

Effective approximations of multiscale PDE based on limited information

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PhD Defense

December 2, 2025

General introduction

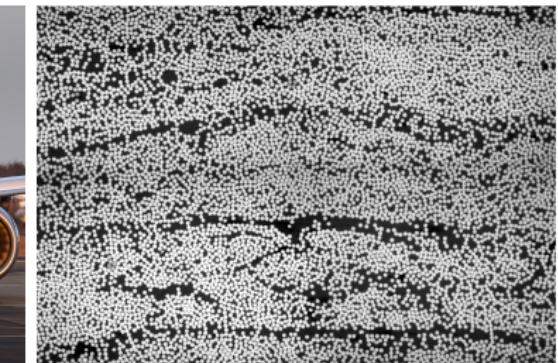
Multiscale systems

Multiscale systems are characterized by the presence of several scales of interest that interact or influence one another.

They may be found in various scientific areas: engineering, biology, physics, ...



airplane wing $\approx 10\text{m}$



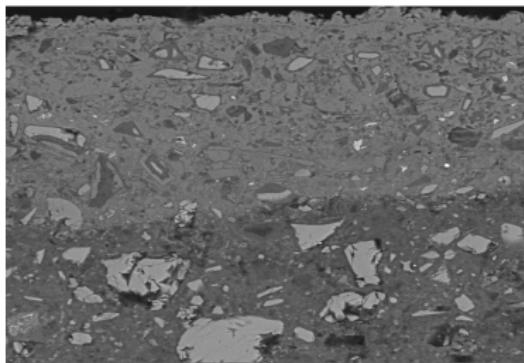
v.s. carbon fibers $\approx 10^{-6}\text{m}$

Figure: Composite material used in the aeronautics industry.

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bridge $\approx 10^3$ m

v.s. mineral aggregate $\approx 10^{-5}$ m

Figure: Concrete: a multiscale material.

Approximation of multiscale PDE

- Consider the problem

$$-\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f \text{ in } \Omega,$$

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

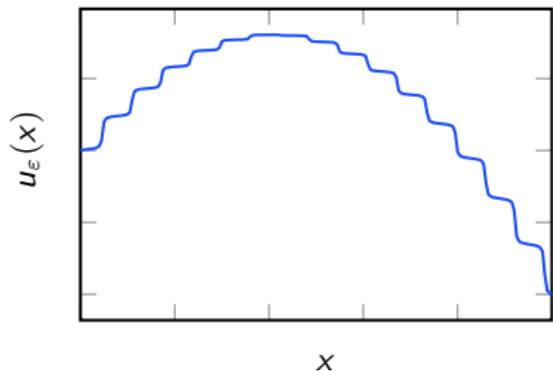
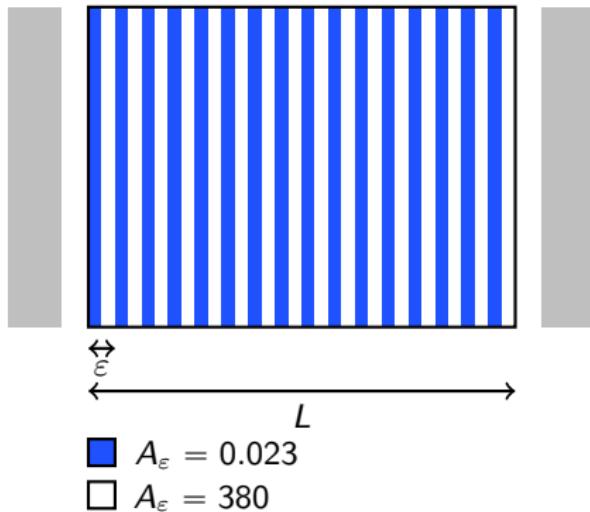
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- Applications: heat transfer in thermal engineering, (simplification of) elastic problem in mechanics, ...



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Based on measurements about the system, construct an approximation of the mapping

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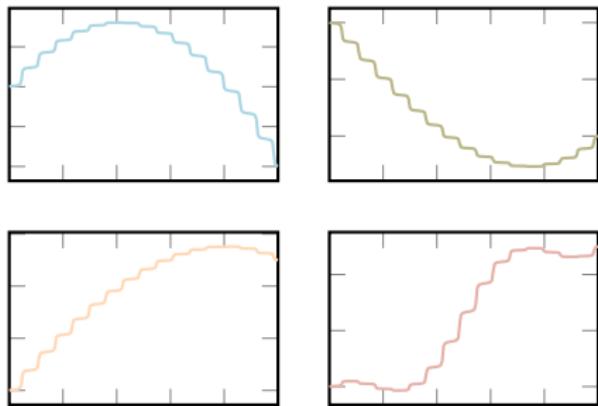
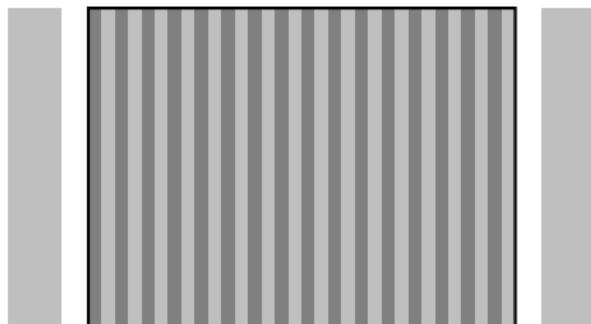
Limited information

Experimental settings:

- little knowledge on microstructure.
- availability of couples (*configuration, system response*).

Settings with limited information:

- No assumptions on microstructure (non periodic case, ε small but not infinitely small, ...).
- Qualitative restrictions (coarse measurements, noisy measurements, ...).
- Quantitative restrictions (limited budget of measurements).



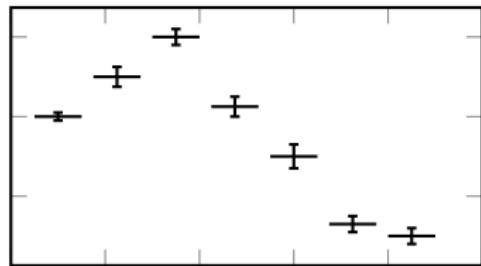
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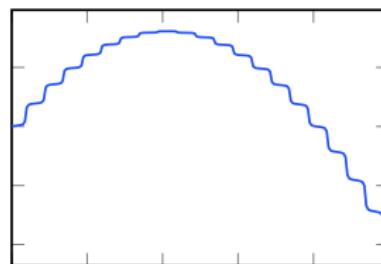
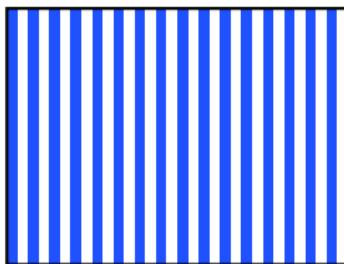
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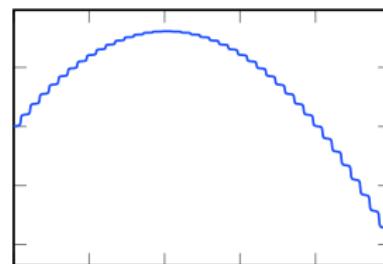
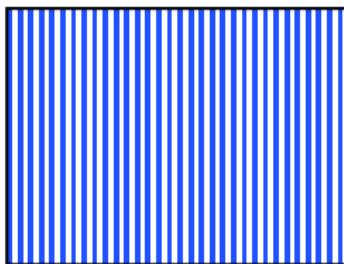
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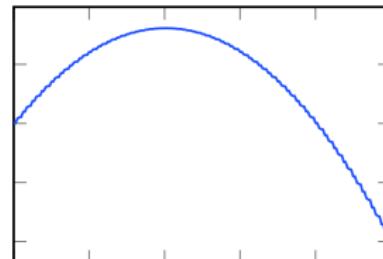
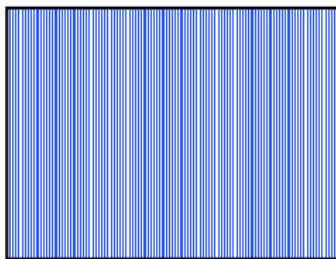


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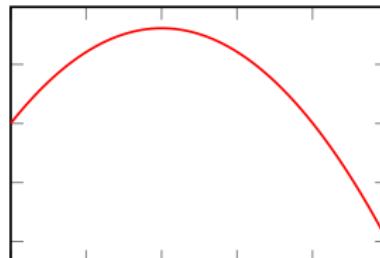


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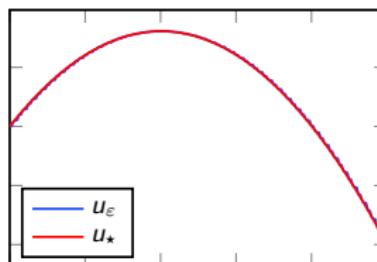
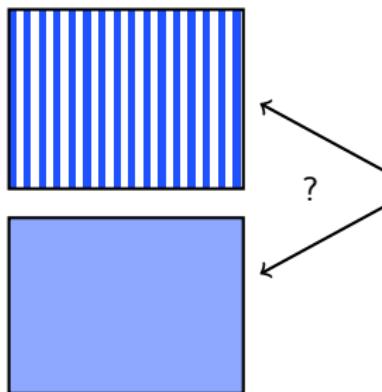
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Oscillating System

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Different approaches

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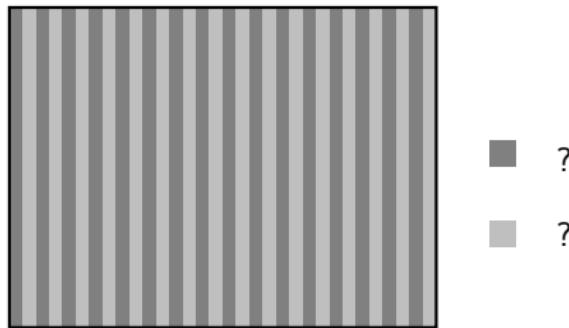
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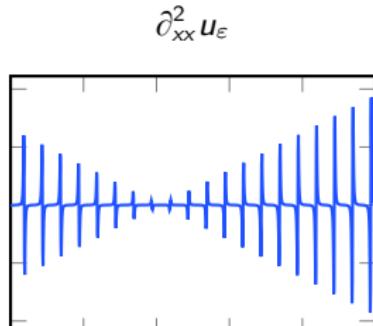
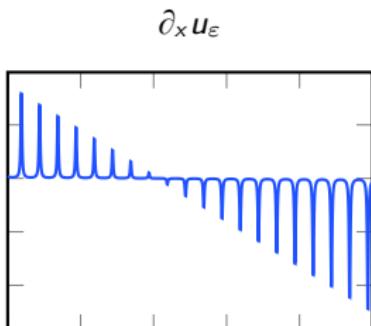
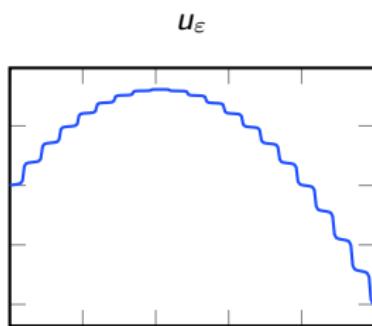
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Issue: how to proceed in contexts of limited information?

Effective coefficients

Effective coefficients are coefficients varying at the macroscopic scale that encapsulate the fine-scale features of highly oscillatory coefficients.

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Example. Homogenization assesses the existence of an **effective coefficient A_*** such that

$$\mathcal{L}_\varepsilon : f \longrightarrow u_\varepsilon(f) \quad \text{sol. to } -\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f$$

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In the periodic case $A_\varepsilon(x) = A_{\text{per}}\left(\frac{x}{\varepsilon}\right)$, with A_{per} Q -periodic:

$$A_\star = \int_Q A_{\text{per}}(\nabla w + \operatorname{Id}),$$

where w is a corrector defined through a PDE involving A_{per} .

In particular, in dimension $d = 1$, it holds that $A_\star = \left(\int_Q \frac{1}{A_{\text{per}}} \right)^{-1}$.

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Two major limitations of homogenization:

- **No formulas** for A_* in the general case.
- Valid only in the regime of **separated scale** (i.e. $\varepsilon \rightarrow 0$).

Objective

Based on available observables, define an effective operator $-\operatorname{div}(\bar{A}\nabla \cdot)$ such that, for any f , the solutions $u_\varepsilon(f)$ to

$$-\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f$$

are satisfactorily approximated by the solutions $\bar{u} = u(\bar{A}, f)$ to the coarse problem

$$-\operatorname{div}(\bar{A}\nabla \bar{u}) = f.$$

- Part I** • Construct \bar{A} in the set $\mathbb{R}_{\text{sym}}^{d \times d}$.
- Part II** • Identify \bar{A} in the vicinity of a known coefficient \bar{A}_0 .
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Part IV • Effective approximation of Schrödinger equation.

Part I

Effective modeling from boundary aggregated measurements

A proof of concept [CRAS2013]², [COCV2018]³

For any $g \in L_0^2(\partial\Omega)$, consider the solution $u_\varepsilon = u_\varepsilon(g)$ with vanishing mean to

$$-\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = 0 \text{ in } \Omega, \quad (A_\varepsilon \nabla u_\varepsilon) \cdot n = g \text{ on } \partial\Omega. \quad (1)$$

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

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

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

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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.

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Practical observables

Only *coarser* observables are usually experimentally accessible, such as the energy

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

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Motivation:

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

$$\mathcal{E}(A_\varepsilon, g) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{E}(A_\star, g) \text{ in } \mathbb{R},$$

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** at the **boundary**, thus it presents the characteristics of a quantity that is experimentally accessible.
- $\mathcal{E}(A_\varepsilon, g)$ is a scalar, thus it provides **no direct insights about the microscale**.

A new formulation

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

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$$\sup_{\|g\|_{L^2(\partial\Omega)}=1} \|u_\varepsilon(g) - u(\bar{A}, g)\|_{L^2(\Omega)}^2 \rightarrow \sup_{\|g\|_{L^2(\partial\Omega)}=1} |\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}, g)|^2.$$

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

Theoretical analysis

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

$$I_\varepsilon = \inf_{\substack{\bar{A} \in \mathbb{R}_{\text{sym}}^{d \times d} \\ \alpha \leq \bar{A} \leq \beta}} \underbrace{\sup_{\|g\|_{L^2(\partial\Omega)}=1} |\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}, g)|^2}_{J_\varepsilon(\bar{A})}$$

Proposition (Asymptotic consistency, periodic case)

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

$$I_\varepsilon \leq J_\varepsilon(\bar{A}_\varepsilon^\#) \leq I_\varepsilon + \text{err}(\varepsilon),$$

the following convergence holds:

$$\lim_{\varepsilon \rightarrow 0} \bar{A}_\varepsilon^\# = A_\star. \tag{4}$$

Sketch of proof

Three ingredients:

- Optimization over **compact set** $\mathcal{S}_{\alpha,\beta}$ $\implies \overline{A}_\varepsilon^\#$ converges to $\overline{A}_\#$ up to an extraction.

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Polarization relation implies that for any $f, g \in L_0^2(\partial\Omega)$:

$$\int_{\partial\Omega} f \ u(A_\star, g) = \int_{\partial\Omega} f \ u(\bar{A}_\#, g).$$

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- Use that $A_\star, \bar{A}_\#$ are **constant coefficients** and exploit (5) evaluated at **particular loadings** $(g_i)_{1 \leq i \leq \frac{d(d+1)}{2}}$ to conclude that

$$A_\star = A_\#.$$

Computational procedure

We apply an **iterative algorithm** to solve

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

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Given an iterate \bar{A}^n ,

- ① Define g^n , the argsup to

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In practice, $\sup_{g \in L_0^2(\Omega)} \rightarrow \sup_{g \in V_P}$ on $V_P = \text{Span}\{P \text{ loadings}\}$, with $P \approx \frac{d(d+1)}{2}$.

This step requires computing P solutions to a coarse PDE in order to get the energy $\mathcal{E}(\bar{A}^n, \cdot)$.

We next solve a $P \times P$ eigenvalue problem.

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In practice, we perform a gradient descent together with a line search.

The gradient can be expressed with solutions computed in previous step, hence no additional costs.

Choice of the loadings

We identify P appropriate loadings $(g_i)_{1 \leq i \leq P}$ such that

$$\sup_{g \in L_0^2(\partial\Omega)} |\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}, g)| \approx \sup_{\substack{g \in \text{Span}(g_i) \\ 1 \leq i \leq P}} |\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}, g)|.$$

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Rayleigh quotient: we optimize

$$\sup_{\|g\|_{L^2(\partial\Omega)}=1} |\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}, g)| = \sup_{g \in L_0^2(\partial\Omega)} \left| \frac{\int_{\partial\Omega} g (\mathcal{T}_\varepsilon - \mathcal{T}_{\bar{A}}) g}{\int_{\partial\Omega} g^2} \right|,$$

where

$$\mathcal{T}_\varepsilon : g \in L_0^2(\partial\Omega) \longrightarrow u_\varepsilon(g)|_{\partial\Omega} \quad \text{with } u_\varepsilon(g) \text{ sol. to (1),}$$

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Thus, we seek the eigenmode of $\mathcal{T}_\varepsilon - \mathcal{T}_{\bar{A}}$ with largest eigenvalue in absolute value.

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Case of spheric, periodic coefficients: it holds that

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with $\mathcal{T} : g \in L_0^2(\partial\Omega) \longrightarrow w(g)|_{\partial\Omega}$ where $w(g)$ is solution to

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Practical choice: We select the $P \gtrapprox P_d = \frac{d(d+1)}{2}$ first eigenmodes of \mathcal{T} .

Numerical results (periodic)

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

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

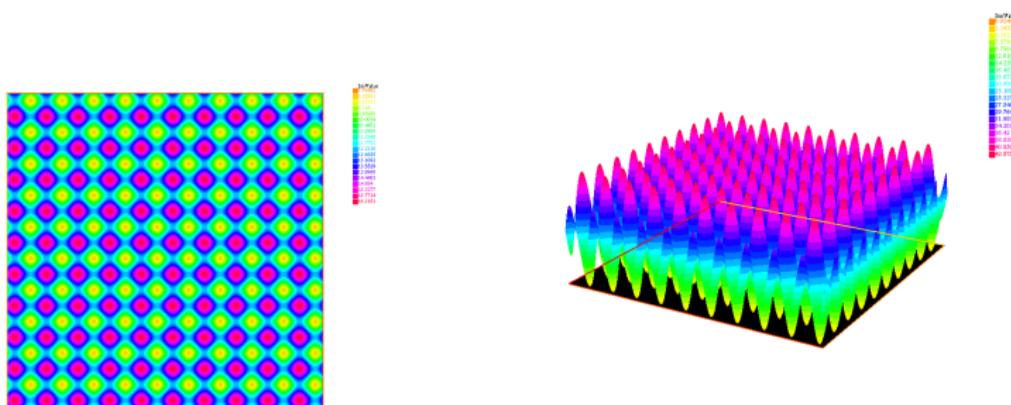


Figure: Components 11 and 22 of coefficient A_ε .

Numerical results (periodic)

$$\frac{|\bar{A} - A_*|_2}{|A_*|_2}$$

$$\text{Err}_{\varepsilon, Q}(\bar{A}) = \sup_{g \in \text{Span}(g_1, \dots, g_Q)} \left(\frac{\|u_\varepsilon(g) - u(\bar{A}, g)\|_{L^2(\Omega)}}{\|u_\varepsilon(g)\|_{L^2(\Omega)}} \right)$$

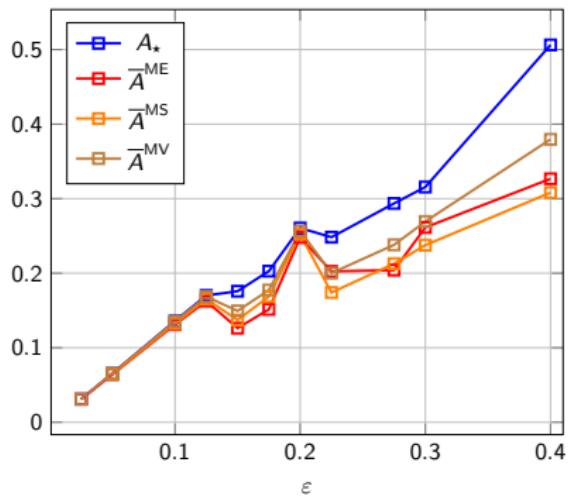
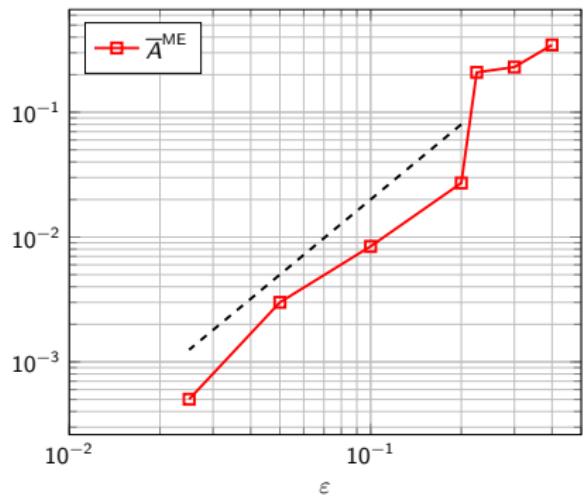


Figure: (left) Error between coefficients A_* and $\bar{A}_{\varepsilon, P}^{\text{ME}}$.

(right) Criterion $\text{Err}_{\varepsilon, Q}(\bar{A})$ for $\bar{A} \in \{A_*, \bar{A}_{\varepsilon, P}^{\text{MV}}, \bar{A}_{\varepsilon, P}^{\text{ME}}, \bar{A}_{\varepsilon, P}^{\text{MS}}\}$ (with $Q = 11$).

Numerical results (stochastic)

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

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

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

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

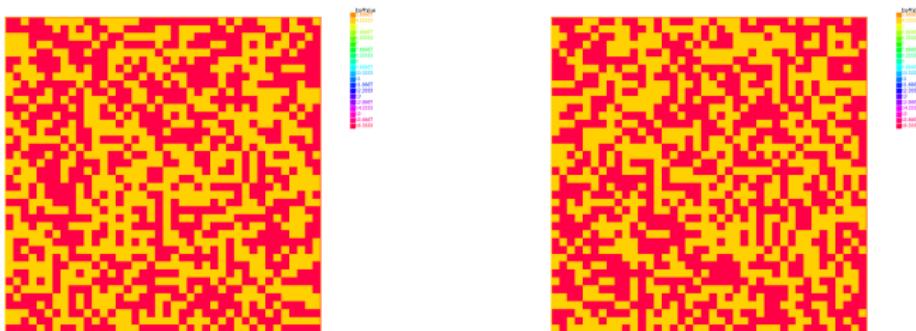
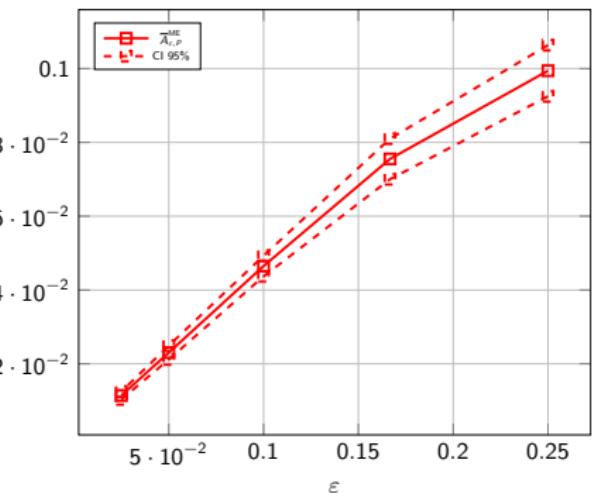


Figure: Two realizations of coefficient A_ε .

Our strategy rewrites $I_\varepsilon = \inf \sup |\mathbb{E}(\mathcal{E}(A_\varepsilon(\cdot, \omega), f)) - \mathcal{E}(\bar{A}, f)|$. Confidence intervals are computed from 40 realizations of the expectation (itself approximated by its empirical mean using 40 realizations of the coefficient a^{sto}).

Numerical results (stochastic)

$$\frac{|\bar{A} - A_\star|_2}{|A_\star|_2}$$



$$\text{Err}_{\varepsilon, Q}^{\mathbb{E}}(\bar{A}) = \sup_{g \in \text{Span}(g_1, \dots, g_Q)} \left(\frac{\|\mathbb{E}(u_\varepsilon(g)) - u(\bar{A}, g)\|_{L^2(\Omega)}}{\|\mathbb{E}(u_\varepsilon(g))\|_{L^2(\Omega)}} \right)$$

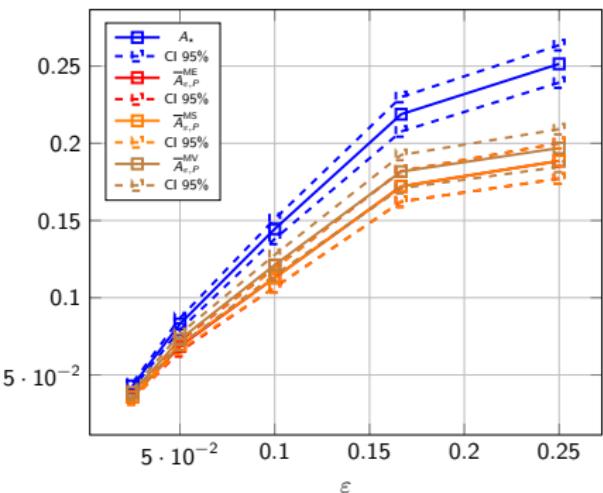


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Noise

Motivation: The value of the energy may not be known exactly.

Formulation: Consider a multiplicative noise in the energy:

$$\mathcal{E}(A_\varepsilon, g; \sigma) = (1 + \sigma \eta) \mathcal{E}(A_\varepsilon, g).$$

where A_ε is a deterministic periodic coefficient, and η follows a Gaussian distribution.

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Results:

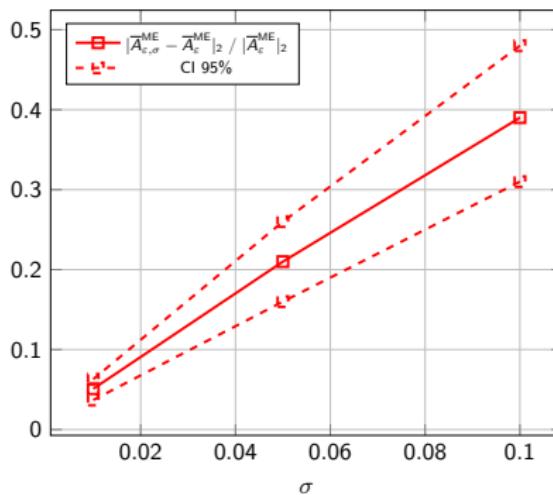


Figure: Error $\frac{|\bar{A}_{\varepsilon,\sigma}^{\text{ME}} - \bar{A}_\varepsilon^{\text{ME}}|_2}{|\bar{A}_\varepsilon^{\text{ME}}|_2}$ as a function of the noise magnitude σ (for $\varepsilon = 0.025$).

Part II

Perturbative reconstruction of effective coefficients

Perturbative reconstruction of effective coefficients

- **Assumption:** The effective coefficient lies in neighboorhood of a known coefficient \bar{A}_0 .

Perturbative reconstruction of effective coefficients

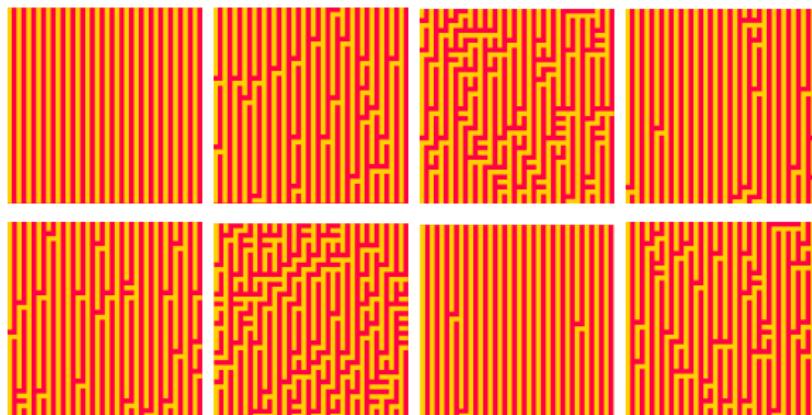
- **Assumption:** The effective coefficient lies in neighbourhood of a known coefficient \bar{A}_0 .
- **Example:** Periodic material with random defect

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

with $C_{\varepsilon}^{\text{per}}$ possibly not negligible, but

$$A_{*, \eta} = \bar{A}_0 + \eta \bar{A}_1 + o(\eta),$$

where \bar{A}_0 is known (e.g. given as an industrial reference).



Perturbative reconstruction of effective coefficients

- **Assumption:** The effective coefficient lies in neighboorhood of a known coefficient \bar{A}_0 .
- **Issue:** Computing the effective coefficient using previous methods for many realizations ω and different defect rates η may lead to **prohibitive computational costs...**

Question

How can we use the a priori knowledge of \bar{A}_0 to guide and speed up the optimization ?

Perturbative development

Consider the problem

$$-\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f \text{ in } \Omega, \quad \text{and} \quad u_\varepsilon = 0 \text{ on } \partial\Omega,$$

and its approximation by

$$-\operatorname{div}(\bar{A} \nabla \bar{u}) = f \text{ in } \Omega, \quad \text{and} \quad \bar{u} = 0 \text{ on } \partial\Omega.$$

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$u(\bar{A}, f)$	$u_0 + \eta v$

where $u_0 = u(\bar{A}_0, f)$ and $v = v(\bar{A}_0, \bar{B}, f)$ is solution to

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Linearity implies that $v = \sum_{ij} \bar{B}_{ij} v_{ij}$ with $v_{ij} = v_{ij}(\bar{A}_0, f)$ solution to

$$\begin{cases} -\operatorname{div}(\bar{A}_0 \nabla v_{ij}) = \operatorname{div}(E_{ij} \nabla u_0) & \text{in } \Omega, \\ v_{ij} = 0 & \text{on } \partial\Omega. \end{cases}$$

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where $\mathcal{E}(\bar{A}_0, f) = -\frac{1}{2} \int_{\Omega} f u_0$ and

$$\begin{aligned} \mathcal{F}_{ij}(\bar{A}_0, f) &= -\frac{1}{2} \int_{\Omega} f v_{ij} \\ &= \frac{1}{2} \int_{\Omega} \partial_i u_0 \partial_j u_0. \end{aligned}$$

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We formulate the optimization problem

$$\inf_{\substack{\bar{B} \in \mathbb{R}_{\text{sym}}^{d \times d}, \\ \|\bar{B}\|_{L^2(\Omega)} = 1.}} \left(\mathcal{E}(A_{\varepsilon, \eta}, f) - \mathcal{E}(\bar{A}_0, f) - \sum_{1 \leq i, j \leq d} [\bar{B}]_{ij} \mathcal{F}_{ij}(\bar{A}_0, f) \right)^2.$$
$$\alpha \leq \bar{A}_0 + \bar{B} \leq \beta$$

- **Offline stage:**

- Compute $u(\bar{A}_0, f)$.
- Compute $\mathcal{E}(\bar{A}_0, f)$ and $\mathcal{F}_{ij}(\bar{A}_0, f)$ for any $1 \leq i \leq j \leq d$.

↳ computing $P \approx \frac{d(d+1)}{2}$ solutions to a coarse PDE and $P(1 + \frac{d(d+1)}{2})$ integrals.

Implementation aspects

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Observe that J_ε^n is quadratic.

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- Define \mathbf{f}^n , the argsup to

$$\sup_{f \text{ s.t. } \|f\|_{L^2(\Omega)} = 1} \left(\mathcal{E}(A_\varepsilon, f) - \mathcal{E}(\bar{A}_0, f) - \sum_{ij} [\bar{B}^n]_{ij} \mathcal{F}_{ij}(\bar{A}_0, f) \right)^2.$$

In practice, $\sup_{f \in L^2(\Omega)} \rightarrow \sup_{f \in V_P}$ on $V_P = \text{Span}\{P \text{ loadings}\}$, with $P \approx \frac{d(d+1)}{2}$.
This step amounts to solving a $P \times P$ eigenvalue problem.

- Define

$$\bar{B}^{n+1} = \bar{B}^n - \mu \nabla_{\bar{B}} J_\varepsilon^n(\bar{B}^n)$$

with

$$J_\varepsilon^n(\bar{B}) = \left(\mathcal{E}(A_\varepsilon, \mathbf{f}^n) - \mathcal{E}(\bar{A}_0, \mathbf{f}^n) - \sum_{ij} [\bar{B}]_{ij} \mathcal{F}_{ij}(\bar{A}_0, \mathbf{f}^n) \right)^2.$$

Observe that J_ε^n is quadratic.

↳ **no additional computations of coarse PDE !**

Numerical results

- Preserve the quality of the approximation.
- Reduction of computational costs (by a factor of ≈ 80 to 400).

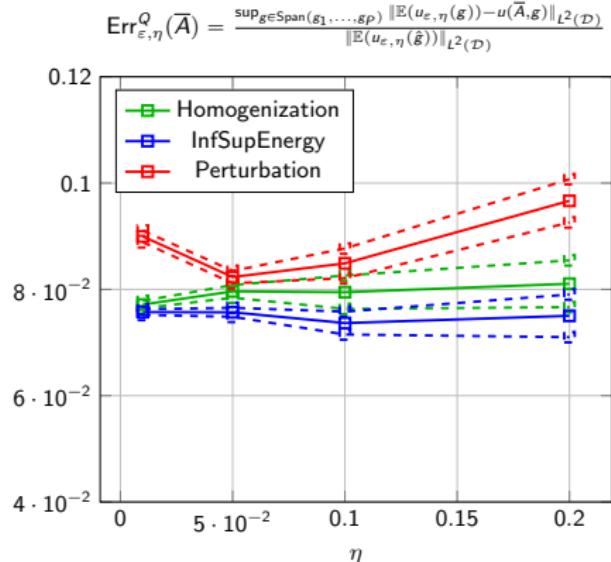
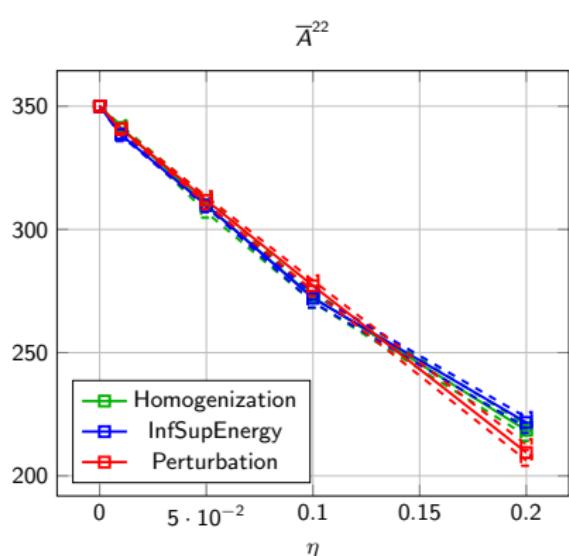


Figure: (left) Component 22 for various approximations of the effective coefficient.
(right) Criterion $\text{Err}_{\varepsilon, Q}^{\mathbb{E}}(\bar{A})$ for different constant coefficients (with $Q = 9$ and $\varepsilon = 0.025$).

Part III

Efficient selection of effective coefficients

- **Setting:** we are given

- a list of candidate coefficients $\mathcal{A} = \{\bar{A}_1, \dots, \bar{A}_N\}$.
- a list of admissible loadings $\mathcal{F} = \{f_1, \dots, f_P\}$.
- a measurement operator $\mathcal{O} : \mathcal{A} \times \mathcal{F} \rightarrow \mathbb{R}$ or $L^2(\Omega)$ (e.g. $\mathcal{O}(A_\varepsilon, f) = u_\varepsilon(f)$ or $\mathcal{E}(A_\varepsilon, f)$).

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- **Challenge:**

- Expensive measurement costs \implies budget of $Q \ll P$ measurements.
- (Unknown) decomposition of \mathcal{F} into $\mathcal{F}_{\text{disc}}$ and $\mathcal{F}_{\text{non-disc}}$ such that

$$\text{card}(\mathcal{F}_{\text{disc}}) \ll \text{card}(\mathcal{F}),$$

and for any $f \in \mathcal{F}_{\text{non-disc}}$ and any $\bar{A}, \bar{B} \in \mathcal{A}^2$,

$$\|\mathcal{O}(A_\varepsilon, f) - \mathcal{O}(\bar{A}, f)\|_{\mathcal{O}} \approx \|\mathcal{O}(A_\varepsilon, f) - \mathcal{O}(\bar{B}, f)\|_{\mathcal{O}}.$$

Framework

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Objective

Select the coefficient in \mathcal{A} that provides the best effective approximation of the underlying system while simultaneously minimizing the number of measurement operations $\mathcal{O}(A_\varepsilon, f)$ with $f \in \mathcal{F}$.

Work inspired by discussions with H. Ammari (ETH Zürich).

Selection algorithm

Iterative algorithm: each step k selects a loading f^k in \mathcal{F} and update the choice of the best coefficient \bar{A}^k in \mathcal{A} .

Selection algorithm

Iterate k :

① Compute discrimination rate $\Delta^k(f)$ for any f in $\mathcal{F}^k = \mathcal{F} \setminus \{f^p\}_{p=1,\dots,k-1}$.

② Select

$$f^k \in \arg \max_{f \in \mathcal{F}^k} \Delta^k(f).$$

③ Measure $\mathcal{O}(A_\varepsilon, f^k)$.

④ Define the effective coefficient

$$\bar{A}^k \in \arg \min_{\bar{A} \in \mathcal{A}} \gamma^k(\bar{A}).$$

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Iterate k :

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$$f^k \in \arg \max_{f \in \mathcal{F}^k} \Delta^k(f).$$

③ *Measure $\mathcal{O}(A_\varepsilon, f^k)$.*

④ *Define the effective coefficient*

$$\bar{A}^k \in \arg \min_{\bar{A} \in \mathcal{A}} \gamma^k(\bar{A}).$$

Core components:

- **Discrimination rate:** Δ^k estimates how a loadings is discriminative w.r.t \mathcal{O} and \mathcal{A} .
- **Effectiveness score :** γ^k assesses the quality of a coefficient as an effective coefficient for the system.

Conclusion and perspectives

Our strategies

- aim at **determining effective approximations** for multiscale PDEs through effective coefficients,
- are designed for context where only **limited information** is available,
- are **inspired by homogenization theory** and **consistent with it** (numerically and theoretically),
- can be **extended outside the regime of separated scale**.

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Perspectives

- Application to real **experimental data**.
- Extension to **non-constant** effective coefficients.
- **Convergence analysis** of \bar{A} to A_* .
- **Convergence analysis** of selection algorithm.

Conclusion and perspectives

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- **Convergence analysis** of \bar{A} to A_* .
- **Convergence analysis** of selection algorithm.

Thank you !

A different perspective on noise

Motivation: anticipate on reproducibility errors during model deployment.

Idea: treat \bar{A} as a random field and optimize upon its mean.

Formulation: consider the problem

$$\inf_{\bar{A} \in \mathcal{S}_{\alpha, \beta}} \sup_{\|g\|_{L^2(\partial\Omega)} = 1} \left| \mathcal{E}(A_\varepsilon, g) - \mathbb{E}(\mathcal{E}(\bar{A} + \sigma\eta, g)) \right|^2,$$

where η is a Gaussian variable.

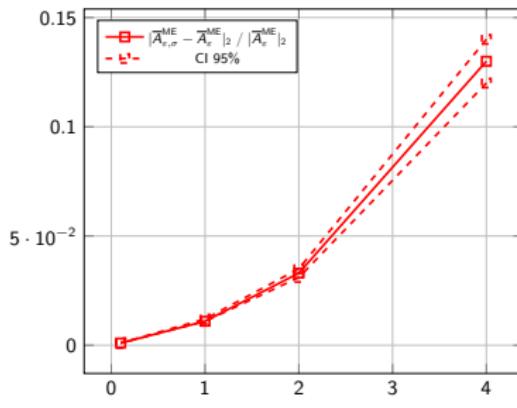


Figure: Error between $\bar{A}_{\varepsilon, \sigma}^{ME}$ and $\bar{A}_{\varepsilon}^{ME}$ as a function of the noise magnitude σ (for $\varepsilon = 0.05$).

Convergence analysis

We consider the slightly modified

$$\inf_{\overline{A} \in \mathbb{R}_{\text{sym}}^{d \times d}, \text{ blue } 1 \leq i \leq j \leq d} |\mathcal{E}(A_\varepsilon, \mathbf{g}_{i,j}) - \mathcal{E}(\overline{A}, \mathbf{g}_{i,j})|,$$
$$\alpha \leq \overline{A} \leq \beta$$

where $(g_{i,j})_{1 \leq i \leq j \leq d}$ are preselected loadings.

For an appropriate choice of loadings $(g_{i,j})_{1 \leq i \leq j \leq d}$, it holds that

$$|\overline{A}_\varepsilon^{\text{opt}} - A_\star| \leq C\delta(\varepsilon),$$

where $\delta(\varepsilon)$ is any function such that

$$|\mathcal{E}(A_\varepsilon) - \mathcal{E}(A_\star)| \leq C\delta(\varepsilon).$$

Loading selection

We define

$$g_{i,j} = \left(\frac{\mathbf{e}_i + \mathbf{e}_j}{2} \right) \cdot \mathbf{n},$$

where $(\mathbf{e}_i)_{1 \leq i \leq d}$ is the canonical basis of \mathbb{R}^d .

For any $\bar{\mathbf{A}} \in \mathbb{R}_{\text{sym}}^{d \times d}$, the solution to

$$-\operatorname{div}(\bar{\mathbf{A}} \nabla \bar{u}) = 0 \text{ in } \Omega, \quad (\bar{\mathbf{A}} \nabla \bar{u}) \cdot \mathbf{n} = g_{i,j} \text{ on } \partial\Omega.$$

writes

$$\bar{u}_{i,j} = (\bar{\mathbf{A}}^{-1} \mathbf{e}_{i,j}) \cdot \mathbf{x}.$$

Thus the energy writes:

$$\mathcal{E}(\bar{\mathbf{A}}, g_{i,j}) = \int_{\Omega} \underbrace{(\bar{\mathbf{A}}^{-1} \mathbf{e}_{i,j})^T}_{(\nabla u_{i,j})^T} \bar{\mathbf{A}} \underbrace{(\bar{\mathbf{A}}^{-1} \mathbf{e}_{i,j})}_{\nabla u_{i,j}} = |\Omega| \mathbf{e}_{i,j}^T \bar{\mathbf{A}}^{-1} \mathbf{e}_{i,j}$$

Then, we get

$$\begin{aligned} \|\bar{\mathbf{A}} - \mathbf{A}_\star\| &\leq C \|\bar{\mathbf{A}}^{-1} - \mathbf{A}_\star^{-1}\| \\ &\leq C \sum_{1 \leq i \leq j \leq d} |\mathbf{e}_{ij}^T (\bar{\mathbf{A}}^{-1} - \mathbf{A}_\star^{-1}) \mathbf{e}_{ij}| \\ &\leq \dots \\ &\leq C \delta(\varepsilon). \end{aligned}$$

Efficient selection of effective coefficients

Framework

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Select the coefficient in \mathcal{A} that provides the best effective approximation of the underlying system while simultaneously minimizing the number of measurement operations $\mathcal{O}(A_\varepsilon, f)$ with $f \in \mathcal{F}$.

Iterative algorithm: each step k selects a loading f^k in \mathcal{F} and update the choice of the best coefficient \bar{A}^k in \mathcal{A} .

Core components:

- **Discrimination rate:** it estimates how a loadings is discriminative w.r.t observable \mathcal{O} .
- **Effectiveness score:** it assesses the quality of a coefficient as an effective coefficient for the system.

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$\Delta_1(f)$	$\max_{(\bar{A}, \bar{B}) \in \mathcal{A}^2} \text{Err}(\bar{A}, \bar{B}, f)$	$\text{Err}(\bar{A}, \bar{B}, f) = \frac{\ \mathcal{O}(\bar{A}, f) - \mathcal{O}(\bar{B}, f)\ _{\mathcal{O}}}{\ \mathcal{O}(\bar{A}, f)\ _{\mathcal{O}}}$
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$\Delta_3(f)$	$\max_{(\bar{A}, \bar{B}) \in \mathcal{A}^2} \text{Err}_\varepsilon(\bar{A}, f) - \text{Err}_\varepsilon(\bar{B}, f) $	$\text{Err}_\varepsilon(\bar{A}, f) = \frac{\ \mathcal{O}(A_\varepsilon, f) - \mathcal{O}(\bar{A}, f)\ _{\mathcal{O}}}{\ \mathcal{O}(A_\varepsilon, f)\ _{\mathcal{O}}}$

- **Effectiveness score:** it assesses the quality of a coefficient as an effective coefficient for the system.

↳ e.g.

$$\gamma^k(\bar{A}) = \max_{f \in \{f_1, \dots, f_k\}} \text{Err}_\varepsilon(\bar{A}, f).$$

Strategy

Selection algorithm

Initialization:

Select $f^1 \in \mathcal{F}$ by solving

$$f^1 = \arg \max_{f \in \mathcal{F}} \max_{(\bar{A}, \bar{B}) \in \mathcal{A}^2} \frac{\|\mathcal{O}(\bar{A}, f) - \mathcal{O}(\bar{B}, f)\|_{\mathcal{O}}}{\|\mathcal{O}(\bar{A}, f)\|_{\mathcal{O}}}.$$

Iterate k :

- ① Compute discrimination rate $\Delta^k(f)$ for any f in $\mathcal{F}^k = \mathcal{F} \setminus \{f^p\}_{p=1, \dots, k-1}$.
- ② Select $f^k \in \arg \max_{f \in \mathcal{F}^k} \Delta^k(f).$
- ③ Measure $\mathcal{O}(A_\varepsilon, f^k).$
- ④ Define the effective coefficient

$$\bar{A}^k \in \arg \min_{\bar{A} \in \mathcal{A}} \gamma^k(\bar{A}).$$

Numerical results

- **Microstructure.** Consider

$$A_\varepsilon(x) = \begin{cases} \gamma_1 + \gamma_2 \sin\left(\frac{2\pi x}{\varepsilon}\right) & \text{if } x \in D_1, \\ \gamma_3 & \text{if } x \in D_2. \end{cases}$$

with

$$\gamma_3 = a_\star$$

the limit in the sense of homogenization of
 $x \mapsto \gamma_1 + \gamma_2 \sin\left(\frac{2\pi x}{\varepsilon}\right)$.

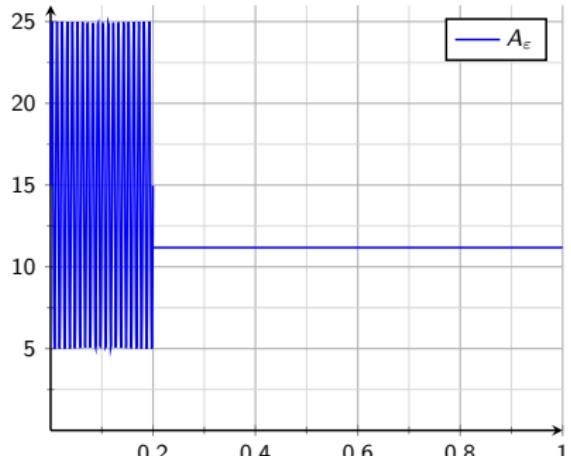


Figure: Coefficient A_ε with $\varepsilon = 0.01$.

Numerical results

- Microstructure.
- Set \mathcal{F} . Consider

$$f_n = \mathbb{1}_{\left(\frac{n-1}{N}, \frac{n}{N}\right)}$$

and

$$\mathcal{F} = \underbrace{\{f_n \text{ s.t. } \text{Supp}(f_n) \subset D_1\}}_{\mathcal{F}_{\text{disc}}} \cup \underbrace{\{f_n \text{ s.t. } \text{Supp}(f_n) \subset D_2\}}_{\mathcal{F}_{\text{non-disc}}}.$$

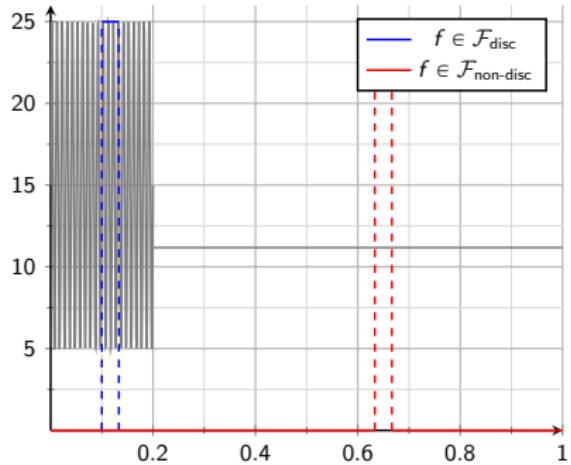


Figure: Admissible loadings.

Numerical results

Microstructure.

Set \mathcal{F} .

Set \mathcal{A} . Consider

$$\bar{A}(x) = \begin{cases} \bar{A}^1 & \text{if } x < 0.2, \\ \bar{A}^2 & \text{if } x > 0.2. \end{cases}$$

with \bar{A}^1 and \bar{A}^2 are constants.

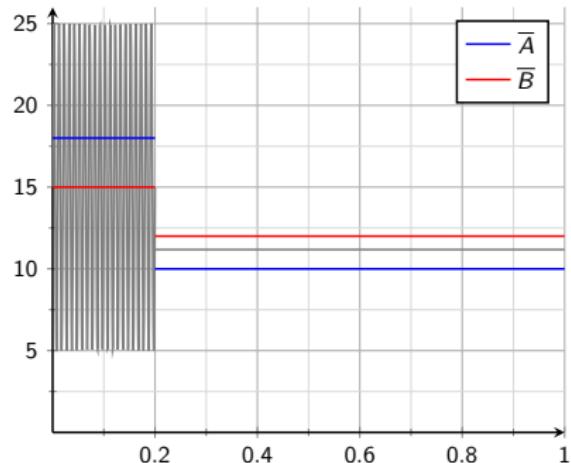
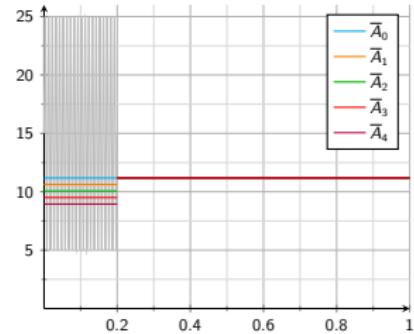


Figure: Effective coefficients.

Numerical results: case 1

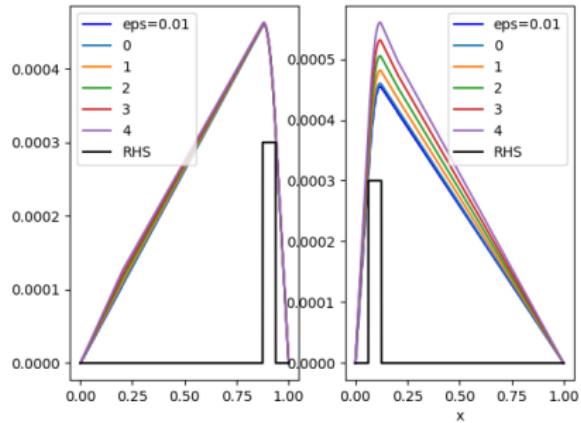
Setting:

$$\begin{aligned}\mathcal{A}_1 = \{ \bar{A}_0 &= (a_*, a_*), \\ \bar{A}_1 &= (0.95a_*, a_*), \\ \bar{A}_2 &= (0.9a_*, a_*), \\ \bar{A}_3 &= (0.85a_*, a_*), \\ \bar{A}_4 &= (0.8a_*, a_*) \},\end{aligned}$$



and

$$\frac{\text{card}(\mathcal{F}_{\text{disc}})}{\text{card}(\mathcal{F})} \approx 0.2.$$



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and

$$\frac{\text{card}(\mathcal{F}_{\text{disc}})}{\text{card}(\mathcal{F})} \approx 0.2.$$

Conclusions:

- Δ_1 , Δ_2 and Δ_ε perform the same selection.
- Loadings in $\mathcal{F}_{\text{disc}}$ are first identified.
- $\bar{A}_0 = (a_*, a_*)$ is the best coefficient at each step.

Step	Loadings	Best Coefficient
1	$f_1 \in \mathcal{F}_{\text{disc}}$	\bar{A}_0
2	$f_2 \in \mathcal{F}_{\text{disc}}$	\bar{A}_0
3	$f_3 \in \mathcal{F}_{\text{disc}}$	\bar{A}_0
4	$f_4 \in \mathcal{F}_{\text{disc}}$	\bar{A}_0
5	$f_{12} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
6	$f_{13} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
7	$f_{14} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
8	$f_{15} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
9	$f_{16} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
10	$f_{17} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
11	$f_{18} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
12	$f_{19} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
13	$f_{20} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
14	$f_{21} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0
15	$f_{22} \in \mathcal{F}_{\text{non-disc}}$	\bar{A}_0

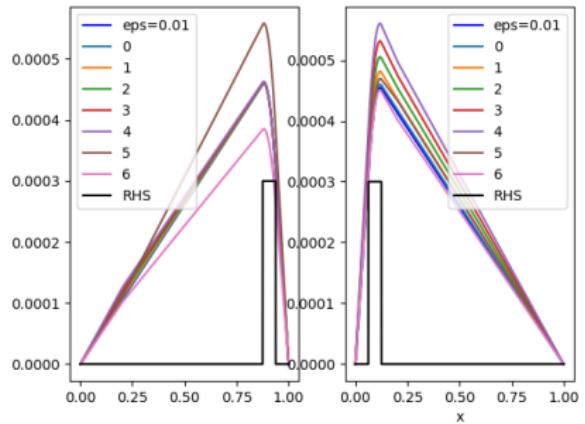
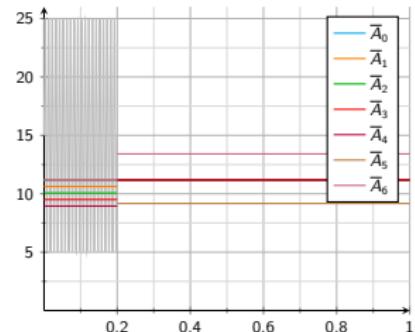
Numerical results: case 2

Setting:

$$\mathcal{A}_2 = \mathcal{A}_1 \cup \{\bar{A}_5 = (a_*, 0.82a_*), \bar{A}_6 = (a_*, 1.2a_*)\},$$

and

$$\frac{\text{card}(\mathcal{F}_{\text{disc}})}{\text{card}(\mathcal{F})} \approx 0.2.$$



Numerical results: case 2

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and

$$\frac{\text{card}(\mathcal{F}_{\text{disc}})}{\text{card}(\mathcal{F})} \approx 0.2.$$

Conclusions:

- Δ_2 better replicates Δ_ε than Δ_1 .
- $\bar{A}_0 = (a_*, a_*)$ is the best coefficient at each step.
- Δ_1 selects loadings that do not precisely discriminate \bar{A}_0 from other coefficients in \mathcal{A}_1 .

Step	Δ_ε	Δ_2
1	$f_1 \in \mathcal{F}_{\text{disc}}$	$f_{29} \in \mathcal{F}_{\text{non-disc}}$
2	$f_2 \in \mathcal{F}_{\text{disc}}$	$f_1 \in \mathcal{F}_{\text{disc}}$
3	$f_3 \in \mathcal{F}_{\text{disc}}$	$f_2 \in \mathcal{F}_{\text{disc}}$
4	$f_4 \in \mathcal{F}_{\text{disc}}$	$f_3 \in \mathcal{F}_{\text{disc}}$
5	$f_{29} \in \mathcal{F}_{\text{non-disc}}$	$f_{28} \in \mathcal{F}_{\text{non-disc}}$
6	$f_{28} \in \mathcal{F}_{\text{non-disc}}$	$f_4 \in \mathcal{F}_{\text{disc}}$
7	$f_{12} \in \mathcal{F}_{\text{non-disc}}$	$f_{27} \in \mathcal{F}_{\text{non-disc}}$
8	$f_{27} \in \mathcal{F}_{\text{non-disc}}$	$f_{12} \in \mathcal{F}_{\text{non-disc}}$
9	$f_{26} \in \mathcal{F}_{\text{non-disc}}$	-
10	$f_{25} \in \mathcal{F}_{\text{non-disc}}$	-
11	$f_{24} \in \mathcal{F}_{\text{non-disc}}$	-
12	$f_{23} \in \mathcal{F}_{\text{non-disc}}$	-
13	$f_{22} \in \mathcal{F}_{\text{non-disc}}$	-
14	$f_{21} \in \mathcal{F}_{\text{non-disc}}$	-
15	$f_{20} \in \mathcal{F}_{\text{non-disc}}$	-
16	$f_{19} \in \mathcal{F}_{\text{non-disc}}$	-
17	$f_{18} \in \mathcal{F}_{\text{non-disc}}$	-
17	$f_{17} \in \mathcal{F}_{\text{non-disc}}$	-

Numerical results: case 2

Setting:

$$\mathcal{A}_2 = \mathcal{A}_1 \cup \{\bar{A}_5 = (a_*, 0.82a_*), \\ \bar{A}_6 = (a_*, 1.2a_*)\},$$

and

$$\frac{\text{card}(\mathcal{F}_{\text{disc}})}{\text{card}(\mathcal{F})} \approx 0.2.$$

Conclusions:

- Δ_2 better replicates Δ_ε than Δ_1 .
- $\bar{A}_0 = (a_*, a_*)$ is the best coefficient at each step.
- Δ_1 selects loadings that do not precisely discriminate \bar{A}_0 from other coefficients in \mathcal{A}_1 .

Step	Δ_ε	Δ_1
1	$f_1 \in \mathcal{F}_{\text{disc}}$	$f_{29} \in \mathcal{F}_{\text{non-disc}}$
2	$f_2 \in \mathcal{F}_{\text{disc}}$	$f_{28} \in \mathcal{F}_{\text{non-disc}}$
3	$f_3 \in \mathcal{F}_{\text{disc}}$	$f_{27} \in \mathcal{F}_{\text{non-disc}}$
4	$f_4 \in \mathcal{F}_{\text{disc}}$	$f_{26} \in \mathcal{F}_{\text{non-disc}}$
5	$f_{29} \in \mathcal{F}_{\text{non-disc}}$	$f_{25} \in \mathcal{F}_{\text{non-disc}}$
6	$f_{28} \in \mathcal{F}_{\text{non-disc}}$	$f_{24} \in \mathcal{F}_{\text{non-disc}}$
7	$f_{12} \in \mathcal{F}_{\text{non-disc}}$	$f_{23} \in \mathcal{F}_{\text{non-disc}}$
8	$f_{27} \in \mathcal{F}_{\text{non-disc}}$	$f_{22} \in \mathcal{F}_{\text{non-disc}}$
9	$f_{26} \in \mathcal{F}_{\text{non-disc}}$	$f_{21} \in \mathcal{F}_{\text{non-disc}}$
10	$f_{25} \in \mathcal{F}_{\text{non-disc}}$	$f_{20} \in \mathcal{F}_{\text{non-disc}}$
11	$f_{24} \in \mathcal{F}_{\text{non-disc}}$	$f_{19} \in \mathcal{F}_{\text{non-disc}}$
12	$f_{23} \in \mathcal{F}_{\text{non-disc}}$	$f_{18} \in \mathcal{F}_{\text{non-disc}}$
13	$f_{22} \in \mathcal{F}_{\text{non-disc}}$	$f_{17} \in \mathcal{F}_{\text{non-disc}}$
14	$f_{21} \in \mathcal{F}_{\text{non-disc}}$	$f_{16} \in \mathcal{F}_{\text{non-disc}}$
15	$f_{20} \in \mathcal{F}_{\text{non-disc}}$	$f_{15} \in \mathcal{F}_{\text{non-disc}}$
16	$f_{19} \in \mathcal{F}_{\text{non-disc}}$	$f_{14} \in \mathcal{F}_{\text{non-disc}}$
17	$f_{18} \in \mathcal{F}_{\text{non-disc}}$	$f_{13} \in \mathcal{F}_{\text{non-disc}}$
17	$f_{17} \in \mathcal{F}_{\text{non-disc}}$	$f_1 \in \mathcal{F}_{\text{non-disc}}$

Schrödinger equation

Schrödinger equation

Homogenization. Consider the Schrödinger equation

$$-\Delta u_\varepsilon + V_\varepsilon u_\varepsilon = f \text{ in } \Omega, \quad u_\varepsilon = 0 \text{ on } \partial\Omega.$$

In the periodic case (i.e. $V_\varepsilon(x) = \frac{1}{\varepsilon} V_{\text{per}}\left(\frac{x}{\varepsilon}\right)$), we define

$$-\Delta u_* + V_* u_* = f \text{ in } \Omega, \quad u_* = 0 \text{ on } \partial\Omega,$$

with $V_* \in \mathbb{R}$ defined through a corrector w , periodic solution to

$$-\Delta w = V_{\text{per}} \text{ in } \mathbb{R}^d.$$

Homogenization assesses that

$$\begin{aligned} u_\varepsilon - u_* &\rightarrow 0 \text{ in } L^2(\Omega), \\ u_\varepsilon - \underbrace{\left(1 + \varepsilon w\left(\frac{x}{\varepsilon}\right)\right) u_*}_{u_{\varepsilon,1}} &\rightarrow 0 \text{ in } H^1(\Omega). \end{aligned}$$

Effective approximation in $H^1(\Omega)$. Based on measurements of solutions $(u_\varepsilon(f_p))_{1 \leq p \leq P}$ and their gradients, we proceed in two steps:

1. a *best* potential \bar{V} is defined through an optimization problem.
2. a *corrector term* is built using measurements of solution $(u_\varepsilon(f_p))_{1 \leq p \leq P}$.

Defining a best potential \bar{V}

We consider the optimization problem

$$\inf_{\bar{V} \in \mathbb{R}} \sup_{f \in L^2(\Omega)} \left\| (-\Delta)^{-1} (-\Delta + \bar{V}) (u_\varepsilon(f) - u(\bar{V}, f)) \right\|_{L^2(\Omega)}^2,$$

with $\bar{u} = u(\bar{V}, f)$ solution to

$$-\Delta \bar{u} + \bar{V} \bar{u} = f \text{ in } \Omega, \quad \bar{u} = 0 \text{ on } \partial\Omega.$$

It holds that

Proposition (Existence and uniqueness)

In the periodic setting, there exists a unique minimizer $\bar{V}_\varepsilon^{\text{opt}}$ for sufficiently small ε .

Proposition (Asymptotic consistency)

In the periodic setting, the following convergence holds:

$$\lim_{\varepsilon \rightarrow 0} \bar{V}_\varepsilon^{\text{opt}} = V_*$$

Defining a corrector term

By homogenization, we know that

$$\nabla u_\varepsilon \approx \nabla u_\star + u_\star (\nabla w) \left(\frac{x}{\varepsilon} \right) \text{ in } L^2(\Omega).$$

We define a corrector

$$\inf_{\bar{C} \in (L^2(\Omega))^d \times d} \sup_{f \in L^2(\Omega)} \|\nabla u_\varepsilon(f) - \nabla \bar{u}(f) - \bar{C} \bar{u}(f)\|_{L^2(\Omega)}^2,$$

where $\bar{u}(f) = u(\bar{V}_\varepsilon^{\text{opt}}, f)$.

$$\text{Err}_{\varepsilon, Q}(\bar{V}) = \sup_{f \in V_n^Q(\Omega)} \|u_\varepsilon(f) - u(\bar{V}, f)\|_{L^2(\Omega)} / \|u_\varepsilon(\hat{f})\|_{L^2(\Omega)} \quad \text{Err}_{\varepsilon, Q}^{\text{corr}}(\bar{V}, \bar{C}) = \sup_{f \in V_n^Q(\Omega)} \|\nabla u_\varepsilon(f) - \nabla u(\bar{V}, f) - \bar{C} u(\bar{V}, f)\|_{L^2(\Omega)} / \|\nabla u_\varepsilon(\hat{f})\|_{L^2(\Omega)}$$

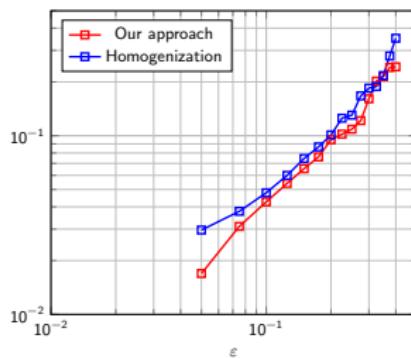
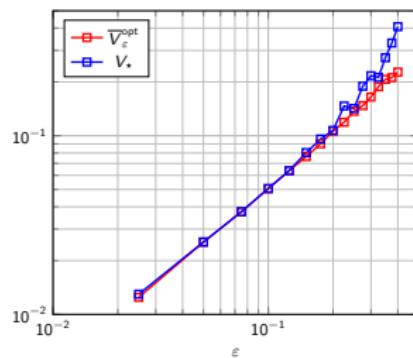


Figure: Comparison of our approach and homogenization in L^2 -norm (left) and H^1 -norm (right).