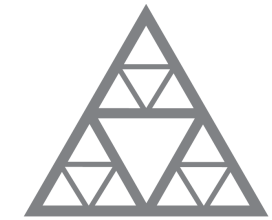

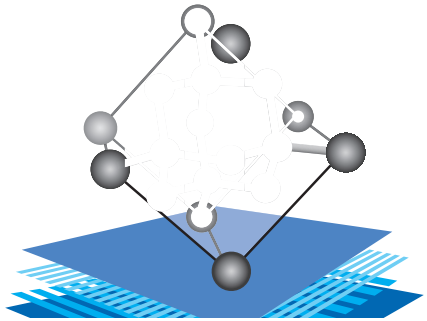

Effective Approximation for Elliptic PDEs with Highly Oscillating Coefficients

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Outline

1. An inverse multiscale problem
2. Recovering an effective coefficient
3. Linearization through perturbative approaches

Inverse problem

Our study focuses on inverse problems for PDEs.
Consider an equation of the type

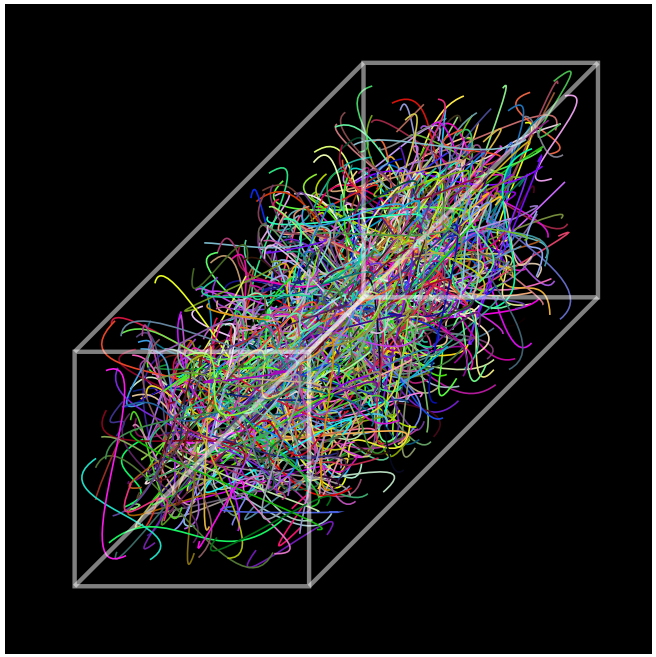
$$\mathcal{L}u = f.$$

- Is it possible to reconstruct the operator $\mathcal{L}$ (namely its coefficients) from the knowledge of some solutions u ?
- Can other (coarser) observables be used to reconstruct $\mathcal{L}$?

Inverse multiscale problem

Our study focuses on inverse problems for multiscale PDEs:

$$\mathcal{L}_\varepsilon u_\varepsilon = f.$$



Determining the fine-scale structure from measurements is an ill-posed problem... but identifying effective parameters is possible !

Inverse multiscale problem and ill-posedness

Consider the prototypical linear equation oscillating at the small length scale ε,

$$\mathcal{L}_\varepsilon u_\varepsilon = -\mathrm{div}\,(A_\varepsilon \nabla u_\varepsilon) = f \text{ in } \Omega, \quad u_\varepsilon = 0 \text{ on } \partial\Omega, \tag{1}$$

with A_ε a bounded coercive coefficient.

Homogenization[1] assesses the existence of a limit equation when $\varepsilon \to 0$,

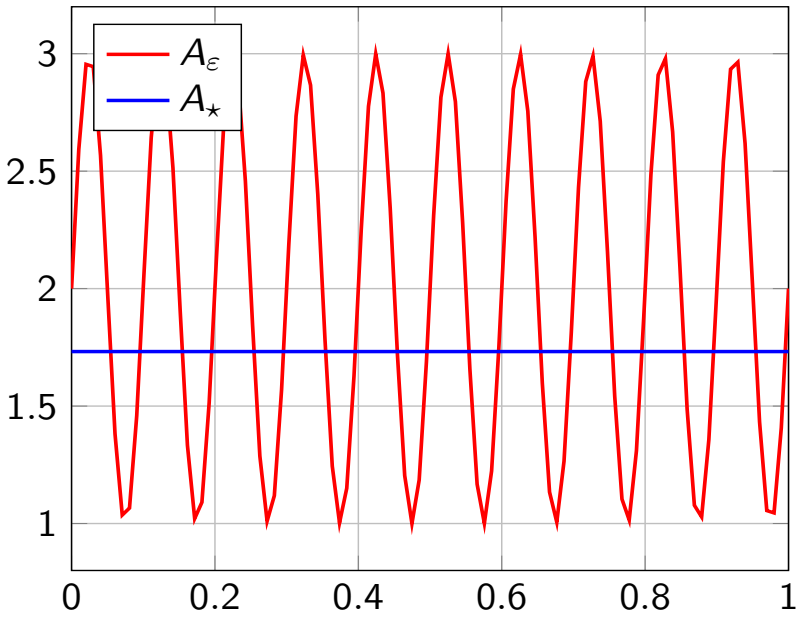
$$\mathcal{L}_\star u_\star = -\mathrm{div}\,(A_\star \nabla u_\star) = f \text{ in } \Omega, \quad u_\star = 0 \text{ on } \partial\Omega, \tag{2}$$

with $A_\star$ an effective coefficient for which, in general, there exists no formula (abstract compactness result).

[1] see e.g. A. Benssoussan, J.-L. Lions, G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, 1978.

Inverse multiscale problem and ill-posedness

Issue: in the limit $\varepsilon \to 0$, the observable u_ε is very close to $u_\star$ whereas the operator we seek to reconstruct, $\mathcal{L}_\varepsilon$, is very different from $\mathcal{L}_\star$, its homogenized version.



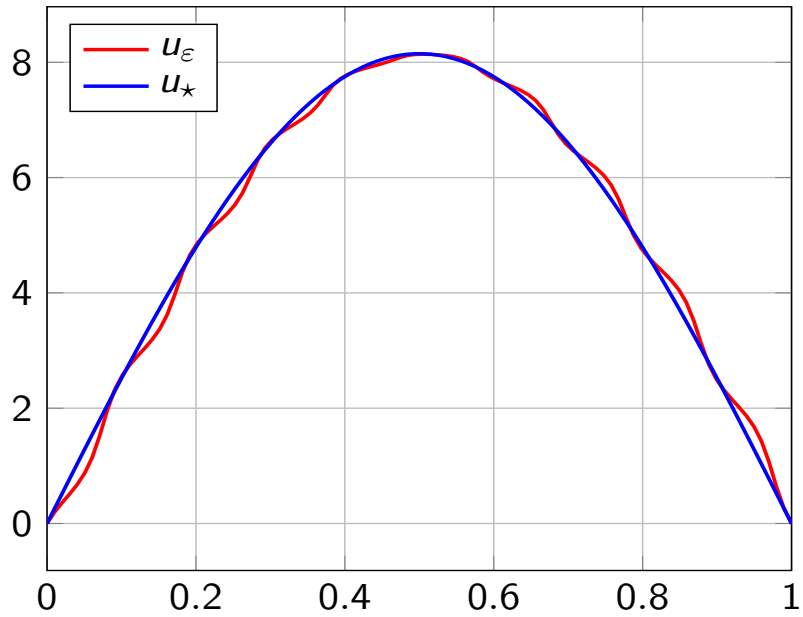


Figure 3: Two similar solutions associated to two distinct diffusion coefficients

Building an effective coefficient

Consider the multiscale diffusion problem (3)

$$\mathcal{L}_\varepsilon u_\varepsilon = -\text{div}\left(A_\varepsilon \nabla u_\varepsilon\right) = f \text{ in } \Omega, \qquad u_\varepsilon = 0 \text{ on } \partial\Omega. \tag{3}$$

From the knowledge of *observables* (to be explicited latter) associated to solutions u_ε for various r.h.s. f, our aim is to propose a numerical methodology to build an effective operator $\overline{\mathcal{L}}$ approaching $\mathcal{L}_\varepsilon$.

Our strategy

- is inspired by homogenization theory,
- does not rely on classical hypothesis for homogenization (such as periodicity) which may be too restrictive in practical situations,
- is valid outside the regime of homogenization (i.e. $\varepsilon \to 0$),
- requires *few* prior information about the underlying system (the knowledge of $P \approx 3$ averaged observables is sufficient).

Previous work [CRAS2013][2], [COCV2018][3]

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

$$\overline{\mathcal{L}}\overline{u} = -\text{div}\left(\overline{A}\nabla\overline{u}\right) = f \text{ in } \Omega, \qquad \overline{u} = 0 \text{ on } \partial\Omega. \tag{4}$$

The quality of the approximation of $\mathcal{L}_\varepsilon$ by $\overline{\mathcal{L}}$ can be quantified through the functional

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

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

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

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.

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

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

Exploiting the energy

Coarser observables can be considered, such as the energy

$$\mathcal{E}(A_\varepsilon, f) = \frac{1}{2}\int_\Omega A_\varepsilon \nabla u_\varepsilon \cdot \nabla u_\varepsilon - \int_\Omega f u_\varepsilon. \tag{5}$$

Homogenization theory guarantees the convergence for energy:

$$\mathcal{E}(A_\varepsilon, f) \underset{\varepsilon \to 0}{\longrightarrow} \mathcal{E}(A_\star, f) \text{ in } \mathbb{R}, \tag{6}$$

with

$$\mathcal{E}(A_\star, f) = \frac{1}{2}\int_\Omega A_\star \nabla u_\star \cdot \nabla u_\star - \int_\Omega f u_\star,$$

and where $u_\star$ still denotes the solution to

$$\mathcal{L}_\star u_\star = -\mathrm{div}\,(A_\star \nabla u_\star) = f \quad \text{in } \Omega, \qquad u_\star = 0 \text{ on } \partial\Omega.$$

Our strategy

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

$$\overline{\mathcal{L}}\overline{u} = -\text{div}\left(\overline{A}\nabla\overline{u}\right) = f \text{ in } \Omega, \qquad \overline{u} = 0 \text{ on } \partial\Omega. \tag{7}$$

To assess the quality of the approximation of $\mathcal{L}_\varepsilon$ by $\overline{\mathcal{L}}$, we use the functional

$$\cancel{\sup_{\|f\|_{L^2(\Omega)}=1} \|u_\varepsilon(f) - u(\overline{A}, f)\|_{L^2(\Omega)}} \longrightarrow \sup_{\|f\|_{L^2(\Omega)}=1} |\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(\overline{A}, f)|$$

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

$$\inf_{\overline{A}\in\mathbb{R}^{d\times d}_{\text{sym}}} \sup_{\|f\|_{L^2(\Omega)}=1} |\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(\overline{A}, f)|$$

In the limit of separated scales

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

$$I_\varepsilon = \inf_{\overline{A} \in \mathbb{R}^{d\times d}_{\text{sym}}} \sup_{\|f\|_{L^2(\Omega)}=1} |\mathcal{E}\left(A_\varepsilon, f\right) - \mathcal{E}\left(\overline{A}, f\right)|. \tag{8}$$

Proposition (Asymptotic consistency, periodic case)

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

$$I_\varepsilon \leq J_\varepsilon(\overline{A}^{\#}_\varepsilon) \leq I_\varepsilon + \varepsilon, \tag{9}$$

the following convergence holds:

$$\lim_{\varepsilon\to 0} \overline{A}^{\#}_\varepsilon = A_\star. \tag{10}$$

Proof for consistency proposition

Let $J_\varepsilon(\overline{A}) = \sup_{\|f\|_{L^2(\Omega)}=1} |\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(\overline{A}, f)|$.

Lemma (Convergence for the energy)

In the periodic setting, we have

$$\lim_{\varepsilon \to 0} J_\varepsilon(A_\star) = 0.$$

We also use in the proof that the injection $H^1(\Omega) \subset L^2(\Omega)$ is compact.

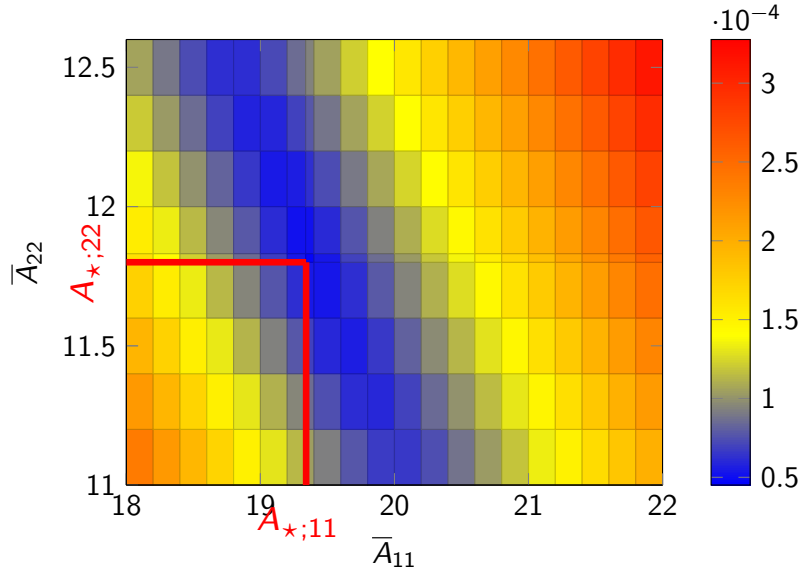


Figure 1: Isovalue of $J_\varepsilon(\overline{A})$.

Computational procedure

To solve

$$I_\varepsilon = \inf_{\overline{A} \in \mathbb{R}^{d\times d}_{\text{sym}}} \sup_{\|f\|_{L^2(\Omega)}=1} \left(\mathcal{E}\left(A_\varepsilon, f\right) - \mathcal{E}\left(\overline{A}, f\right)\right)^2 .$$

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

① Define f^n, the argsup to

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

In practice, $\sup_{f\in L^2(\Omega)} \to \sup_{f\in V_P}$ on $V_P = \text{Span}\{P \text{ r.h.s.}\}$, with $P \approx 3$. This step requires computing P solutions to a coarse 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

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

In practice, we perform a gradient descent. The gradient can be expressed with solutions computed in step ①, hence no additionnal costs.

In practice, we perform $N \approx 10$ iterations of both steps.

Numerical results

We use an alternating direction algorithm in 2D ($\Omega = [0,1]^2$) using 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

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

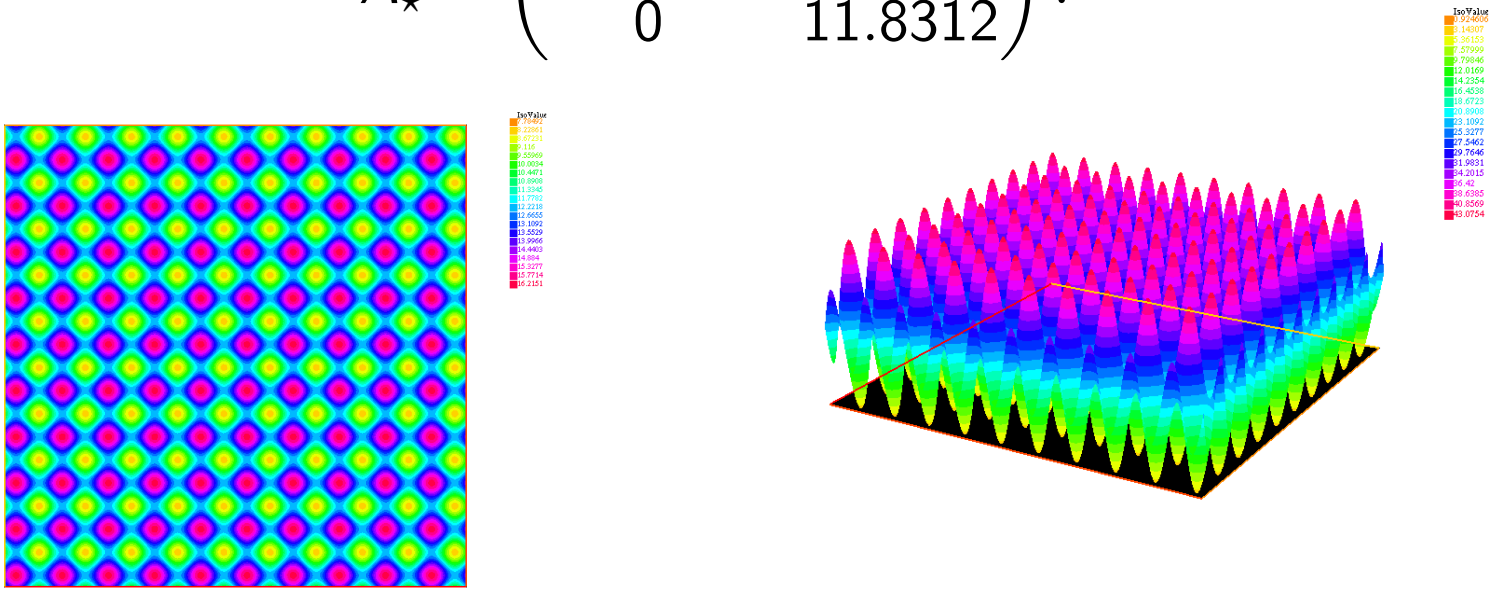


Figure 2: Components 11 and 22 of coefficient A_ε.

Consistency with homogenization theory

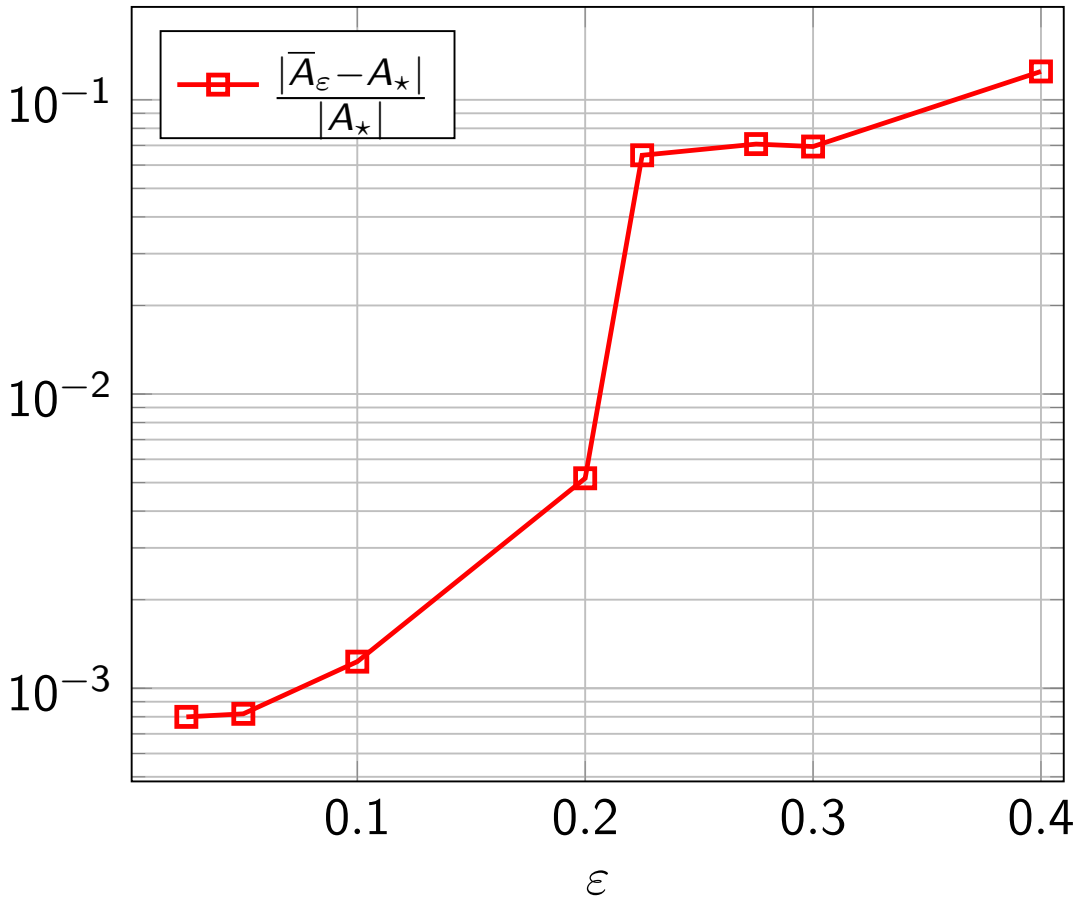


Figure 3: Error between the homogenized coefficient $A_\star$ and the effective coefficient $\overline{A}_\varepsilon$ as a function of ε.

Beyond the regime of separated scales

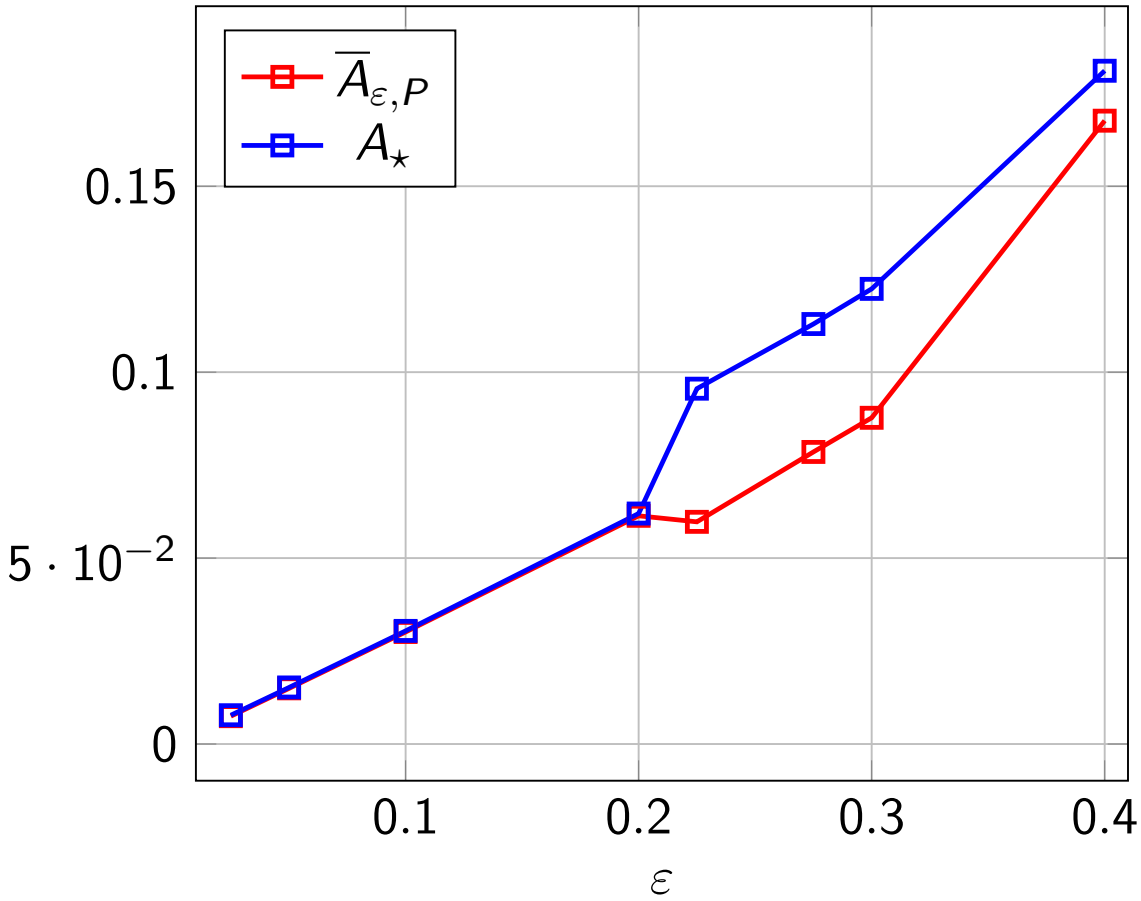


Figure 4: Error $\frac{\sup_{f \in V_Q} \|u_\varepsilon(f) - u(\overline{A}_{\varepsilon,P}, f)\|_{L^2(\Omega)}}{\|u_\varepsilon(\bar{f})\|_{L^2(\Omega)}}$ as a function of ε. ($\overline{A}_\varepsilon$ is computed with $P \ll Q = 16$ r.h.s)

Beyond periodicity

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

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

with X_k i.i.d random variables such that $\mathbb{P}(X_k = 4) = \mathbb{P}(X_k = 16) = \frac{1}{2}$.

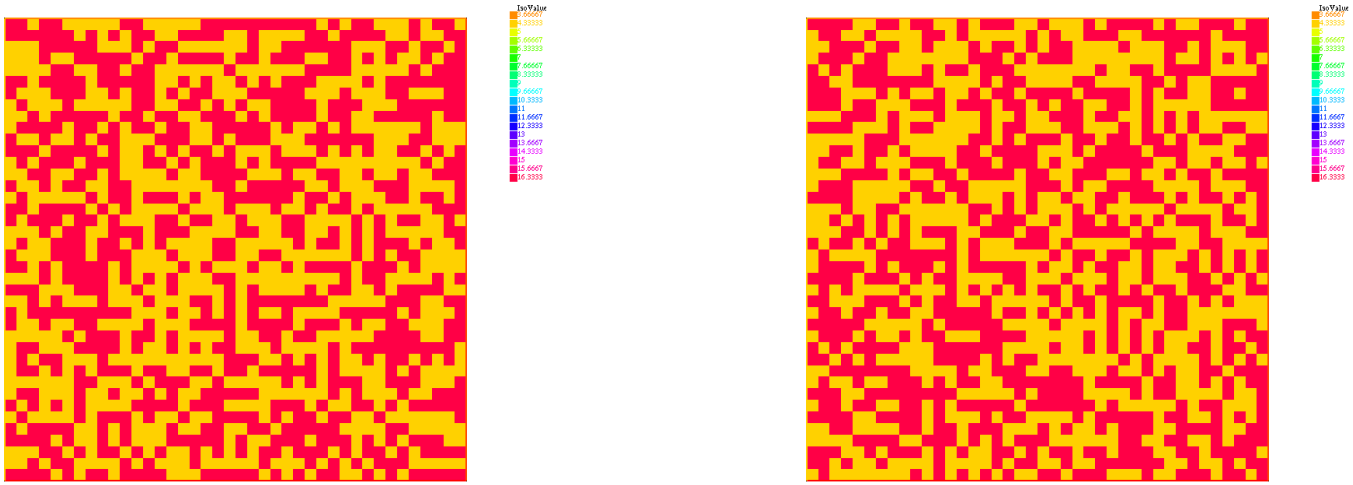


Figure 5: Two realizations of coefficient A_ε.

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}).

Consistency with homogenization theory

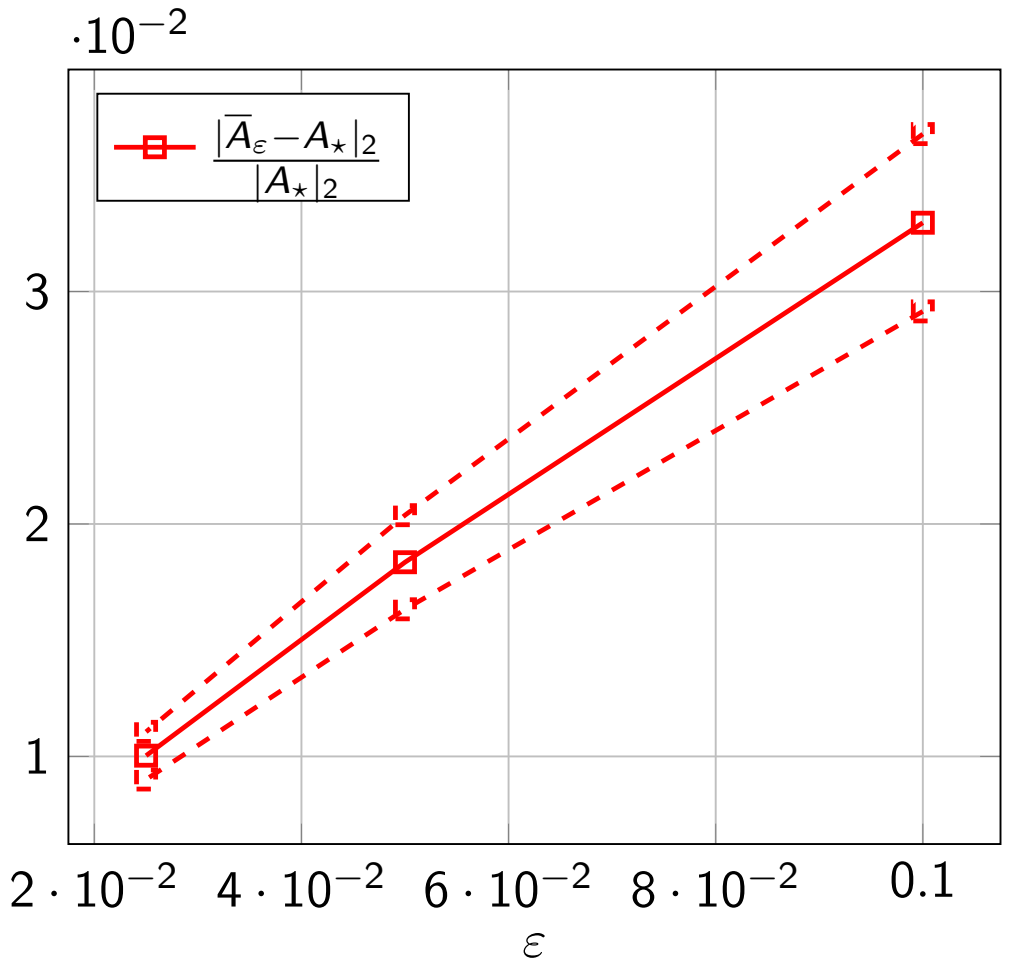


Figure 6: Error between the homogenized coefficient $A_\star$ and the effective coefficient $\overline{A}_\varepsilon$ as a function of ε.

Beyond periodicity and the regime of separated scales

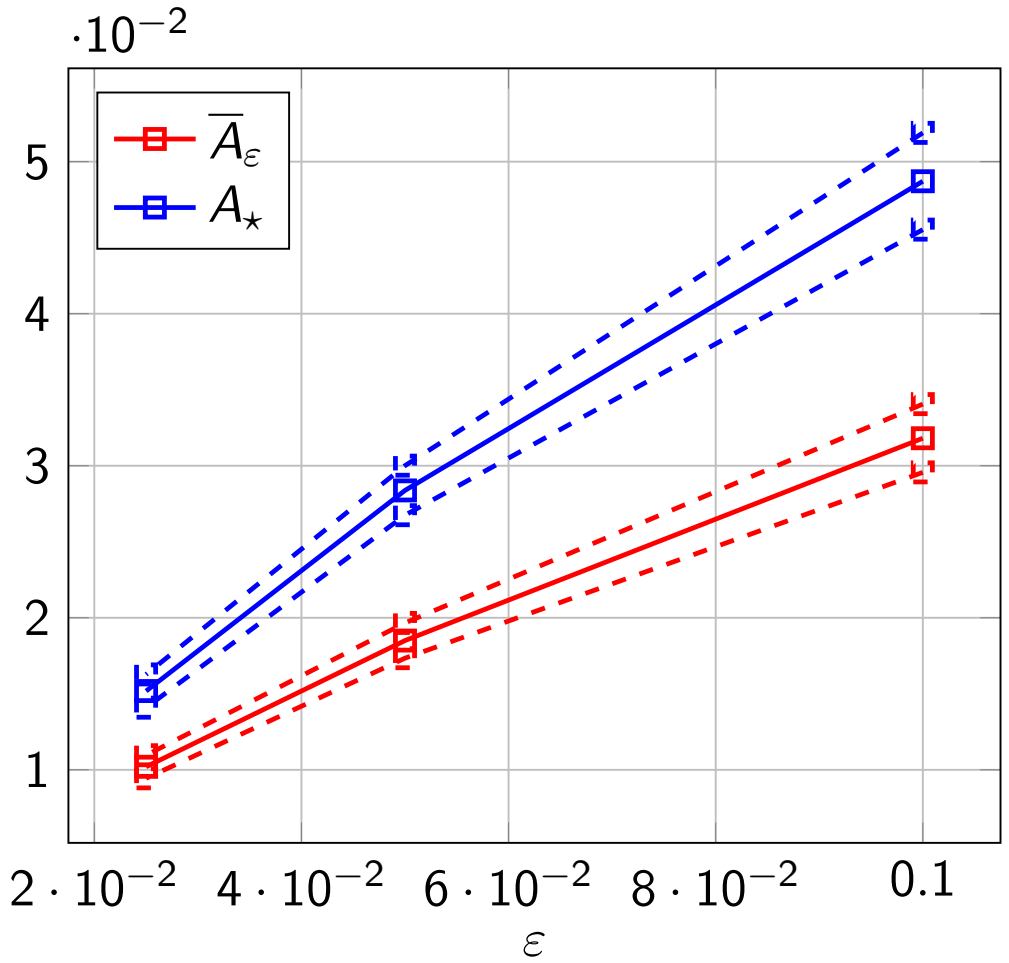


Figure 7: Error $\frac{\sup_{f \in V_Q} \|\mathbb{E}(u_\varepsilon(f,\omega)) - u(\overline{A}_{\varepsilon,P}, f)\|_{L^2(\Omega)}}{\|\mathbb{E}(u_\varepsilon(\bar{f},\omega))\|_{L^2(\Omega)}}$ as a function of ε. ($\overline{A}_\varepsilon$ is computed with $P \ll Q = 16$ r.h.s)

Perturbative approach

In some situations, we may initially know that A_ε is close to a reference coefficient A_ε^0, and therefore that the coefficient $A_\star$ we are looking for is close to a reference coefficient A_0.

To take into account such information, we look for an effective coefficient in the form

$$\overline{A} = A_0 + \eta \overline{B} \tag{11}$$

and assume A_0 and η are known (η may represent the probability of defect in a material[4]).
For such $\overline{A}$, we have the perturbative development

$$\mathcal{E}(\overline{A}, f) \approx \mathcal{E}(A_0, f) + \eta \sum_{ij} \overline{B}_{ij} \int_\Omega f \, v_{ij}(A_0, f). \tag{12}$$

with v_{ij} depending only on A_0 and f.

[4] see e.g. A. Anantharaman, C. Le Bris, MMS, 2011.

Linearization through a perturbative approach

The problem rewrites

$$\inf_{\overline{A}=A_0+\eta\overline{B}\in\mathbb{R}^{d\times d}} \sup_{\|f\|_{L^2(\Omega)}=1} \left(\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(A_0, f) - \eta \sum_{ij} \overline{B}_{ij} \int_\Omega f\, v_{ij}(A_0, f) \right)^2$$

An advantage of this formulation is that the functional to optimize is quadratic in $\overline{B}$ in contrast to the previous formulation.

This significantly reduces the computational costs provided the offline resolution of $P \times \frac{d(d+1)}{2}$ PDE to identify $v_{ij}(A_0, f_p)$.

Computational Procedure

Offline: Precompute $v_{ij}(A_0, f_p)$.
Online: Given an iterate $\overline{A}^n = A_0 + \eta \overline{B}^n$:

① Define f^n, the argsup to

$$\sup_{\|f\|_{L^2(\Omega)}=1} (\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(A_0, f) - \eta \sum_{ij} \overline{B}_{ij} \int_\Omega f v_{ij}(A_0, f))^2$$

In practice, $\sup_{f \in L^2(\Omega)} \to \sup_{f \in V_P}$ with $P \approx 3$ r.h.s.

① Define $\overline{A}^{n+1} = A_0 + \eta \overline{B}^{n+1}$, the optimizer to

$$\inf_{\overline{A}=A_0+\eta\overline{B}} (\mathcal{E}(A_\varepsilon, f^n) - \mathcal{E}(A_0, f^n) - \eta \sum_{ij} \overline{B}_{ij} \int_\Omega f^n v_{ij}(A_0, f^n))^2$$

In practice, we perform a gradient descent. The gradient can be expressed with the quantity computed offline, hence no additionnal costs.

In practice, we need more iterations ($N_{\text{iter}} \approx 10^4$), but each iteration is essentially for free (no PDE to solve).

Numerical results

Let us consider a perturbed material

$$A_{\varepsilon,\eta}(x,y,\omega) = A_\varepsilon(x,y) + b_\eta(\omega) C_\varepsilon(x,y)$$

for which, in each cell of size ε, the probability of a defect from A_ε to $A_\varepsilon + C_\varepsilon$ is η.

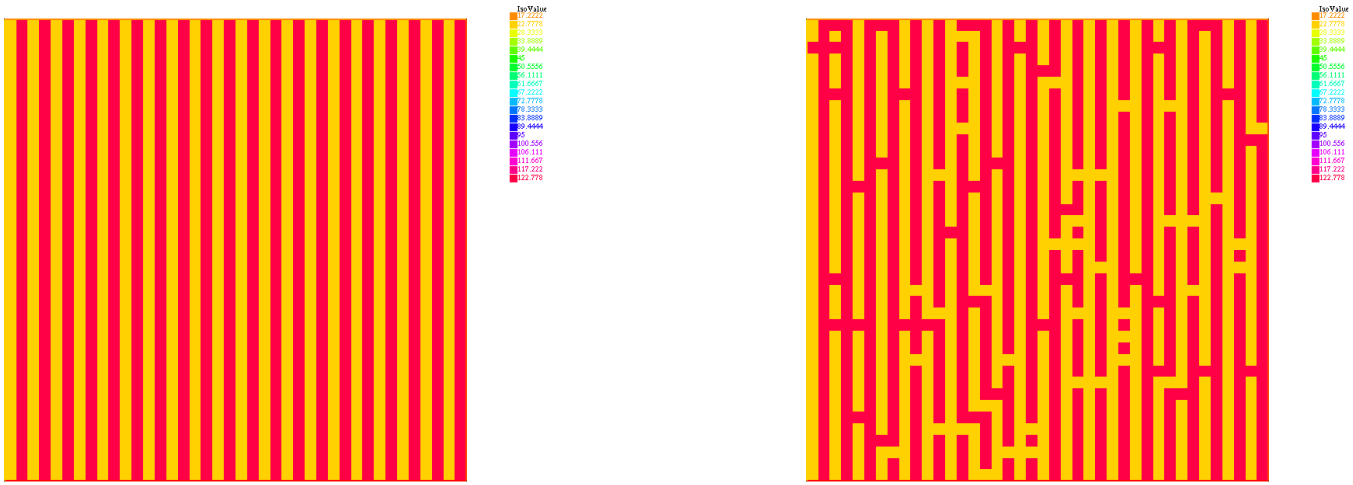


Figure 8: Coefficient $A_{\varepsilon,\eta}$ with $\eta = 0$ (left) and with $\eta = 0.1$ (right).

Recovering Effective Coefficient

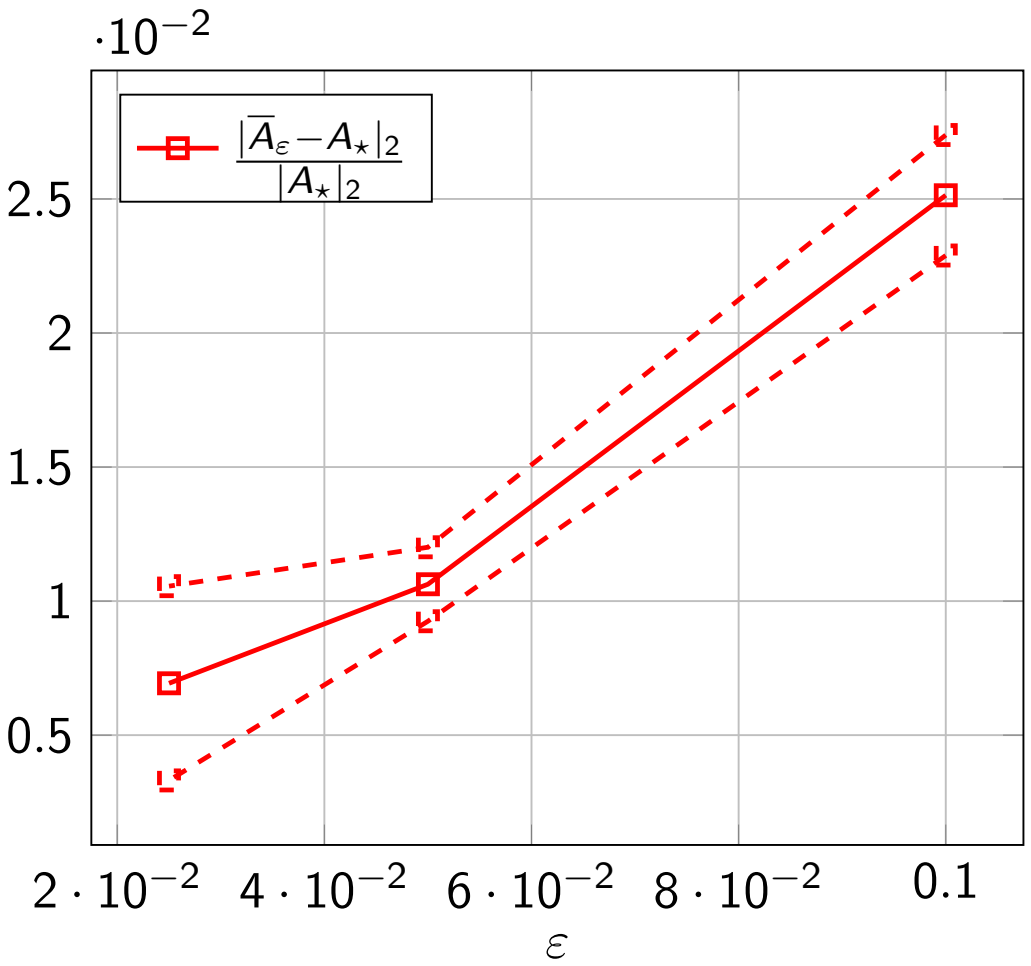


Figure 9: Error between the effective coefficient $\overline{A}_{\varepsilon,\eta}$ and the homogenized coefficient $A_{\star,\eta}$ ($\eta = 0.1$) as a function of ε.

Conclusion and ongoing works

Our strategy

- aims at determining effective coefficients for multiscale PDEs,
- is inspired by homogenization theory and consistent with it (numerically and theoretically),
- can be extended outside the regime of separated scale,
- requires *few* prior information on the system (coarse averages are sufficient),
- can be linearized in a perturbative context (hence reducing the computationnal cost).

Future works include selection of effective coefficient among a given list rather than identification.