Spectral approach for a homogenization problem using boundary integral operators

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Summary

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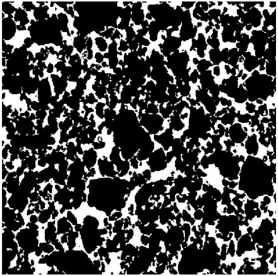
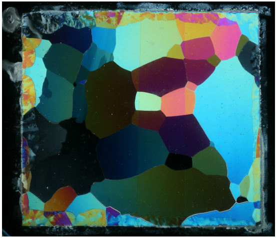
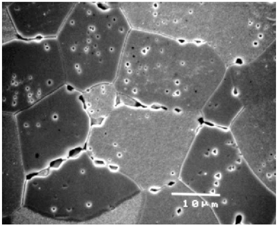
Motivation : Heterogeneous materials



(a) Fe-Ag alloy

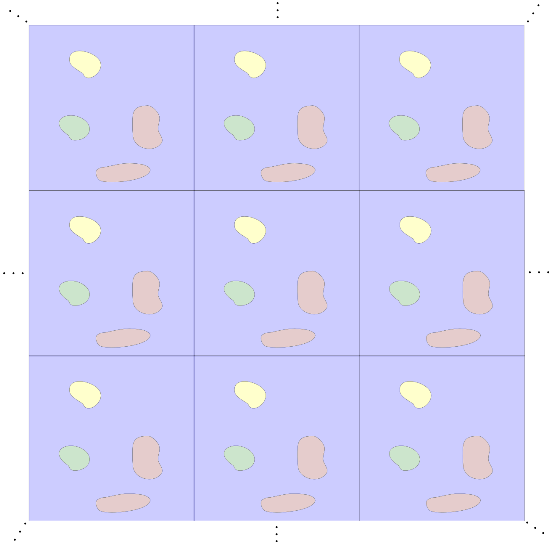


(b) Ice



(c) UO_2

Periodic material



Homogenization

Effective conductivity :

$$\langle C \nabla U \rangle_\Omega =: C_{\text{eff}} \langle \nabla U \rangle_\Omega$$

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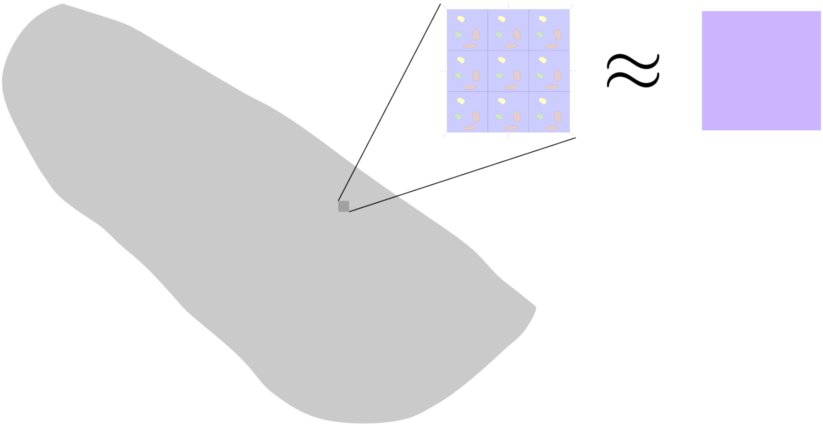
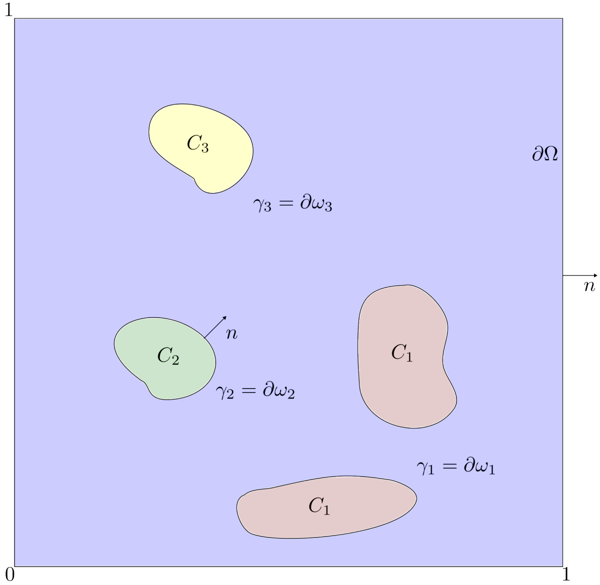


Problem setting



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- Conductivities : $C_1, \dots, C_p > 0$

$$C := \sum_{k=1}^{p} C_k \mathbb{1}_{\omega_k},$$

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Weak formulation

- It is :

$$\int_\Omega C \nabla u \cdot \nabla v \, \mathrm{d}\lambda = - \int_\Omega C \overline{\varepsilon} \cdot \nabla v \, \mathrm{d}\lambda$$

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$$\langle A_0 u, v\rangle := \int_\Omega C_0 \nabla u \cdot \nabla v \,\mathrm{d}\lambda$$

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- We have :

$$A = b$$
$$A_0 \left(I + A_0^{-1} (A - A_0)\right) = b$$

Lippmann-Schwinger formulation : volumic approach

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Proposition (e.g. Bellis, Moulinec 2025)

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C_0 may be chosen such that $\|S\| < 1$.

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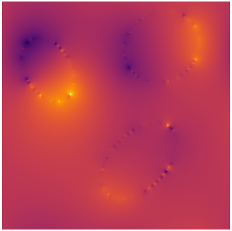
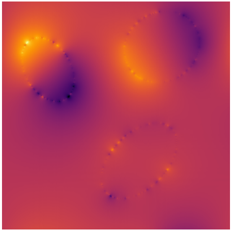
However S self-adjoint but not compact...

Numerical results : Lippmann-Schwinger



(a) Non-spurious



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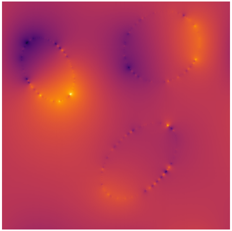

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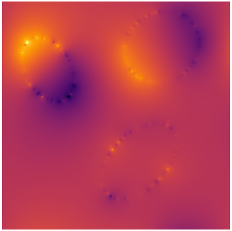

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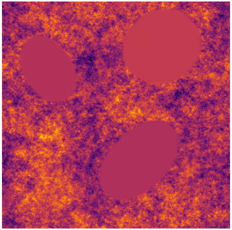
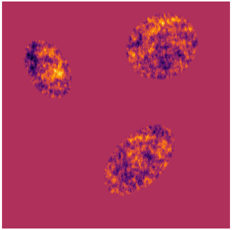


(c) Spurioux



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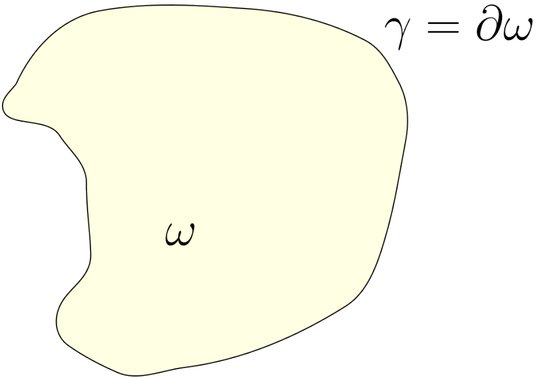

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- Double and single layer potentials : boundary integral operators

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- Problems of Dirichlet, Neumann, transmission... (see e.g. Rjasanow, Steinbach 2007 or McLean 2000)

The periodic fundamental solution

- Definition :

$$G_{\#}(x) := -\frac{1}{4\pi^2} \sum_{\xi \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{|\xi|^2} e^{2i\pi x \cdot \xi},$$

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- Handle periodic conditions!

Reformulation

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$\rightarrow$ Transmission problem

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$\rightarrow$ Transmission problem $\rightarrow$ Boundary integral operators

Boundary integral equation

$$
\begin{cases}
\Delta u = 0 & \text{in } \Omega \setminus \gamma \\
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\langle u \rangle_\Omega = 0 & \\
u & \text{is } \Omega\text{-periodic} \\
\partial_n u & \text{is } \partial\Omega\text{-antiperiodic.}
\end{cases}
$$

Then,

$$u = \mathscr{S}_{\#,\gamma} q,$$

solves

$$\left(C_i \partial_n^- \mathscr{S}_{\#,\gamma} - C_p \partial_n^+ \mathscr{S}_{\#,\gamma}\right) q = -\overline{\varepsilon} \cdot n \qquad \text{on } \gamma_i.$$

Boundary integral equation

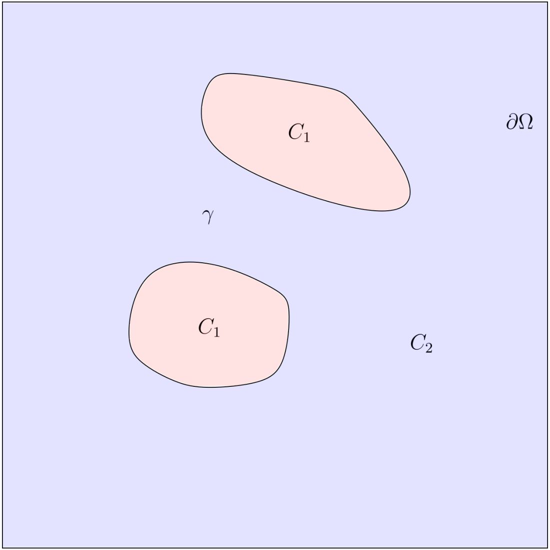
Reduces to :

$$\begin{cases} \left(K'_\gamma - D\right) q = -\overline{\varepsilon} \cdot n & \text{on } \gamma \\ \langle q, 1 \rangle_\gamma = 0, \end{cases}$$

where

$$D \coloneqq \operatorname{diag}\left(\frac{C_1 + C_p}{2\left(C_1 - C_p\right)}, \ldots, \frac{C_{p-1} + C_p}{2\left(C_{p-1} - C_p\right)}\right).$$

Two phases



Boundary integral equation

Reduces to :

$$\begin{cases} \left(K'_\gamma - \dfrac{C_1 + C_2}{2(C_1 - C_2)} I\right) q = -\overline{\varepsilon} \cdot n & \text{on } \gamma \\ \langle q, 1 \rangle_\gamma = 0. \end{cases}$$

Boundary integral equation

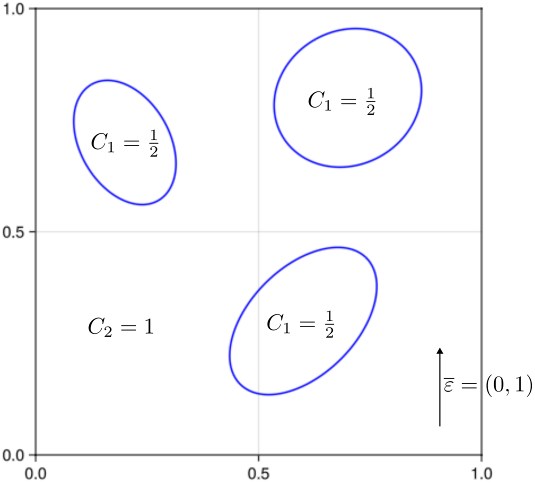
Reduces to :

$$\begin{cases} \left(K'_\gamma - \widetilde{C} I\right) q = -\overline{\varepsilon} \cdot n & \text{on } \gamma \\ \langle q, 1 \rangle_\gamma = 0. \end{cases}$$

Now, $K'_\gamma : H_0^{-\frac{1}{2}}(\gamma) \longrightarrow H_0^{-\frac{1}{2}}(\gamma)$ is compact and self-adjoint !

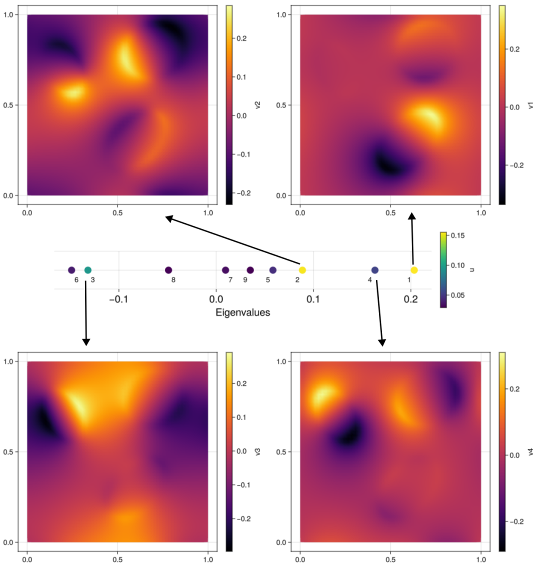
$$u = \sum_{k=0}^{+\infty} \frac{(\overline{\varepsilon} \cdot n, e_k)}{\widetilde{C} - \mu_k} \mathscr{S}_{\#,\gamma} e_k.$$

Numerical results



Study case

Numerical results



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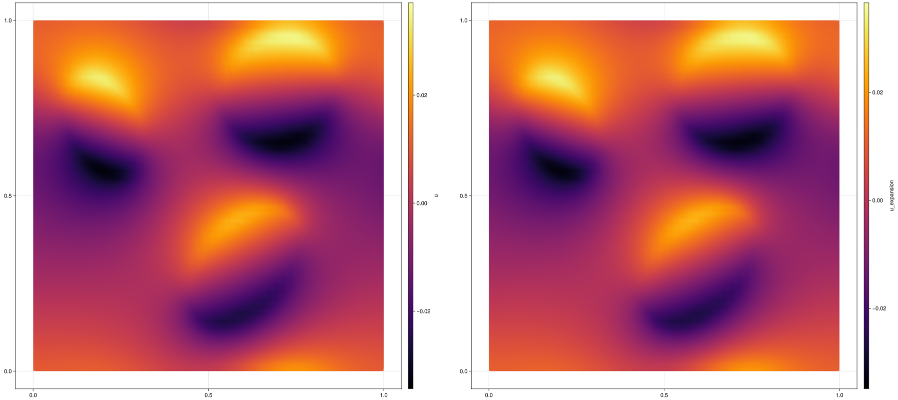


(a) Inverting the boundary equation

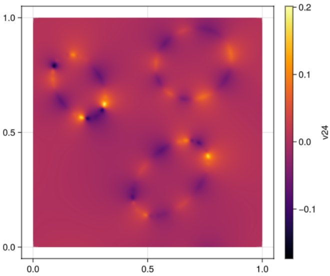
(b) Using the modal decomposition

Implementation

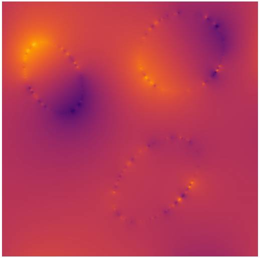
- Nyström method
- Julia : `Inti.jl`
- Execution time : few seconds

Summary

Link between the approaches



(a) Boundary operators



(b)
Lippmann-Schwinger

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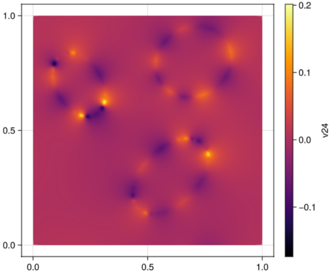

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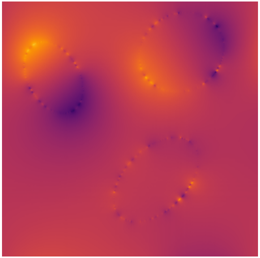

(b) Lippmann-Schwinger

Proposition

(λ, ϕ) : eigenpair of the Lippmann-Schwinger operator S, two cases :

1. *ϕ is constant in ω_i, arbitrary in ω_j, $j \neq i$ $\rightarrow$* $\dim\left(\mathrm{Ker}\left(S - \lambda I\right)\right) = +\infty$
2. *$\exists \mu_k$; $\lambda = a\mu_k + b$ and $\phi \in \mathrm{Vect}\left(e_{k_1}, \ldots, e_{k_N}\right) = \mathrm{Ker}\left(K'_\gamma - \mu_k I\right)$ ($\dim < +\infty$)*

Comparison

Boundary operators

- Filter mods

Lippmann-Schwinger operator

- Spurious mods

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Boundary operators

- Filter mods
- Executed in few seconds

Lippmann-Schwinger operator

- Spurious mods
- Executed in hours

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Lippmann-Schwinger operator

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- Filter mods
- Executed in few seconds
- Smooth borders
- Compact operator (and self-adjoint when $p = 2$)

Lippmann-Schwinger operator

- Spurious mods
- Executed in hours
- Corners allowed
- Self-adjoint operator

Perspectives

- Iterative methods (in the way of Moulinec, Suquet 1994)
- $p > 2$
- Linear elasticity