

Effective approximations of multiscale PDE based on limited information

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Supervisors: Claude Le Bris, Frédéric Legoll

PhD Defense

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General introduction

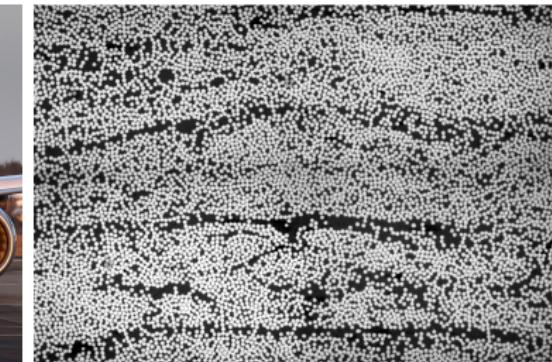
Multiscale systems

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 $\approx 10\text{m}$



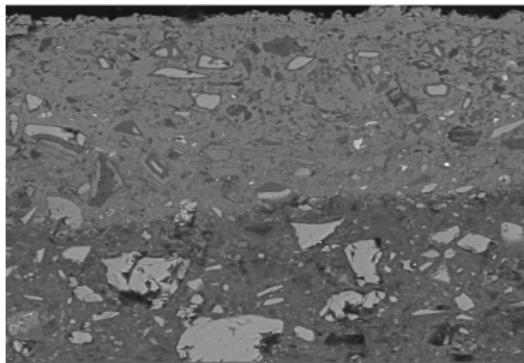
v.s. carbon fibers $\approx 10^{-6}\text{m}$

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

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

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

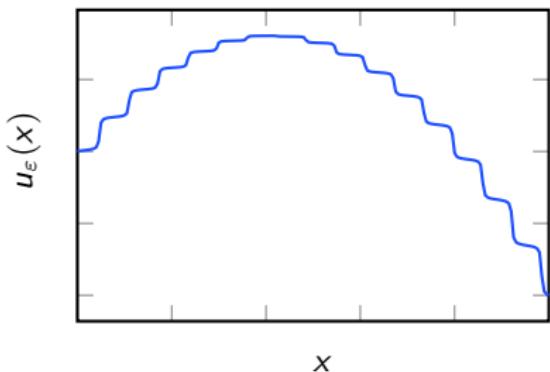
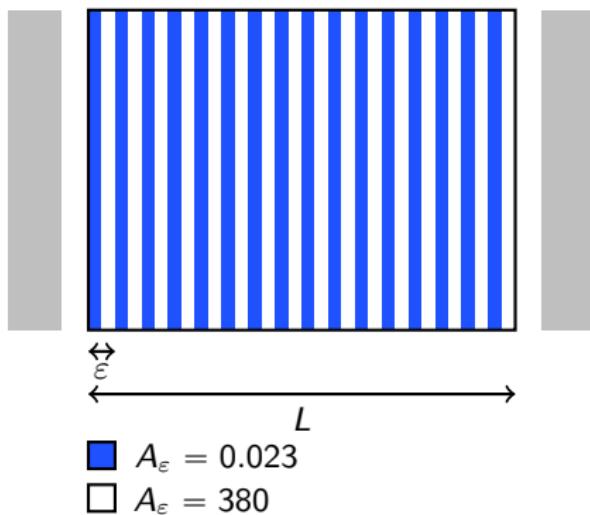
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- Applications: heat transfer in thermal engineering, (simplification of) elastic problem in mechanics, ...



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

$$\mathcal{L}_\varepsilon : f \rightarrow u_\varepsilon(f).$$

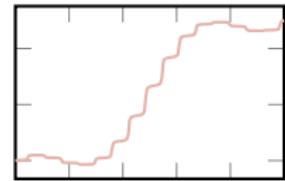
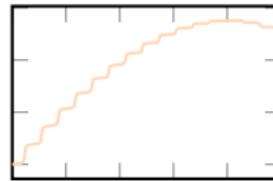
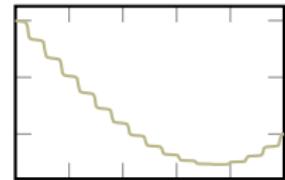
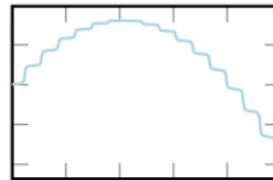
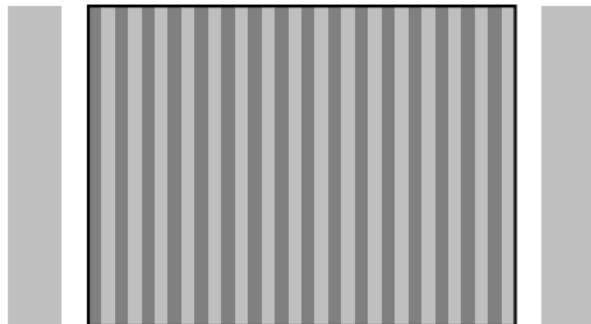
Limited information

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, ...).
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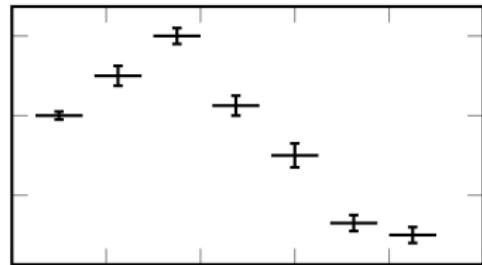
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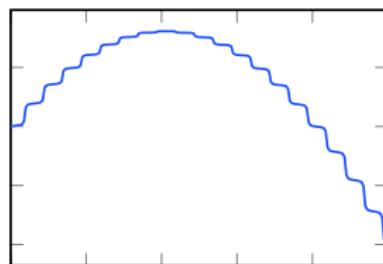
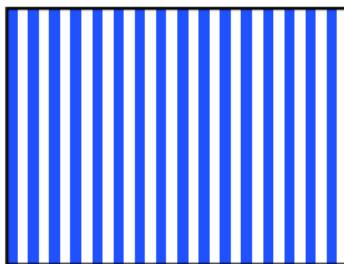
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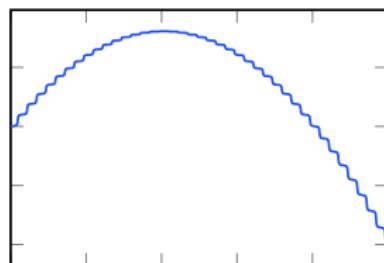
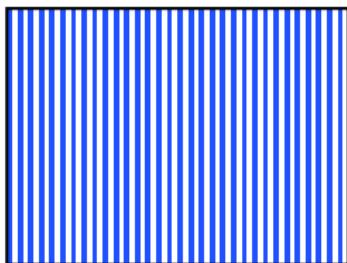
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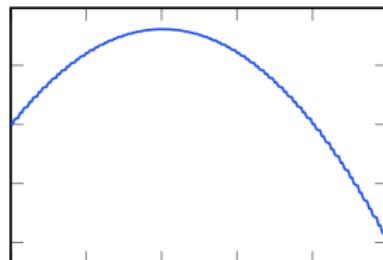
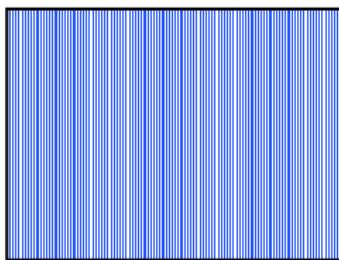
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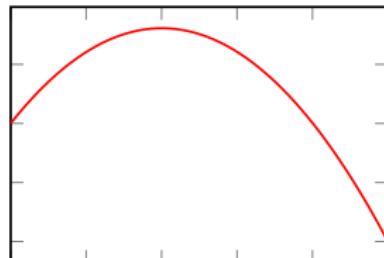


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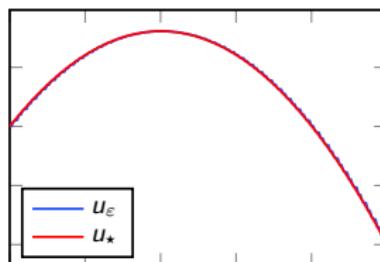
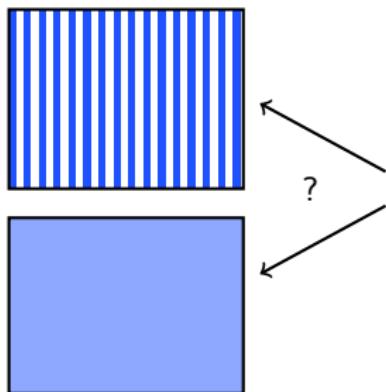
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Oscillating System

$$\xrightarrow[\varepsilon \rightarrow 0]{} \begin{cases} -\operatorname{div}(\mathbf{A}_\star \nabla u_\star) = f & \text{in } \Omega, \\ u_\star = 0 & \text{on } \partial\Omega. \end{cases}$$

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Different approaches

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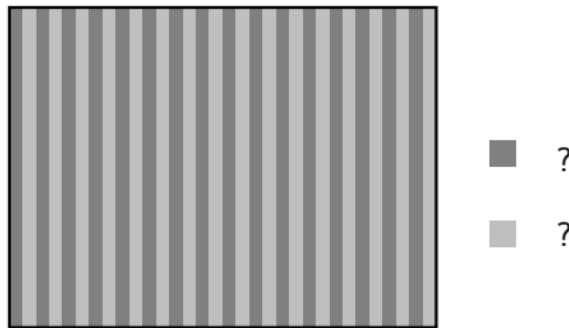
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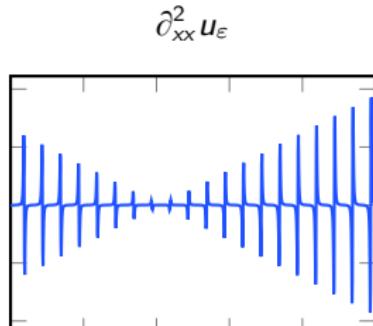
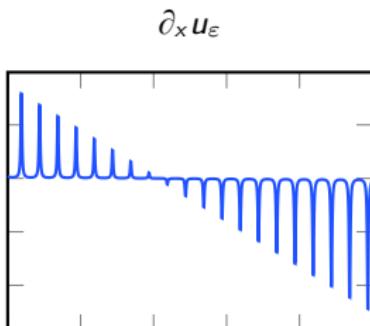
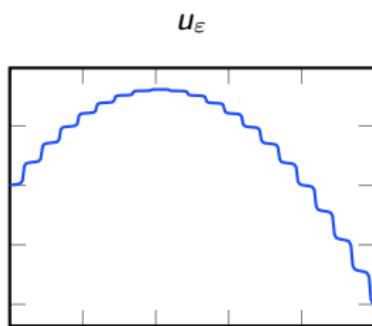
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Issue: how to proceed in contexts of limited information?

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

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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**:

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

where $\mathcal{E}(A_*, g) = \frac{1}{2} \int_{\Omega} A_* \nabla u_* \cdot \nabla u_* - \int_{\partial\Omega} g u_*$ and where u_* 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

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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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- **Homogenization** $\implies \mathcal{E}_\varepsilon(g) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{E}_\#(g) \implies I_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} 0 \implies \mathcal{E}_\varepsilon(g) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{E}_\#(g).$

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

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

Thus,

$$u(A_\star, g) = u(\bar{A}_\#, g) \text{ in } L^2(\partial\Omega). \quad (5)$$

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Thus,

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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

$$\sup_{\begin{array}{c} g \text{ s.t. } \|g\|_{L^2(\partial\Omega)} = 1 \end{array}} \left(\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\bar{A}^n, g) \right)^2.$$

- ② Define \bar{A}^{n+1} , the optimizer to

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

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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.

- ② Define \bar{A}^{n+1} , the optimizer to

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

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

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

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

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

$$\mathcal{T}_\varepsilon - \mathcal{T}_{\bar{A}} \xrightarrow[\varepsilon \rightarrow 0]{} (A_\star - \bar{A}) \mathcal{T}$$

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

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

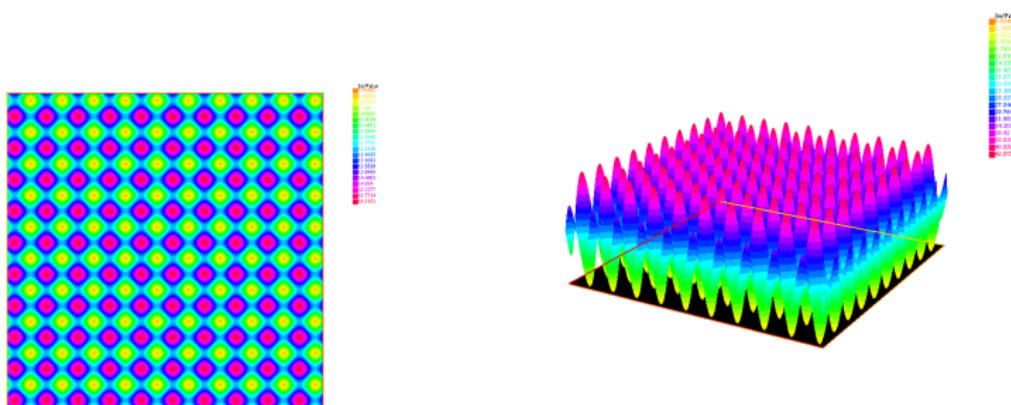


Figure: Components 11 and 22 of coefficient A_ε .

Numerical results (periodic)

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

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

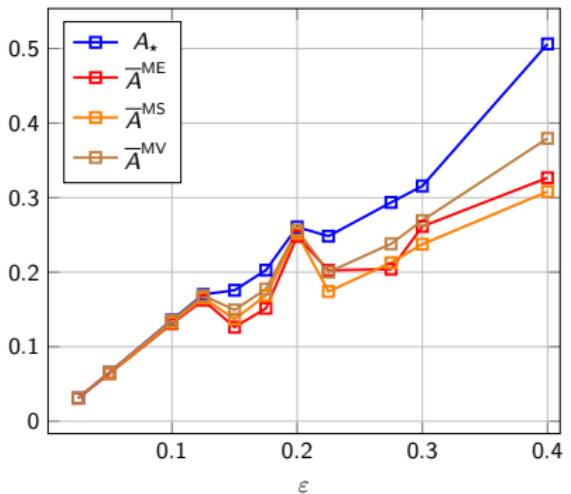
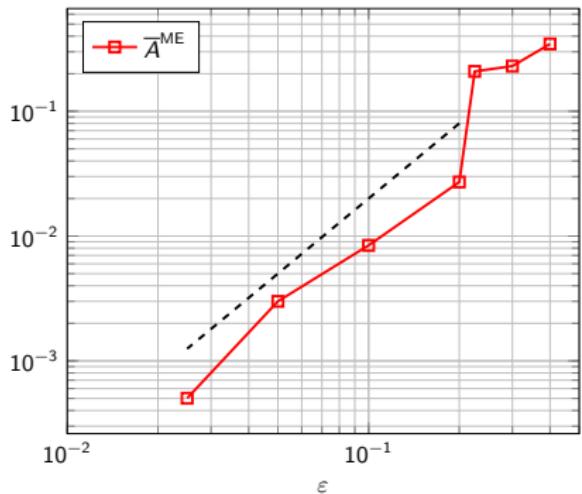


Figure: (left) Error between coefficients A_* and $\bar{A}_{\varepsilon, P}^{\text{ME}}$.

(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

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

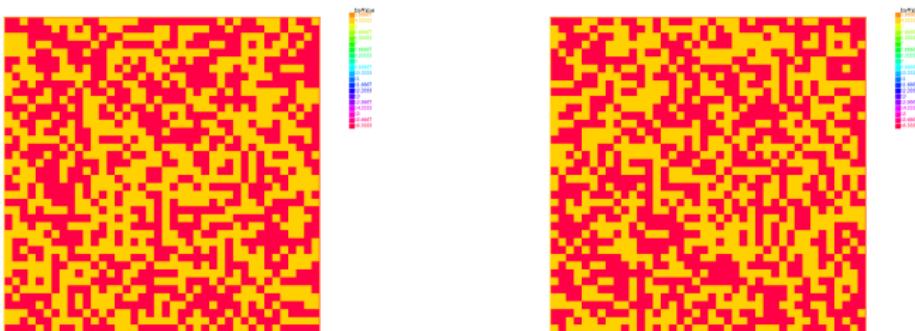
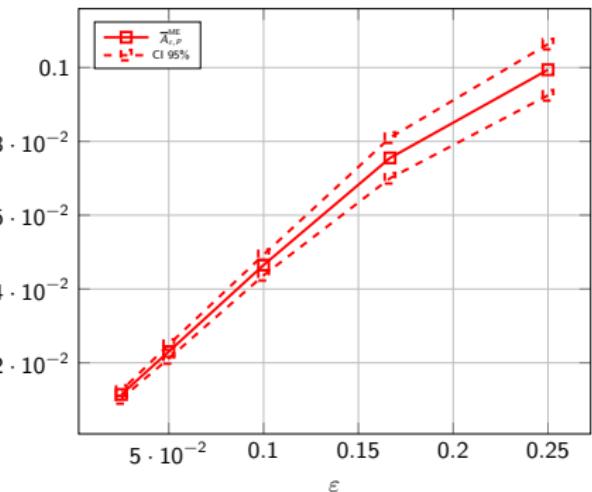


Figure: Two realizations of coefficient A_ε .

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)

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



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

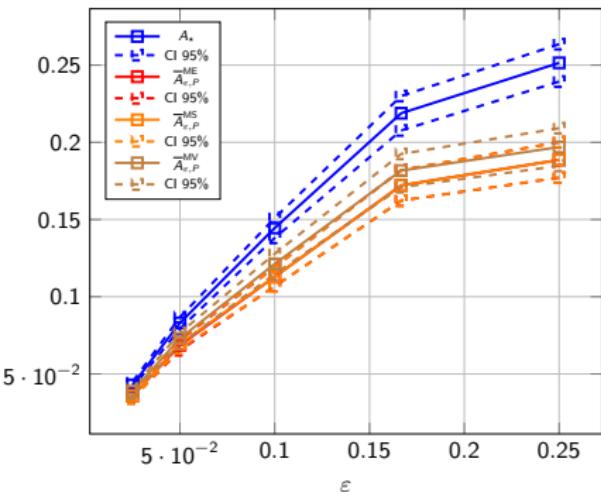


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Noise

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:

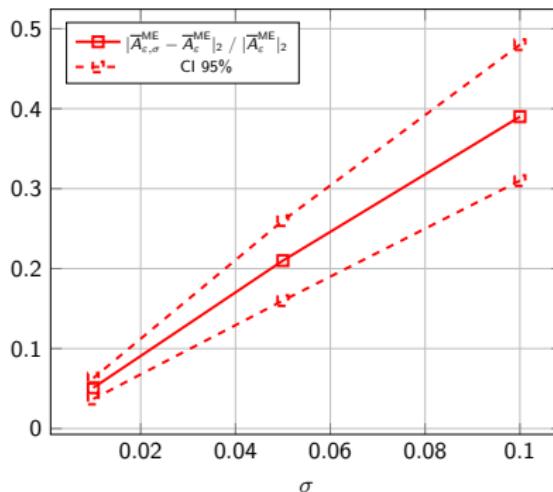


Figure: Error $\frac{|A_{\varepsilon,\sigma}^{ME} - A_\varepsilon^{ME}|_2}{|A_\varepsilon^{ME}|_2}$ as a function of the noise magnitude σ (for $\varepsilon = 0.025$).

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

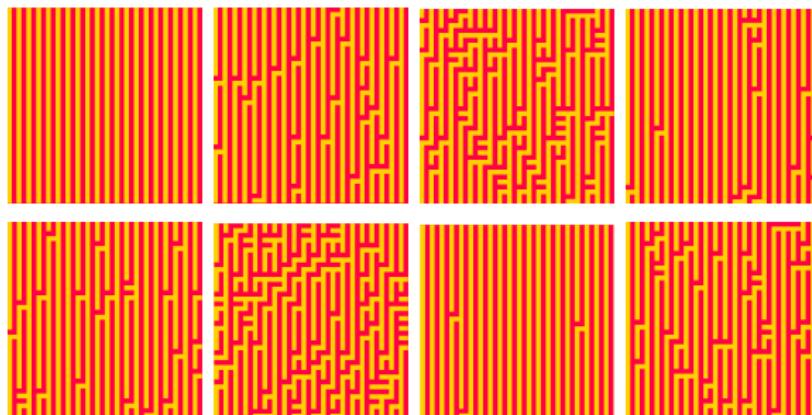
- **Assumption:** The effective coefficient lies in neighbourhood of a known coefficient \bar{A}_0 .
- **Example:** Periodic material with random defect

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

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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Exact	Perturbative expansion
\bar{A}	$\bar{A}_0 + \eta \bar{B}$
$u(\bar{A}, f)$	$u_0 + \eta v$

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

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

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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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$\mathcal{E}(\bar{A}, f)$	$\mathcal{E}(\bar{A}_0, f) + \eta \sum_{ij} \bar{B}_{ij} \mathcal{F}_{ij}(\bar{A}_0, f)$

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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$\mathcal{E}(\bar{A}, f)$	$\mathcal{E}(\bar{A}_0, f) + \eta \sum_{ij} \bar{B}_{ij} \mathcal{F}_{ij}(\bar{A}_0, f)$

We formulate the optimization problem

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

Implementation aspects

- **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.

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- Define

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

with

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

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This step amounts to solving a $P \times P$ eigenvalue problem.

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Observe that J_ε^n is quadratic.

Implementation aspects

- **Offline stage:**

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- 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.

- **Online stage:** we apply a **gradient descent**

- Define 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

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

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).

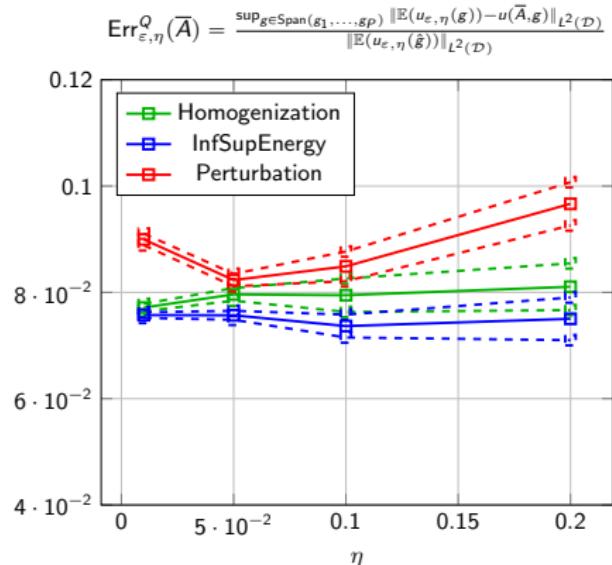
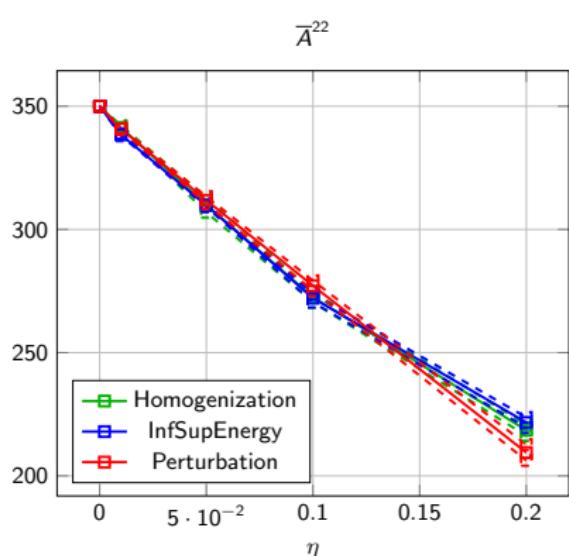


Figure: (left) Component 22 for various approximations of the effective coefficient.
(right) Criterion $\text{Err}_{\varepsilon, Q}^E(\bar{A})$ for different constant coefficients (with $Q = 9$ and $\varepsilon = 0.025$).

Part III

Efficient selection of effective coefficients

Framework

- **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 $\bar{A}, \bar{B} \in \mathcal{A}^2$,

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

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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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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

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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- Application to real experimental data.
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- 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.

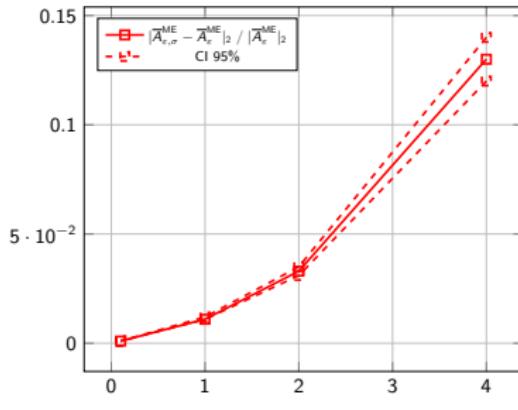


Figure: Error between $\bar{A}_{\varepsilon, \sigma}^{\text{ME}}$ and $\bar{A}_\varepsilon^{\text{ME}}$ as a function of the noise magnitude σ (for $\varepsilon = 0.05$).

Convergence analysis

We consider the slightly modified

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

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

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

writes

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

Thus the energy writes:

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

Then, we get

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

Efficient selection of effective coefficients

Framework

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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.

Strategy

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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
 $x \mapsto \gamma_1 + \gamma_2 \sin\left(\frac{2\pi x}{\varepsilon}\right)$.

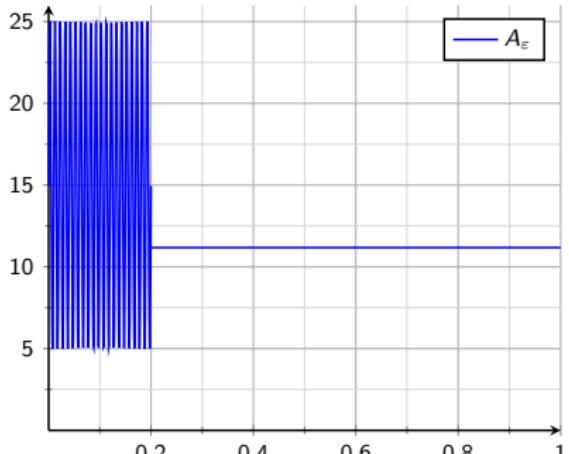


Figure: Coefficient A_ε with $\varepsilon = 0.01$.

Numerical results

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

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

and

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

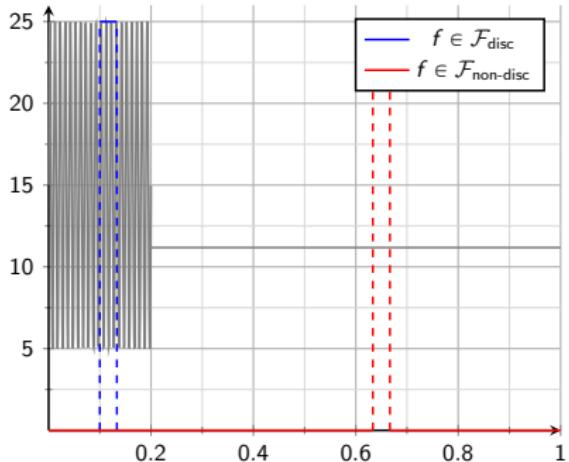


Figure: Admissible loadings.

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.

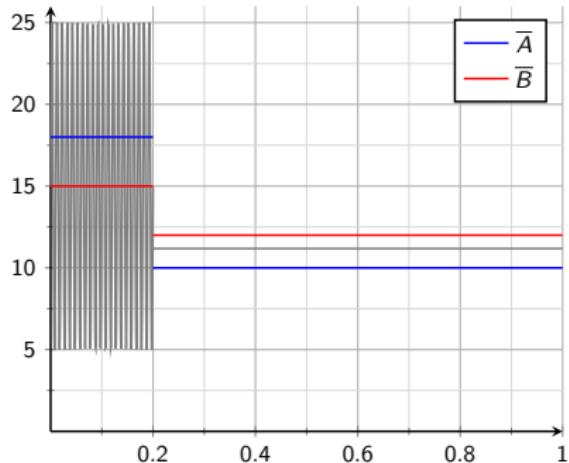


Figure: Effective coefficients.

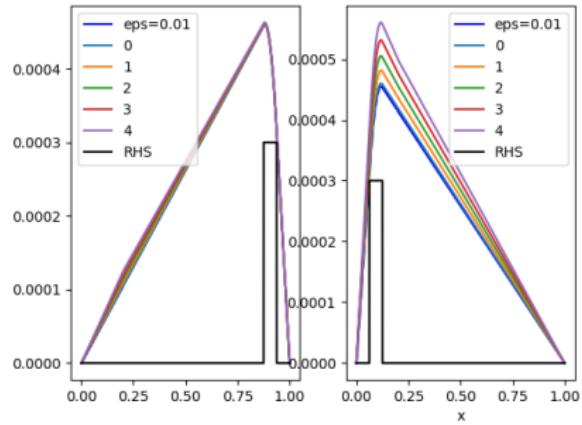
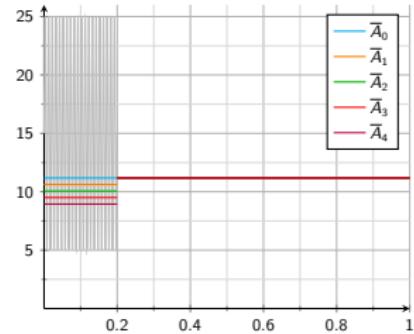
Numerical results: case 1

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

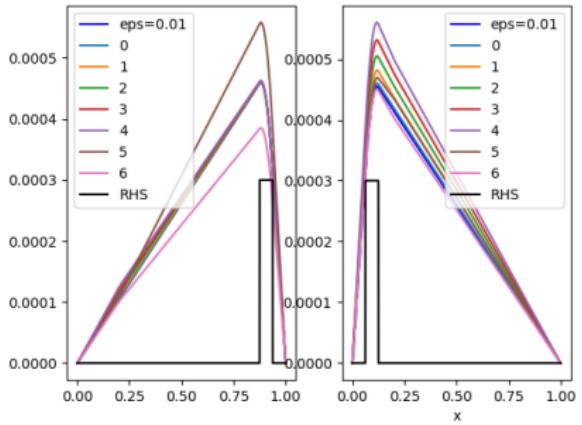
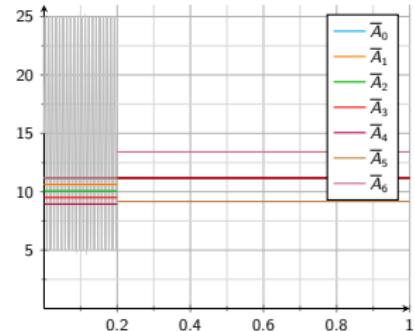
Numerical results: case 2

Setting:

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

and

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



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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	$f_{28} \in \mathcal{F}_{\text{non-disc}}$	$f_4 \in \mathcal{F}_{\text{disc}}$
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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:

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

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

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

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

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

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

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

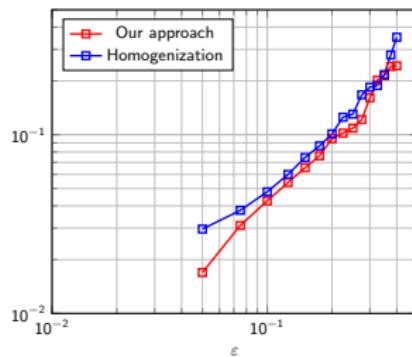
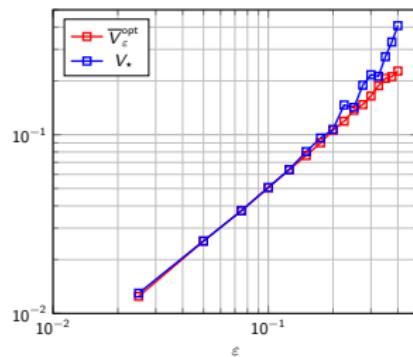


Figure: Comparison of our approach and homogenization in L^2 -norm (left) and H^1 -norm (right).