Effective Approximation for Elliptic PDEs with highly oscillating coefficients

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ECCOMAS 2024

June 3rd – 7th, 2024

Outline

1. An inverse multiscale problem

2. Recovering an effective coefficient

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 $\mathcal{L}$?

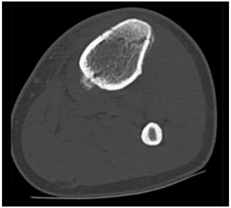


Figure 1: Bones echography showing two inclusions

Inverse multiscale problem

Our study focuses on inverse problems for multiscale PDEs :

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

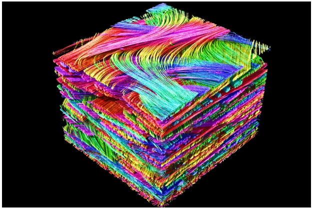


Figure 2: Composite material

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

Homogenization theory as a guideline

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

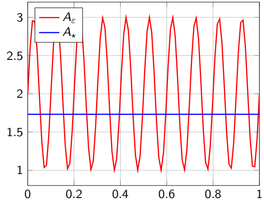
$$\mathcal{L}_\varepsilon u_\varepsilon = -\mathrm{div}\left(A_\varepsilon \nabla u_\varepsilon\right) = f \text{ in } \Omega, \quad u_\varepsilon = 0 \text{ on } \partial\Omega, \tag{1}$$

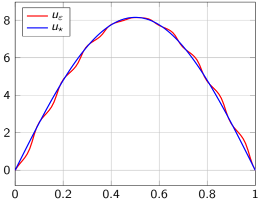
with $A_\varepsilon(\cdot) = A^{\mathrm{per}}(\cdot/\varepsilon)$ a bounded coercive coefficient.

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

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

with $A_\star$ an effective constant coefficient.





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

Building an effective coefficient

Consider the multiscale diffusion problem (3)

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

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 only coarse scale prior information about the underlying system,
- is designed to get satisfying approximation of u_ε (but not of ∇u_ε).

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

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

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 $A_\star$.

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

Proposition (Asymptotic consistency, periodic case)

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

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

the following convergence holds :

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

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

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

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 <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

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

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

In practice, we perform <u>$N \approx 10$ iterations</u> 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

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

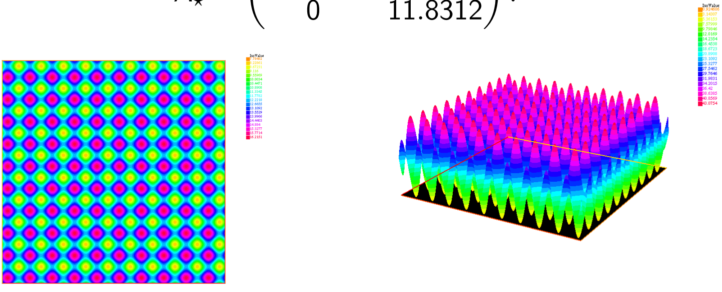


Figure 3: Components 11 and 22 of coefficient A_ε.

Consistency with homogenization theory

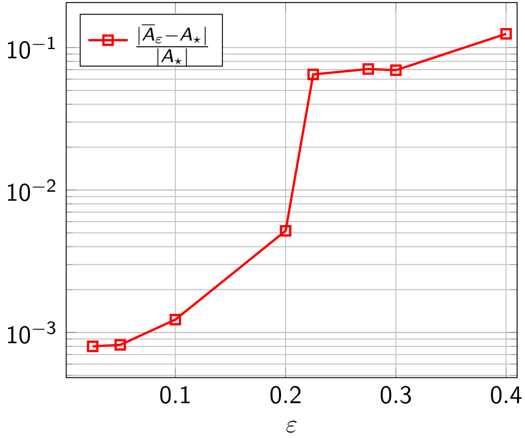


Figure 4: Error between the homogenized coefficient $A_\star$ and the effective coefficient $\overline{A}_\varepsilon$ as a function of ε.

Beyond the regime of separated scales

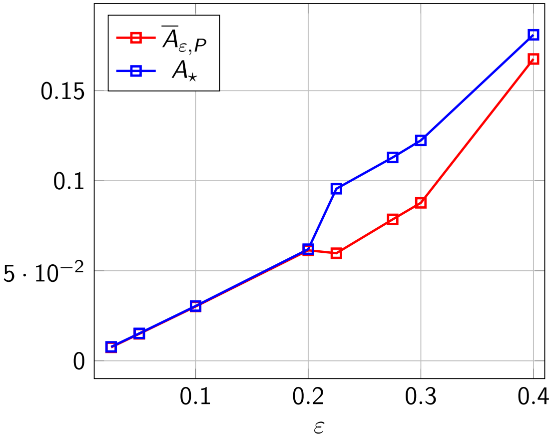


Figure 5: Error $\frac{\sup_{f \in V_Q} \|u_\varepsilon(f) - u(\overline{A}_{\varepsilon,P}, f)\|_{L^2(\Omega)}}{\|u_\varepsilon(\bar{f})\|_{L^2(\Omega)}}$ as a function of ε. ($\overline{A}_\varepsilon$ is computed with $P \ll Q = 16$ r.h.s)

Beyond periodicity

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

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

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

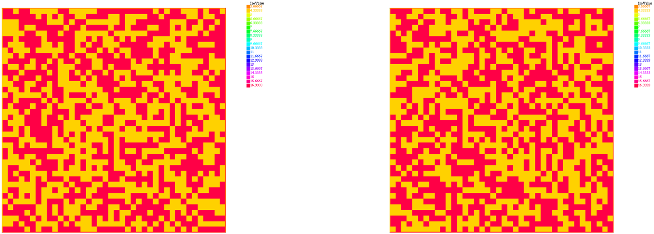


Figure 6: Two realizations of coefficient A_ε.

Our strategy rewrites $I_\varepsilon = \inf\sup\left|\mathbb{E}(\mathcal{E}(A_\varepsilon(\cdot,\omega),f)) - \mathcal{E}(\overline{A},f)\right|$. The expectation is computed from 40 realizations.

Consistency with homogenization theory

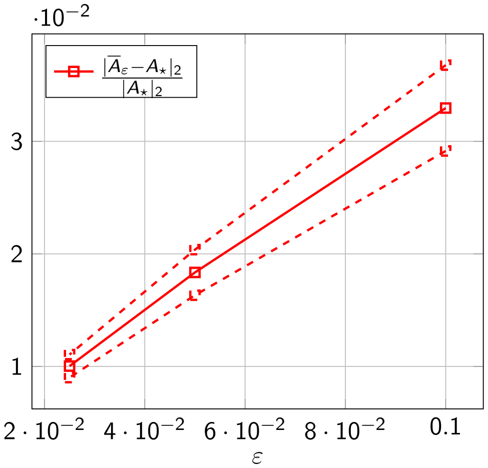


Figure 7: Error between the homogenized coefficient $A_\star$ and the effective coefficient $\overline{A}_\varepsilon$ as a function of ε.

Beyond periodicity and the regime of separated scales

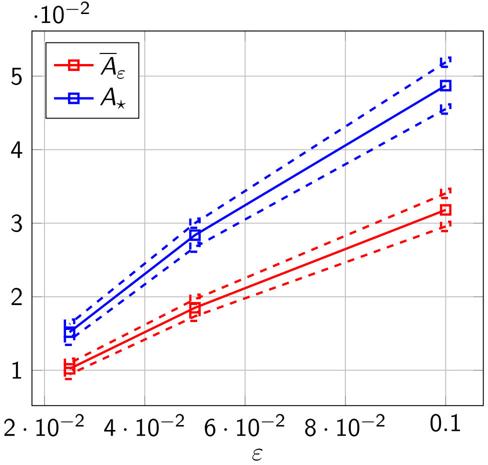


Figure 8: Error $\frac{\sup_{f \in V_Q} \|\mathbb{E}(u_\varepsilon(f,\omega)) - u(\overline{A}_{\varepsilon,P}, f)\|_{L^2(\Omega)}}{\|\mathbb{E}(u_\varepsilon(\bar{f},\omega))\|_{L^2(\Omega)}}$ as a function of ε. ($\overline{A}_\varepsilon$ is computed with $P \ll Q = 16$ r.h.s)

Conclusion and ongoing works

Our strategy

- aims at determining effective coefficients for multiscale PDEs,
- provides an accurate description of u_ε (not of ∇u_ε),
- is inspired by homogenization theory and consistent with it (numerically and theoretically),
- can be extended outside the regime of separated scale,
- requires coarse scale prior information on the system.