Effective Approximations of Oscillating PDE based on Boundary Agregated Measurements

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A Multiscale Problem

- Consider the problem

$$\begin{cases} -\mathrm{div}\,(A_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } \Omega, \\ (A_\varepsilon \nabla u_\varepsilon)\cdot n = g & \text{on } \partial\Omega. \end{cases} \tag{1}$$

where A_ε is oscillating at a small length scale $\varepsilon \ll |\Omega|$.

- Applications: (simplification of) elastic problems in Mechanics.

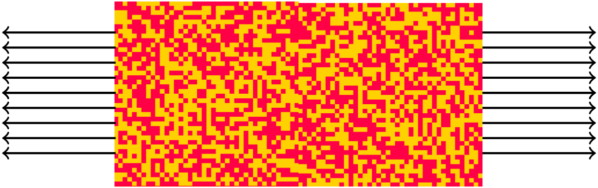


Figure: Traction experiment on a 2D heterogeneous material.

Objective

Construct a constant coefficient $\overline{A} \in \mathbb{R}^{d\times d}$, such that the solutions $u_\varepsilon(g)$ to (1) are satisfyingly approximated by the solutions $\overline{u} = u(\overline{A}, g)$ to the coarse problem

$$\begin{cases} -\mathit{div}\,\left(\overline{A}\nabla \overline{u}\right) = 0 & \text{in } \Omega, \\ \left(\overline{A}\nabla \overline{u}\right)\cdot n = g & \text{on } \partial\Omega. \end{cases} \tag{2}$$

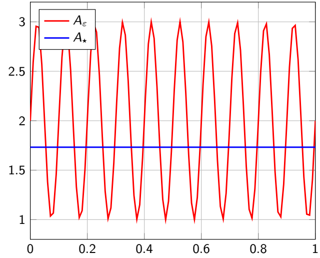
Link with Homogenization Theory

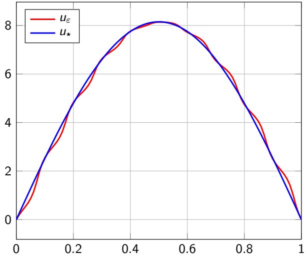
Homogenization seems to be a relevant tool here.

$$\underbrace{\boxed{\begin{cases} -\mathrm{div}\,(A_\varepsilon \nabla u_\varepsilon) = 0 & \text{in } \Omega, \\ (A_\varepsilon \nabla u_\varepsilon)\cdot n = g & \text{on } \partial\Omega. \end{cases}}}_{\text{Oscillating System}} \xrightarrow[\varepsilon\to 0]{} \underbrace{\boxed{\begin{cases} -\mathrm{div}\,(A_\star \nabla u_\star) = 0 & \text{in } \Omega, \\ (A_\star \nabla u_\star)\cdot n = g & \text{on } \partial\Omega. \end{cases}}}_{\text{Homogenized System}}$$

Downsides:

- Valid only in the regime of separated scale (i.e. $\varepsilon \to 0$).
- No formula for $A_\star$ unless strong assumptions on A_ε (e.g. periodicity $A_\varepsilon(x) = A_{\mathrm{per}}(\frac{x}{\varepsilon})$).





Link with Inverse Problems

1. Approaches for **classical inverse problems** are inoperable due to ill-posedness (see Lions 76) or data requirements (see Stuart&al 12).
2. Various approaches for **inverse multiscale problems**.
   - Identify A_ε. **Ill-posed** in general, unless...
     Fine scale data is available. (see Bal&Uhlmann 13)
     Strong assumptions on the structure on A_ε are made (e.g. A_ε depends on a few unknown parameter). (see Frederick&Engquist 17, Abdulle&DiBlasio 19, Lochner&Peter 23)
   - Approximate the map $g \to u_\varepsilon(g)$, and give up on recovering A_ε. (see Chung&al 19, Maier&al 20)
   - Identify effective properties. (Cherkaev 08, LeBris&al 18)

Specificity:
- coarse data (e.g. scalar measurements).
- very few data (e.g. only 3 loadings are available).
  ↳ related to the equation at stake (i.e. linear elasticity)
  $\neq$ data are reasonnably more abundant for other equations (e.g. Helmholtz, Wave, ...)

Effective Modeling from Boundary Agregated Measurements

A first formulation [CRAS2013][1], [COCV2018][2]

For $\overline{A} \in \mathbb{R}^{d\times d}_{\text{sym}}$ a *constant* symmetric coefficient, denote $\overline{u} = u(\overline{A}, g)$ the solution to

$$-\operatorname{div}\left(\overline{A}\nabla\overline{u}\right) = 0 \text{ in } \Omega, \qquad (\overline{A}\nabla\overline{u}) \cdot n = g \text{ on } \partial\Omega.$$

The quality of the effective coefficient $\overline{A}$ can be quantified through the functional

$$\sup_{\|g\|_{L^2(\partial\Omega)}=1} \left\| u_\varepsilon(g) - u(\overline{A}, g) \right\|_{L^2(\Omega)}$$

The strategy consists in minimizing the worst case scenario by looking at the optimization problem

$$\inf_{\overline{A}\in\mathbb{R}^{d\times d}_{\text{sym}}} \sup_{\|g\|_{L^2(\partial\Omega)}=1} \left\| u_\varepsilon(g) - u(\overline{A}, g) \right\|_{L^2(\Omega)}$$

Issue: Using the **full solutions u_ε in the whole domain Ω** as observables is **disproportionate** to estimate a $d \times d$ constant symmetric matrix, and **irrealistic** from an experimental point of view.

[1] C. Le Bris, F. Legoll, K. Li, CRAS, 2013.

[2] C. Le Bris, F. Legoll, S. Lemaire, ESAIM COCV, 2018.

Practical Observables

Only *coarser* observables are usually acquirable, such as the energy

$$\boxed{\mathcal{E}(A_\varepsilon, g) = \frac{1}{2}\int_\Omega A_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon - \int_{\partial\Omega} g \; u_\varepsilon(g) = -\frac{1}{2}\int_{\partial\Omega} g \; u_\varepsilon(g).} \tag{3}$$

Motivation:

- $\mathcal{E}(A_\varepsilon, g)$ passes to the homogenized limit:

$$\mathcal{E}(A_\varepsilon, g) \underset{\varepsilon\to 0}{\longrightarrow} \mathcal{E}(A_\star, g) \text{ in } \mathbb{R},$$

  where $\mathcal{E}(A_\star, g) = \frac{1}{2}\int_\Omega A_\star \nabla u_\star \cdot \nabla u_\star - \int_{\partial\Omega} g \; u_\star$ and where $u_\star$ denotes the homogenized solution.

- $\mathcal{E}(A_\varepsilon, g)$ is an integrated quantity (scalar !), thus it provides no direct insights about the microscale
- $\mathcal{E}(A_\varepsilon, g)$ is tractable.

Practical Strategy

For $\overline{A} \in \mathbb{R}^{d\times d}_{\text{sym}}$ a *constant* symmetric coefficient, denote $\overline{u} = u(\overline{A}, g)$ the solution to

$$-\text{div}\left(\overline{A}\nabla\overline{u}\right) = 0 \text{ in } \Omega, \qquad (\overline{A}\nabla\overline{u}) \cdot n = g \text{ on } \partial\Omega.$$

To assess the quality of the effective coefficient $\overline{A}$, we use the functional

$$\xcancel{\sup_{\|g\|_{L^2(\partial\Omega)}=1} \left\| u_\varepsilon(g) - u(\overline{A}, g) \right\|_{L^2(\Omega)}^2} \longrightarrow \sup_{\|g\|_{L^2(\partial\Omega)}=1} \left|\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g)\right|^2$$

Our strategy consists in minimizing the worst case scenario by looking at the optimization problem

$$\inf_{\substack{\overline{A} \in \mathbb{R}^{d\times d}_{\text{sym}} \\ \alpha \leqslant \overline{A} \leqslant \beta}} \sup_{\|g\|_{L^2(\partial\Omega)}=1} \left|\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g)\right|^2$$

In the limit of vanishing ε, the problem leads to the homogenized diffusion coefficient as shown by the following proposition.

$$I_\varepsilon = \inf_{\substack{\overline{A} \in \mathbb{R}^{d\times d}_{\mathrm{sym}} \\ \alpha \leqslant \overline{A} \leqslant \beta}} \sup_{\substack{g \in L^2(\partial\Omega) \\ \|g\|_{L^2(\partial\Omega)} = 1}} \left| \mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g) \right|^2$$

Proposition (Asymptotic consistency, periodic case)

For any sequence of quasi-minimizer $\left(\overline{A}_\varepsilon^\#\right)_{\varepsilon>0}$, *i.e. sequence such that*

$$I_\varepsilon \leqslant J_\varepsilon(\overline{A}_\varepsilon^\#) \leqslant I_\varepsilon + err(\varepsilon), \tag{4}$$

the following convergence holds:

$$\lim_{\varepsilon\to 0} \overline{A}_\varepsilon^\# = A_\star. \tag{5}$$

Computational procedure

To solve

$$\inf_{\substack{\overline{A} \in \mathbb{R}^{d\times d}_{\mathrm{sym}} \\ \alpha \leqslant \overline{A} \leqslant \beta}} \; \sup_{\substack{g \in L^2(\partial\Omega) \\ \|g\|_{L^2(\partial\Omega)} = 1}} \left|\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g)\right|^2$$

We apply a gradient descent.

Given an iterate $\overline{A}^n$,

1. Define g^n, the argsup to

$$\sup_{g \ \text{ s.t. } \|g\|_{L^2(\partial\Omega)} = 1} \Big(\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}^n, g)\Big)^2 .$$

   In practice, $\sup_{g\in L^2(\Omega)} \to \sup_{g\in V_P}$ on $V_P = \text{Span}\{P \text{ r.h.s.}\}$, with $P \approx 3$.
   This step requires computing P solutions to a <u>coarse</u> PDE in order to get the energy $\mathcal{E}(\overline{A}^n, \cdot)$.
   We next solve a $P \times P$ eigenvalue problem.

2. Define $\overline{A}^{n+1}$, the optimizer to

$$\inf_{\overline{A}\in\mathbb{R}^{d\times d}_{\mathrm{sym}}} \left(\mathcal{E}(A_\varepsilon, g^n) - \mathcal{E}(\overline{A}, g^n)\right)^2 .$$

   In practice, we perform a gradient descent.
   The gradient can be expressed with solutions computed in previous step, hence <u>no additionnal costs</u>.

Numerical Results (periodic)

In 2D ($\Omega = [0,1]^2$), we consider in 2D ($\Omega = [0,1]^2$) the coefficient

$$A_\varepsilon(x,y) = A^{\text{per}}\left(\frac{x}{\varepsilon}, \frac{y}{\varepsilon}\right) = \begin{pmatrix} 22 + 10 \times (\sin(2\pi \frac{x}{\varepsilon}) + \sin(2\pi \frac{y}{\varepsilon})) & 0 \\ 0 & 12 + 2 \times (\sin(2\pi \frac{x}{\varepsilon}) + \sin(2\pi \frac{y}{\varepsilon})) \end{pmatrix}.$$

for which

$$A_\star \approx \begin{pmatrix} 19.3378 & 0 \\ 0 & 11.8312 \end{pmatrix}.$$

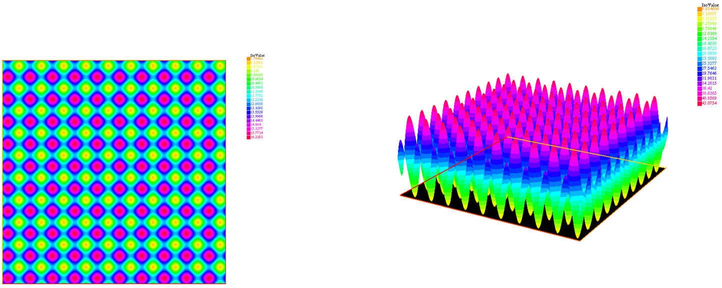


Figure: Components 11 and 22 of coefficient A_ε.

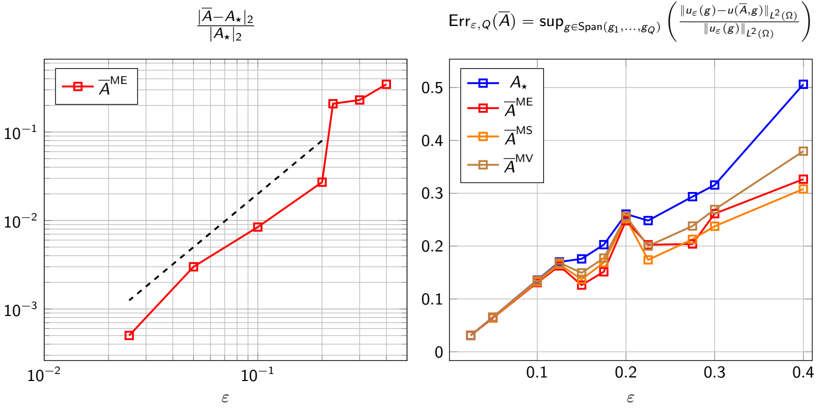


Figure: (left) Error between homogenized coefficient $A_\star$ and coefficients $\overline{A} \in \{\overline{A}^{\mathrm{MV}}_{\varepsilon,P}, \overline{A}^{\mathrm{ME}}_{\varepsilon,P}, \overline{A}^{\mathrm{MS}}_{\varepsilon,P}\}$. (right) Criterion $\mathrm{Err}_{\varepsilon,Q}(\overline{A})$ (with $Q = 11$) for $\overline{A} \in \{A_\star, \overline{A}^{\mathrm{MV}}_{\varepsilon,P}, \overline{A}^{\mathrm{ME}}_{\varepsilon,P}, , \overline{A}^{\mathrm{MS}}_{\varepsilon,P}\}$.

Numerical Results (stochastic)

We now use a non periodic coefficient (random checkerboard),

$$A_\varepsilon(x, y, \omega) = a^{\text{sto}}\left(\frac{x}{\varepsilon}, \frac{y}{\varepsilon}, \omega\right) = \left(\sum_{k \in \mathbb{Z}^2} X_k(\omega) \mathbb{1}_{k+Q}(x, y)\right) \mathrm{Id},$$

with X_k i.i.d random variables such that $\mathbb{P}(X_k = \gamma_1) = \mathbb{P}(X_k = \gamma_2) = \frac{1}{2}$ and $(\gamma_1, \gamma_2) = (4, 16)$.
We have

$$A_\star = \sqrt{\gamma_1 \gamma_2} \mathrm{Id}.$$

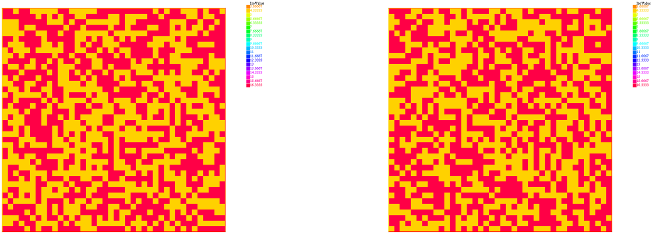
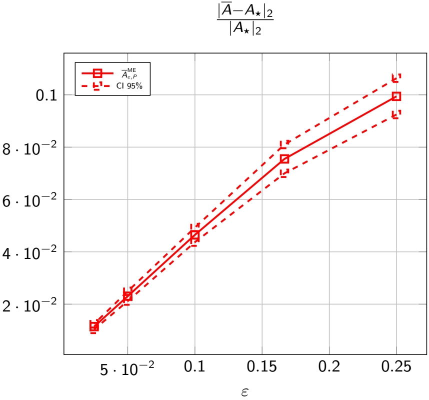


Figure: Two realizations of coefficient A_ε.

Our strategy rewrites $I_\varepsilon = \inf \sup |\mathbb{E}(\mathcal{E}(A_\varepsilon(\cdot, \omega), f)) - \mathcal{E}(\overline{A}, f)|$. Confidence intervals are computed from 40 realizations of the expectation (itself computed with a Monte Carlo method using 40 realizations of the coefficient a^{sto}).



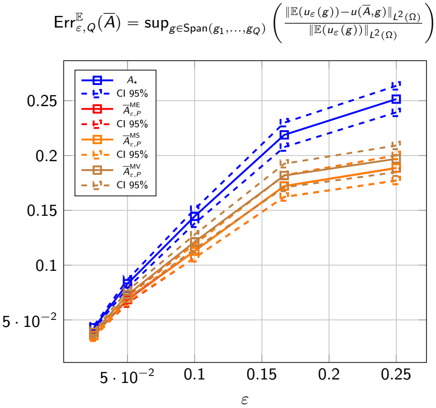


Figure: (left) Error between homogenized coefficient $A_\star$ and coefficients $\overline{A} \in \{\overline{A}^{\mathrm{ME}}_{\varepsilon,P}, \overline{A}^{\mathrm{MS}}_{\varepsilon,P}, \overline{A}^{\mathrm{MV}}_{\varepsilon,P}\}$. (right) Criterion $\mathrm{Err}^{\mathbb{E}}_{\varepsilon,Q}(\overline{A})$ (with $Q = 11$) for $\overline{A} \in \{A_\star, \overline{A}^{\mathrm{ME}}_{\varepsilon,P}, \overline{A}^{\mathrm{MS}}_{\varepsilon,P}, \overline{A}^{\mathrm{MV}}_{\varepsilon,P}\}$.

Perturbative Reconstruction of Effective Coefficients

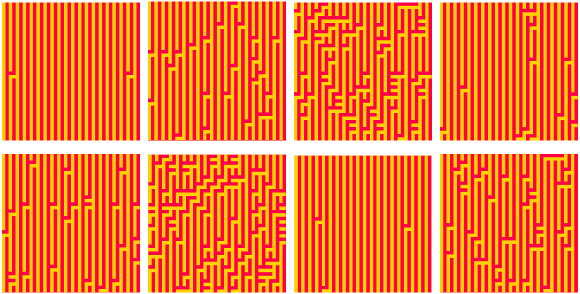
- Setting:
  - Randomly defectuous (periodic) coefficient

$$A_{\varepsilon,\eta}(x,\omega) = A_\varepsilon^{\mathrm{per}}(x) + b_\eta(\omega) C_\varepsilon^{\mathrm{per}}(x).$$

  - $C_\varepsilon^{\mathrm{per}}$ possibly not negligible, but

$$A_{\star,\eta} = \overline{A}_0 + \eta \overline{A}_1 + o(\eta).$$

  - $\overline{A}_0$ is known (e.g. given as an industrial reference).



- Issue:
  - Computing the effective coefficient using previous methods for many realizations ω may end up having a prohibitive computationnal costs...

Objective

Assume that the effective coefficient lies in the neighboorhood of a known coefficient $\overline{A}_0$.
How can we use this a priori knowledge to guide and speed up the optimization ?

- **Perturbative development**:
  - Assume $\overline{A} = \overline{A}_0 + \eta \overline{B}$.
  - Expand $\mathcal{E}(\overline{A}, g) \approx \mathcal{E}(\overline{A}_0, g) + \eta \sum_{ij} [\overline{B}]_{ij} \mathcal{F}_{ij}$, where $\mathcal{F}_{ij} := \mathcal{F}_{ij}(\overline{A}_0, g)$.
  - Consider the optimization problem

$$\inf_{\substack{\overline{B} \in \mathbb{R}^{d\times d}_{\mathrm{sym}}, \\ \alpha \leqslant \overline{A}_0 + \overline{B} \leqslant \beta}} \quad \sup_{\substack{g \in L^2(\Omega), \\ \|g\|_{L^2(\Omega)} = 1.}} \left(\left| \mathcal{E}(A_{\varepsilon,\eta}, g) - \mathcal{E}(\overline{A}_0, g) - \sum_{1 \leqslant i,j \leqslant d} [\overline{B}]_{ij} \mathcal{F}_{ij}(\overline{A}_0, g) \right| \right)^2 . \tag{6}$$

- **Implementation aspects**:
  - Gradient descent.
  - Offline stage to compute $\mathcal{F}_{ij}(\overline{A}_0, g)$.
  - Online stage requires no PDE resolution.

Numerical Results

- Do not damage drastically the quality.
- Reduction of computational costs (by a factor of $\approx$ 80 to 400).

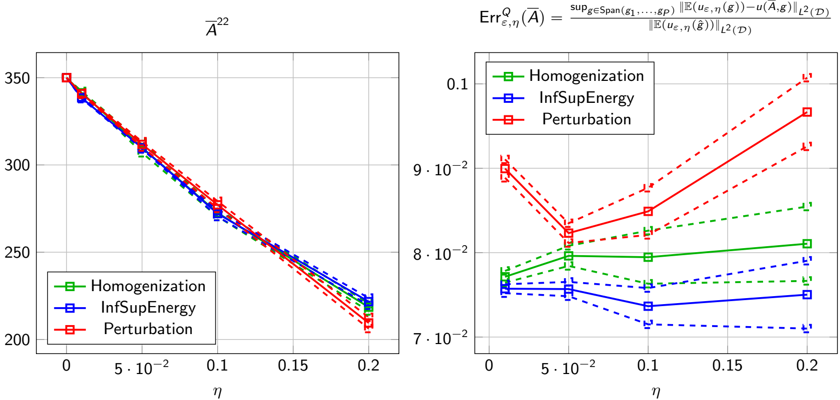


Figure: (left) Component 22 for various approximations of the effective coefficient. (right) Criterion $Err^{\mathbb{E}}_{\varepsilon,Q}(\overline{A})$ (with $Q = 9$) for different constant coefficients.

Conclusion

Our strategy

- aims at determining effective approximation for multiscale PDEs through a constant coefficient,
- is designed for context where *few* and *coarse* information is available,
- is inspired by homogenization theory and consistent with it (numerically and theoretically),
- can be extended outside the regime of separated scale,
- can be slightly modified in a perturbative context (hence reducing the computationnal cost).

Thank you !