Effective approximations of multiscale PDE based on limited information

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Joint work with Claude Le Bris & Frédéric Legoll

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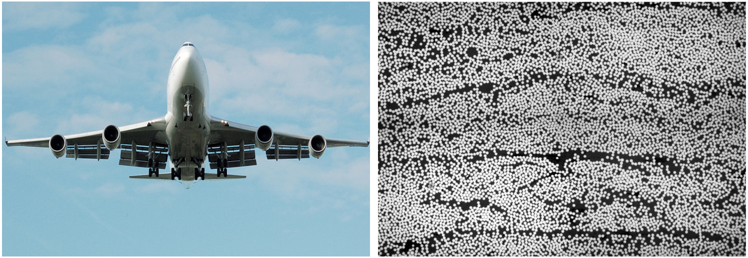
General introduction

Multiscale system are characterized by the presence of multiples scales of interests that interact or influence one another.

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



airplane wing ≈ 10m v.s. carbon fibers $\approx 10^{-6}$m

Figure: Composite material used in the aeronautics industry.

Multiscale systems

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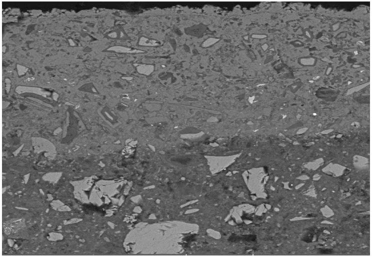


bridge $\approx 10^3$m v.s. mineral aggregate $\approx 10^{-5}$m

Figure: Concrete: a multiscale material.

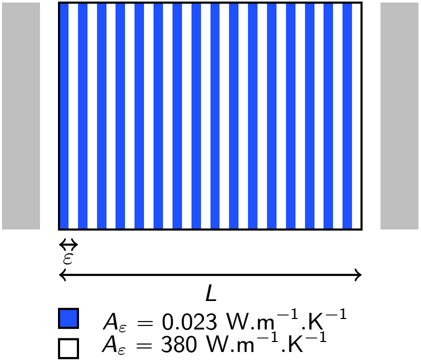
Inverse multiscale problems

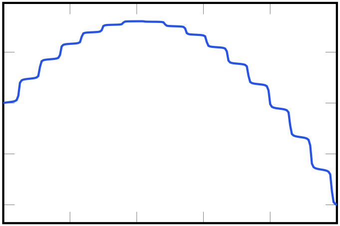
- Consider the problem

$$\begin{cases} -\mathrm{div}\left(A_\varepsilon \nabla u_\varepsilon\right) = f \text{ in } \Omega, \\ u_\varepsilon = g \text{ on } \partial\Omega, \end{cases}$$

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

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





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Question

Based on measurements about the system, can A_ε be reliably reconstructed ? If not, what coefficients may be ?

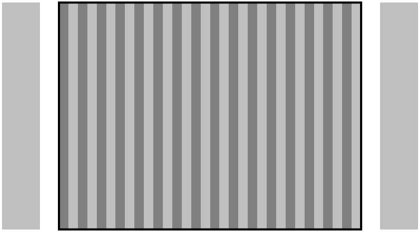
Limited information

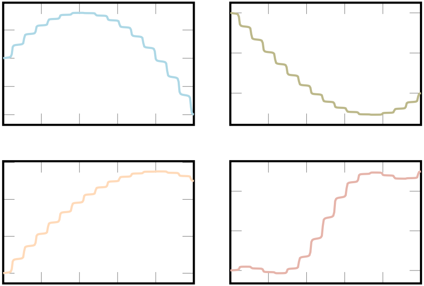
Experimental settings:

- few knowledge on microstructure,
- only couples (*configuration*, *system responses*) are available.

Settings with <u>limited</u> information:

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





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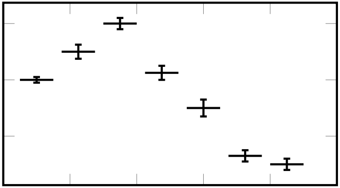

Ill-posedness

Homogenization (see e.g. [BLP78][1]) builds PDE with slowly varying coefficient that accurately approximate the oscillating PDE.

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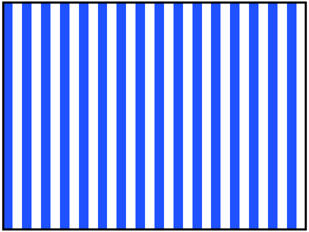

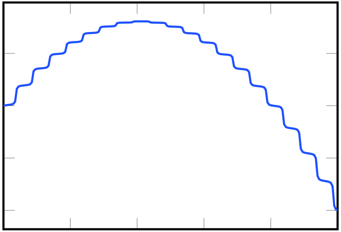

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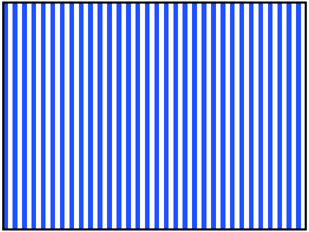

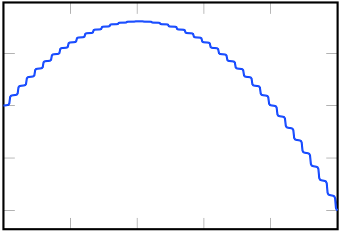

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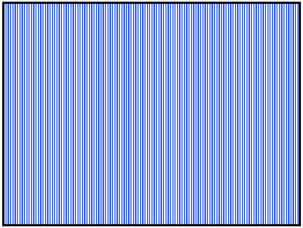

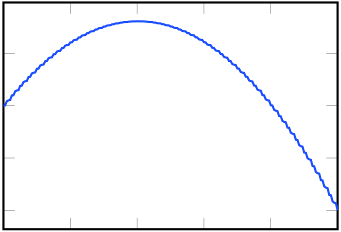

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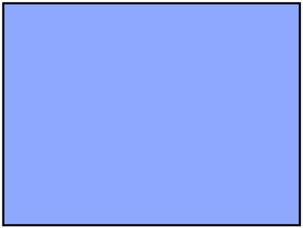

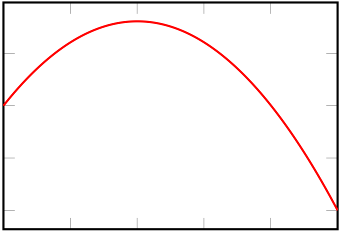

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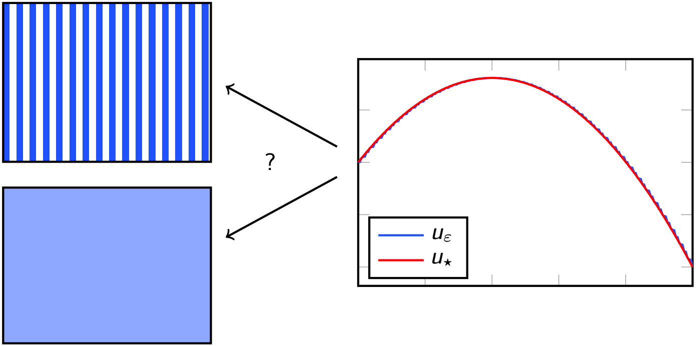

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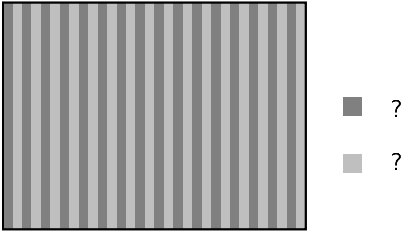

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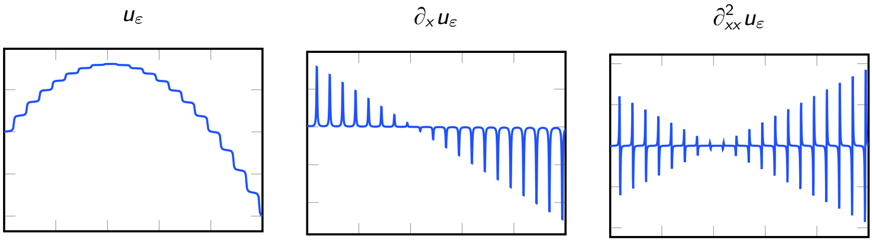

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Issue: how to proceed in contexts of limited information?

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

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

$$\begin{array}{ll} \mathcal{L}_\varepsilon : f \longrightarrow u_\varepsilon(f) & \text{sol. to } -\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f \\ \Big\downarrow \varepsilon \to 0 & \\ \mathcal{L}_{A_\star} : f \longrightarrow u_\star(f) & \text{sol. to } -\operatorname{div}(A_\star \nabla u_\star) = f \end{array}$$

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with respect to the $L^2(\Omega)$ norm.
In the periodic case $A_\varepsilon(x) = A_{\text{per}}\left(\frac{x}{\varepsilon}\right)$, with A_{per} Q-periodic:

- in dimension $d = 1$ $\rightsquigarrow$ $A_\star = \left(\int_Q \frac{1}{A_{\text{per}}}\right)^{-1}$,
- in dimension $d \geqslant 2$ $\rightsquigarrow$ $A_\star = \int_Q A_{\text{per}}(\nabla\omega + \mathrm{Id})$ where ω is a corrector defined through a PDE involving A_{per}.

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Two major limitations of homogenization:

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

Overview

Objective

Based on available observables, define an effective coefficient $\overline{A}$ such that, for any f, the solution $u_\varepsilon(f)$ to

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

are satisfyingly approximated by the solution $\overline{u} = u(\overline{A}, f)$ to the coarse problem

$$-div\left(\overline{A}\nabla\overline{u}\right) = f.$$

Part I — Construct $\overline{A}$ in the whole set $\mathbb{R}^{d\times d}_{\text{sym}}$.

Part II — Identify $\overline{A}$ in the viccinity of a known coefficient $\overline{A}_0$.

Part I

Effective modeling from boundary agregated measurements

A first formulation [CRAS2013][2], [COCV2018][3]

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

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

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

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

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

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

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 acquirable, such as the energy

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

Motivation:

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

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

  where $\mathcal{E}(A_\star, g) = \frac{1}{2}\int_\Omega A_\star \nabla u_\star \cdot \nabla u_\star - \int_{\partial\Omega} g \; u_\star$ and where $u_\star$ denotes the homogenized solution.
- $\mathcal{E}(A_\varepsilon, g)$ is an integrated quantity (scalar !), thus it provides no direct insights about the microscale.

A new formulation

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

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

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

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

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

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

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

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

Proposition (Asymptotic consistency, periodic case)

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

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

the following convergence holds :

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

Computational procedure

We apply a an iterative algorithm to solve

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

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

1. Define g^n, the argsup to

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

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

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

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

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

Choice of the loadings

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

$$\sup_{g\in L^2(\partial\Omega)} \left|\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g)\right| \approx \sup_{g\in \underset{1\leqslant i\leqslant P}{\mathrm{Span}}(g_i)} \left|\mathcal{E}(A_\varepsilon, g) - \mathcal{E}(\overline{A}, g)\right|.$$

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Rayleigh quotient: we optimize

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

where

$$\mathcal{T}_\varepsilon : g \in L^2(\partial\Omega) \longrightarrow \gamma(u_\varepsilon(g)) \qquad \text{with } u_\varepsilon(g) \text{ sol. to (1)},$$
$$\mathcal{T}_{\overline{A}} : g \in L^2(\partial\Omega) \longrightarrow \gamma(u(\overline{A}, g)) \quad \text{with } u(\overline{A}, g) \text{ sol. to (2)}.$$

Thus, we seek the eigenmode of $\mathcal{T}_\varepsilon - \mathcal{T}_{\overline{A}}$ with largest (unsigned) eigenvalue.

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Case of spheric coefficients: it holds that

$$\mathcal{T}_\varepsilon - \mathcal{T}_{\overline{A}} \underset{\varepsilon\to 0}{\longrightarrow} (A_\star - \overline{A})\ \mathcal{T}$$

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

$$-\Delta w = 0 \text{ in } \Omega, \qquad \nabla w \cdot n = g \text{ on } \partial\Omega.$$

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$$-\Delta w=0 \text{ in } \Omega, \qquad \nabla w\cdot n=g \text{ on } \partial\Omega.$$

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

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

for which

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

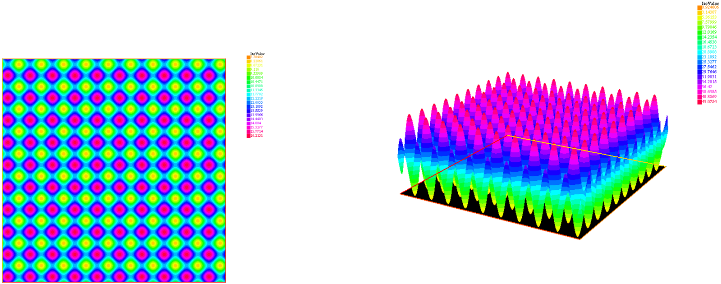


Figure: Components 11 and 22 of coefficient A_ε.

Numerical results (periodic)

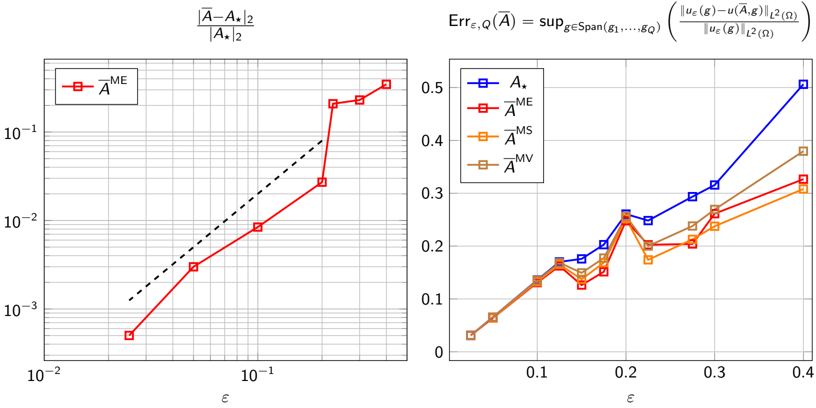


Figure: (left) Error between coefficients $A_\star$ and $\overline{A}^{\mathrm{ME}}_{\varepsilon,P}$.
(right) Criterion $\mathrm{Err}_{\varepsilon,Q}(\overline{A})$ for $\overline{A} \in \{A_\star, \overline{A}^{\mathrm{MV}}_{\varepsilon,P}, \overline{A}^{\mathrm{ME}}_{\varepsilon,P}, , \overline{A}^{\mathrm{MS}}_{\varepsilon,P}\}$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

Numerical results (stochastic)

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

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

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

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

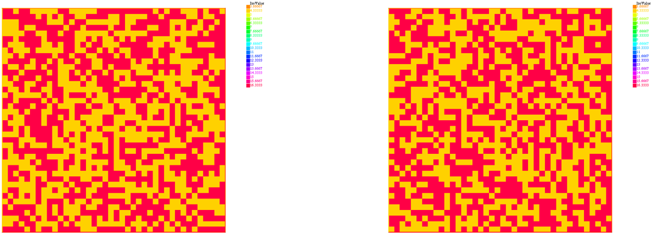
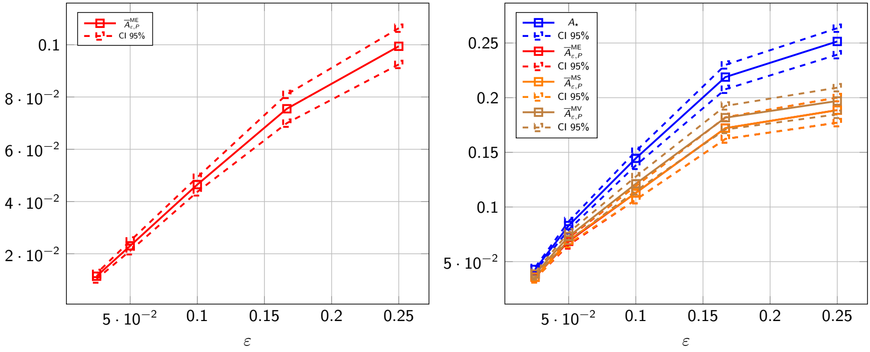


Figure: Two realizations of coefficient A_ε.

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

Numerical results (stochastic)

$$\frac{|\overline{A} - A_\star|_2}{|A_\star|_2} \qquad \mathrm{Err}^{\mathbb{E}}_{\varepsilon,Q}(\overline{A}) = \sup_{g \in \mathrm{Span}(g_1,\dots,g_Q)} \left(\frac{\|\mathbb{E}(u_\varepsilon(g)) - u(\overline{A},g)\|_{L^2(\Omega)}}{\|\mathbb{E}(u_\varepsilon(g))\|_{L^2(\Omega)}} \right)$$



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Noise

Consider a multiplicative Gaussian noise in the energy:

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

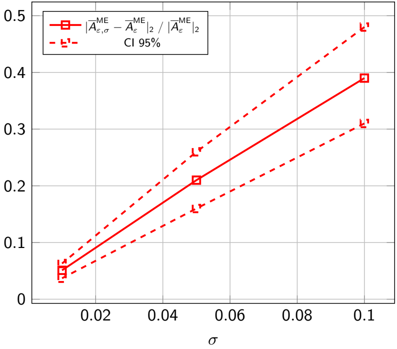


Figure: Error $\frac{|\overline{A}^{\mathrm{ME}}_{\varepsilon,\sigma} - \overline{A}^{\mathrm{ME}}_{\varepsilon}|_2}{|\overline{A}^{\mathrm{ME}}_{\varepsilon}|_2}$ as a function of the noise magnitude σ (for $\varepsilon = 0.025$).

Part II

Perturbative reconstruction of effective coefficients

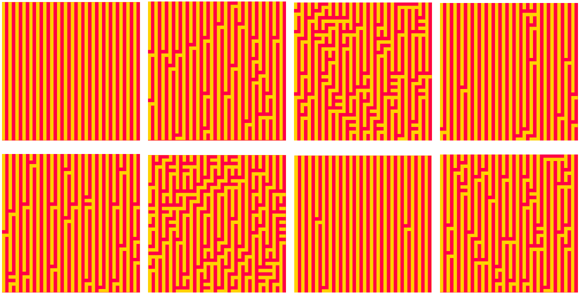
- **Assumption**: The effective coefficient lies in neighboorhood of a known coefficient $\overline{A}_0$.
- **Example**: Randomly defectuous (periodic) material

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

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

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

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



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- **Issue**: Computing the effective coefficient using previous methods for many realizations ω and different defect rates η may end up having a prohibitive computationnal costs...

Question

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

Perturbative development

Consider the problem

$$-\mathrm{div}\left(A_\varepsilon \nabla u_\varepsilon\right) = f \text{ in } \Omega, \qquad \text{and} \qquad u_\varepsilon = 0 \text{ on } \partial\Omega,$$

and its approximation by

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

Exact	Perturbative expansion
$\overline{A}$	$\overline{A}_0 + \eta \overline{B}$

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

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

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

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

$$\begin{cases} -\mathrm{div}\left(\overline{A}_0 \nabla v_{ij}\right) = \mathrm{div}\left(E_{ij} \nabla u_0\right) & \text{in } \Omega, \\ v_{ij} = 0 & \text{on } \partial\Omega. \end{cases} \tag{6}$$

Perturbative development

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

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

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

Perturbative development

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

We formulate the optimization problem

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

- **Offline stage**:
  - Compute $u(\overline{A}_0, f)$.
  - Compute $\mathcal{E}(\overline{A}_0, f)$ and $\mathcal{F}_{ij}(\overline{A}_0, f)$ for any $1 \leqslant i \leqslant j \leqslant d$.

  ↳ computing $P \approx 3$ solutions to a coarse PDE and $P(1 + \frac{d(d+1)}{2})$ domain integrals.

- **Online stage**: We apply a gradient descent. Given an iterate $\overline{B}^n$,
  - Define f^n, the argsup to

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

  In practice, $\sup_{f \in L^2(\Omega)} \to \sup_{f \in V_P}$ on $V_P = \mathrm{Span}\{P \text{ loadings}\}$, with $P \approx 3$.
  This step amounts to solving a $P \times P$ eigenvalue problem.
  - Define

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

  with

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

  ↳ no additional computations of coarse PDE !

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

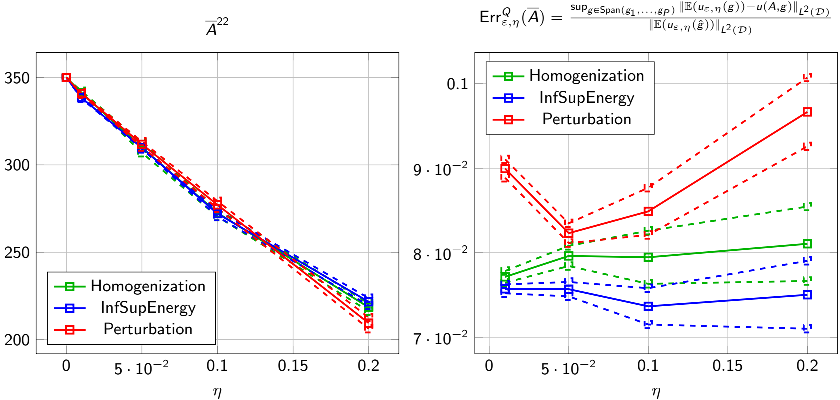

Figure: (left) Component 22 for various approximations of the effective coefficient. (right) Criterion $Err^{\mathbb{E}}_{\varepsilon,Q}(\overline{A})$ for different constant coefficients (with $Q = 9$ and $\varepsilon = 0.025$).

Numerical results

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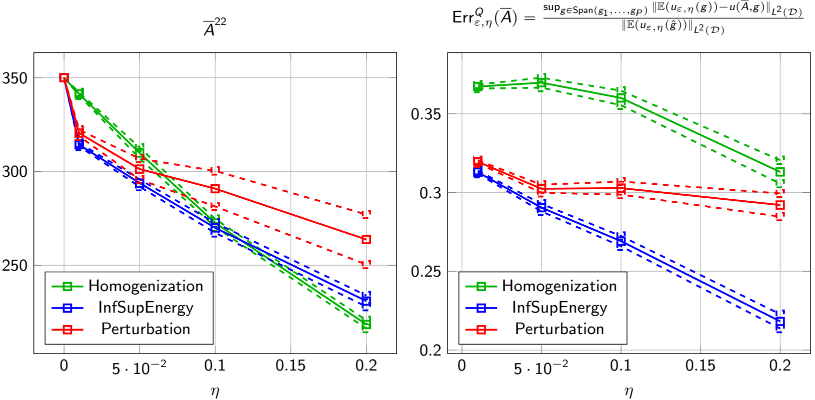

Figure: (left) Component 22 for various approximations of the effective coefficient. (right) Criterion $Err^{\mathbb{E}}_{\varepsilon,Q}(\overline{A})$ for different constant coefficients (with $Q = 9$ and $\varepsilon = 0.1$).

Conclusion and perspectives

Our strategies

- aim at determining effective approximation for multiscale PDEs through coarse coefficients,
- are designed for context with 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.

Perspectives

- Application to real experimental data.
- Extension to non-constant effective coefficients.
- Convergence analysis of $\overline{A}$ to $A_\star$.

Thank you !

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 $\implies \mathcal{E}_{\varepsilon}(g) \underset{\varepsilon\to 0}{\to} \mathcal{E}_{\star}(g) \implies I_{\varepsilon} \underset{\varepsilon\to 0}{\to} 0 \implies \mathcal{E}_{\varepsilon}(g) \underset{\varepsilon\to 0}{\to} \mathcal{E}_{\#}(g)$.

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

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

  Thus,

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

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

  Thus,

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

- Identification of particular couples $(f_i, g_i)_{1 \leqslant i \leqslant \frac{d(d+1)}{2}}$ to get

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

A different perspective on noise

Motivation: anticipate on reproducibility errors during model deployment.

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

Formulation: consider the problem

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

where η is a Gaussian variable.

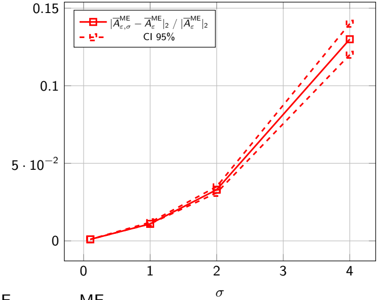

Figure: Error between $\overline{A}^{\mathrm{ME}}_{\varepsilon,\sigma}$ and $\overline{A}^{\mathrm{ME}}_{\varepsilon}$ as a function of the noise magnitude σ (for $\varepsilon = 0.05$).

Part III

Efficient selection of effective coefficients

Framework

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

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

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

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

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 $f \in \mathcal{F}$.

Iterative algorithm: each step k selects a loading f^k in $\mathcal{F}$ and update the choice of the best coefficient $\overline{A}^k$ 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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$\Delta_1(f)$	$\max_{(\overline{A},\overline{B})\in\mathcal{A}^2} \mathrm{Err}(\overline{A},\overline{B},f)$	$\mathrm{Err}(\overline{A},\overline{B},f) = \frac{\|\mathcal{O}(\overline{A},f)-\mathcal{O}(\overline{B},f)\|_{\mathcal{O}}}{\|\mathcal{O}(\overline{A},f)\|_{\mathcal{O}}}$

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

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$\Delta_2^k(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \left\vert\mathrm{Err}^k(\overline{A},f)-\mathrm{Err}^k(\overline{B},f)\right\vert$	$\mathrm{Err}^k(\overline{A},f) = \frac{\Vert\mathcal{O}(\overline{A}^k,f)-\mathcal{O}(\overline{A},f)\Vert_{\mathcal{O}}}{\Vert\mathcal{O}(\overline{A}^k,f)\Vert_{\mathcal{O}}}$

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Core components:

- Discrimination rate: it estimates how a loadings is discriminative w.r.t observable $\mathcal{O}$.

$\Delta_1(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \mathrm{Err}(\overline{A},\overline{B},f)$	$\mathrm{Err}(\overline{A},\overline{B},f) = \frac{\\|\mathcal{O}(\overline{A},f)-\mathcal{O}(\overline{B},f)\\|_{\mathcal{O}}}{\\|\mathcal{O}(\overline{A},f)\\|_{\mathcal{O}}}$
$\Delta_2^k(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \left\lvert\mathrm{Err}^k(\overline{A},f)-\mathrm{Err}^k(\overline{B},f)\right\rvert$	$\mathrm{Err}^k(\overline{A},f) = \frac{\\|\mathcal{O}(\overline{A}^k,f)-\mathcal{O}(\overline{A},f)\\|_{\mathcal{O}}}{\\|\mathcal{O}(\overline{A}^k,f)\\|_{\mathcal{O}}}$
$\Delta_{\varepsilon}(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \left\lvert\mathrm{Err}_{\varepsilon}(\overline{A},f)-\mathrm{Err}_{\varepsilon}(\overline{B},f)\right\rvert$	$\mathrm{Err}_{\varepsilon}(\overline{A},f) = \frac{\\|\mathcal{O}(A_{\varepsilon},f)-\mathcal{O}(\overline{A},f)\\|_{\mathcal{O}}}{\\|\mathcal{O}(A_{\varepsilon},f)\\|_{\mathcal{O}}}$

Strategy

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

Core components:

- Discrimination rate: it estimates how a loadings is discriminative w.r.t observable $\mathcal{O}$.

$\Delta_1(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \mathrm{Err}(\overline{A},\overline{B},f)$	$\mathrm{Err}(\overline{A},\overline{B},f) = \frac{\Vert\mathcal{O}(\overline{A},f)-\mathcal{O}(\overline{B},f)\Vert_{\mathcal{O}}}{\Vert\mathcal{O}(\overline{A},f)\Vert_{\mathcal{O}}}$
$\Delta_2^k(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \left\vert\mathrm{Err}^k(\overline{A},f)-\mathrm{Err}^k(\overline{B},f)\right\vert$	$\mathrm{Err}^k(\overline{A},f) = \frac{\Vert\mathcal{O}(\overline{A}^k,f)-\mathcal{O}(\overline{A},f)\Vert_{\mathcal{O}}}{\Vert\mathcal{O}(\overline{A}^k,f)\Vert_{\mathcal{O}}}$
$\Delta_3(f)$	$\max\limits_{(\overline{A},\overline{B})\in\mathcal{A}^2} \left\vert\mathrm{Err}_\varepsilon(\overline{A},f)-\mathrm{Err}_\varepsilon(\overline{B},f)\right\vert$	$\mathrm{Err}_\varepsilon(\overline{A},f) = \frac{\Vert\mathcal{O}(A_\varepsilon,f)-\mathcal{O}(\overline{A},f)\Vert_{\mathcal{O}}}{\Vert\mathcal{O}(A_\varepsilon,f)\Vert_{\mathcal{O}}}$

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

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

Selection algorithm

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

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

Iterate k:

1. *Compute discrimination rate* $\Delta^k(f)$ *for any* f *in* $\mathcal{F}^k = \mathcal{F} \backslash \{f^p\}_{p=1,\dots,k-1}$.
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*
$$\overline{A}^k \in \arg\min_{\overline{A} \in \mathcal{A}} \gamma^k(\overline{A}).$$

Numerical results

- **Microstructure**. Consider

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

with

$$\gamma_3 = a_\star$$

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

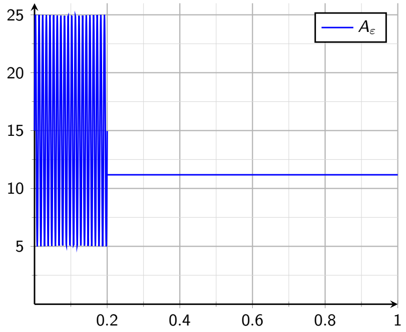


Figure: Coefficient A_ε with $\varepsilon = 0.01$.

Numerical results

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

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

and

$$\mathcal{F} = \begin{array}{c} \overbrace{\{f_n \text{ s.t. } \mathrm{Supp}(f_n) \subset D_1\}}^{\mathcal{F}_{\text{disc}}} \\ \cup \\ \underbrace{\{f_n \text{ s.t. } \mathrm{Supp}(f_n) \subset D_2\}}_{\mathcal{F}_{\text{non-disc}}} \end{array}.$$

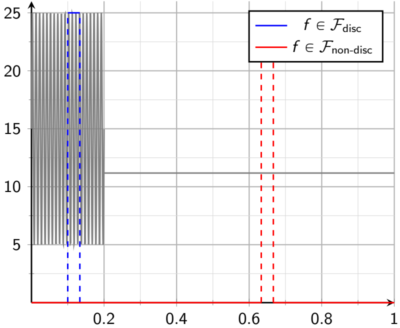


Figure: Admissible loadings.

Microstructure.
Set $\mathcal{F}$.
Set $\mathcal{A}$. Consider

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

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

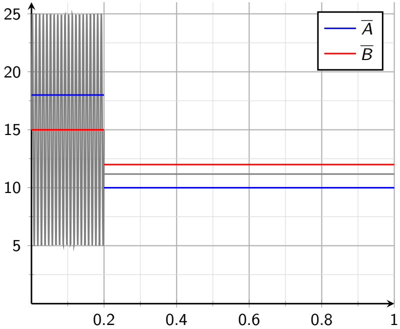


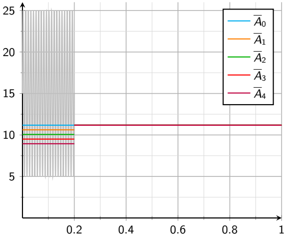
Figure: Effective coefficients.

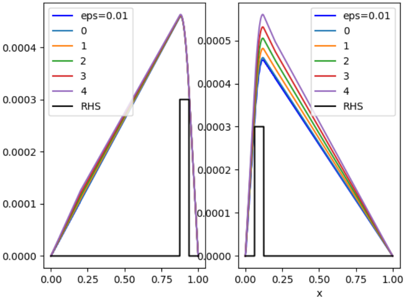
Setting:

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

and

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





Numerical results: case 1

Setting:

$$\mathcal{A}_1 = \{\overline{A}_0 = (a_\star, \quad a_\star),\\ \overline{A}_1 = (0.95a_\star, \quad a_\star),\\ \overline{A}_2 = (0.9a_\star, \quad a_\star),\\ \overline{A}_3 = (0.85a_\star, \quad a_\star),\\ \overline{A}_4 = (0.8a_\star, \quad a_\star)\},$$

and

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

Conclusions:

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

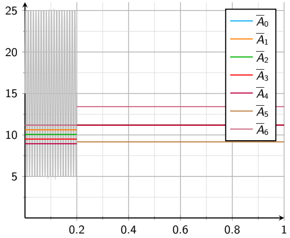
Step	Loadings	Best Coefficient
1	$f_1 \in \mathcal{F}_{\text{disc}}$	$\overline{A}_0$
2	$f_2 \in \mathcal{F}_{\text{disc}}$	$\overline{A}_0$
3	$f_3 \in \mathcal{F}_{\text{disc}}$	$\overline{A}_0$
4	$f_4 \in \mathcal{F}_{\text{disc}}$	$\overline{A}_0$
5	$f_{12} \in \mathcal{F}_{\text{non-disc}}$	$\overline{A}_0$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

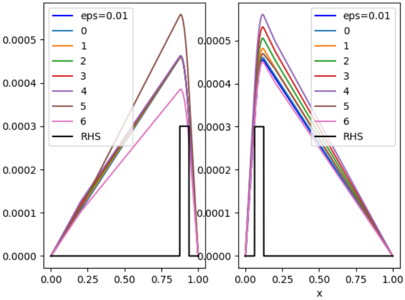
Setting:

$$\mathcal{A}_2 = \mathcal{A}_1 \cup \{\overline{A}_5 = (a_\star, \quad 0.82 a_\star), \\ \overline{A}_6 = (a_\star, \quad 1.2 a_\star)\},$$

and

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





Numerical results: case 2

Setting:

$$\mathcal{A}_2 = \mathcal{A}_1 \cup \{\overline{A}_5 = (a_\star, \quad 0.82a_\star), \\ \overline{A}_6 = (a_\star, \quad 1.2a_\star)\},$$

and

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

Conclusions:

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

Step	Δ_ε	Δ_2
1	$f_1 \in \mathcal{F}_{\mathrm{disc}}$	$f_{29} \in \mathcal{F}_{\text{non-disc}}$
2	$f_2 \in \mathcal{F}_{\mathrm{disc}}$	$f_1 \in \mathcal{F}_{\mathrm{disc}}$
3	$f_3 \in \mathcal{F}_{\mathrm{disc}}$	$f_2 \in \mathcal{F}_{\mathrm{disc}}$
4	$f_4 \in \mathcal{F}_{\mathrm{disc}}$	$f_3 \in \mathcal{F}_{\mathrm{disc}}$
5	$f_{29} \in \mathcal{F}_{\text{non-disc}}$	$f_{28} \in \mathcal{F}_{\text{non-disc}}$
6	$f_{28} \in \mathcal{F}_{\text{non-disc}}$	$f_4 \in \mathcal{F}_{\mathrm{disc}}$
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:

$$\mathcal{A}_2 = \mathcal{A}_1 \cup \{\overline{A}_5 = (a_\star, \quad 0.82 a_\star), \\ \overline{A}_6 = (a_\star, \quad 1.2 a_\star)\},$$

and

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

Conclusions:

- Δ_2 better replicates Δ_ε than Δ_1.
- $\overline{A}_0 = (a_\star, a_\star)$ is the best coefficient at each step.
- Δ_1 selects loadings that do not precisely discriminate $\overline{A}_0$ 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	$f_{17} \in \mathcal{F}_{\text{non-disc}}$	$f_1 \in \mathcal{F}_{\text{non-disc}}$

Convergence analysis

Work with A. Cohen.

Schrödinger equation