{1}{\gamma_4^2}\right)$, $\theta_{1,3} = 0, 90^\circ$, $\theta_{2,4} = \pm 45^\circ$
- Material ratios: $\mu_2/\mu_1 = 6$ and $\rho_2/\rho_1 = 1.5$
- Stopping criterion: $\Theta < 10^{-3}$. Reached for $n = 9$: $\Theta_9 \approx 4.5 \times 10^{-8}$



Minimizing horizontal and vertical and maximizing diagonal dispersions