Coefficient perturbations in diffusion equations

Internship project

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Motivation & Goal

- Manufactured composite materials are often intended to be **periodic**
- Manufacturing process $\Longrightarrow$ **Random defects** $\Longrightarrow$ Non-periodic result
- How such **defects affect** the mechanical integrity of the material ?

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Goal of the talk

- We propose and analyze a **numerical approach** to efficiently solve elliptic PDEs with periodic coefficient that has **random defects**, in **1D** and **2D**
- The methodology uses **pre-computation** of certain configurations in an offline phase allowing **rapid solution** of the problem in the online phase

Problem formulation

- Diffusion equation in $\Omega = [0\,;1]^d$

Perfect coefficient

$$(\mathscr{P}_\varepsilon)\left|\begin{array}{l} \textit{Find } u_\varepsilon : \Omega \to \mathbf{R} \textit{ s.t.} \\ -\operatorname{div}(A_\varepsilon \nabla u_\varepsilon) = f \quad \text{in } \Omega \\ \qquad\qquad u_\varepsilon = 0 \quad \text{on } \partial\Omega \end{array}\right.$$

Perturbed coefficient

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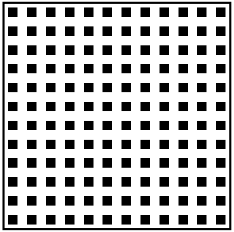
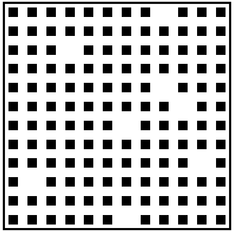
- Setting

$f \in L^2(\Omega)$ $\quad A(x) \in \{\alpha, \beta\}$ $\quad \|A_\varepsilon - A\|_{L^\infty(\Omega)} \approx 1$ $\quad \operatorname{supp}(A_\varepsilon - A) \ll |\Omega|$

- Example



A_ε, perfect coefficient

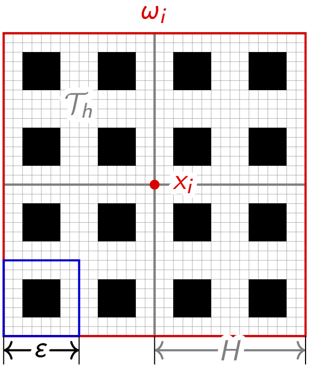


A, perturbed coefficient

Notations

$$(\mathscr{P}) \iff \left| \begin{array}{l} \textit{Find } u \in V := H_0^1(\Omega) \textit{ s.t.} \\ \mathfrak{a}(u,w) := (A\nabla u, \nabla w) = (f,w), \quad \forall w \in V \end{array} \right.$$

- **Fine mesh** $\mathcal{T}_h$ and V_h the corresponding $\mathbb{P}_1$-FEM space
- Let $u_h \in V_h$ solve $\mathfrak{a}(u_h, w) = (f, w), \quad \forall w \in V_h$.
- **Coarse space** $V_H \subset V_h$ with $h < \varepsilon < H$



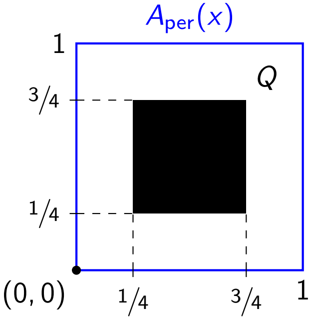
Construction of randomly perturbed coefficient A

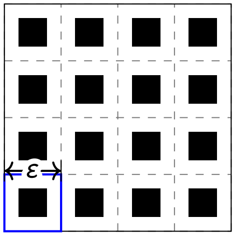
- **Randomly perturbed coefficient**

$$A(x,\omega) = A_\varepsilon(x) + b_{p,\varepsilon}(x,\omega)B_\varepsilon(x),$$

$A_\varepsilon(x) = A_{per}(x/\varepsilon)$ with A_{per} 1-periodic and elliptic and $\varepsilon = 1/n$, B_ε similar

- **Example** : *Sponge*





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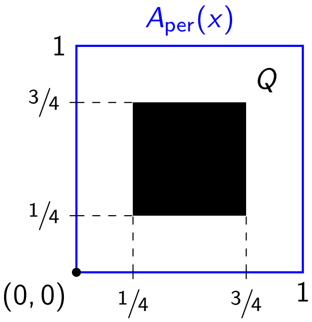

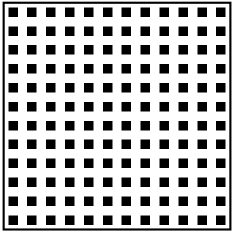

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- **Random character**

$$b_{p,\varepsilon}(x,\omega) = \sum_{j \in I_0} \chi_{\varepsilon(j+Q)}(x) \widehat{b}_p^j(\omega) \quad \text{where} \quad \widehat{b}_p^j(\omega) \sim \mathscr{B}\text{er}(p) \text{ i.i.d.}$$

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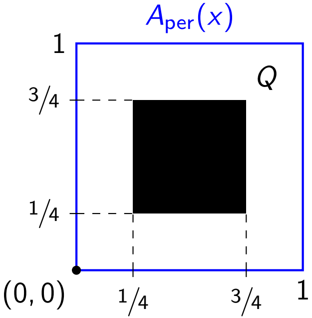

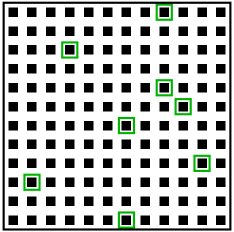

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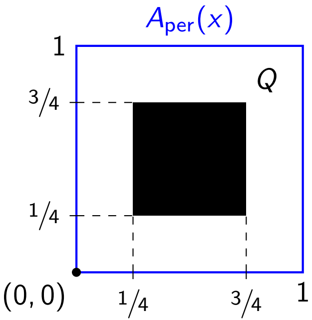

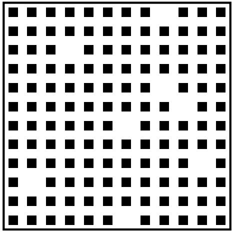

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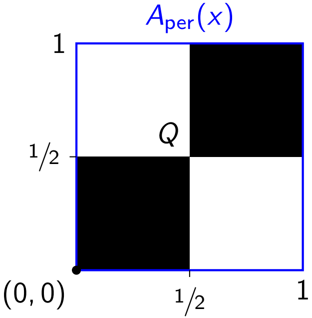
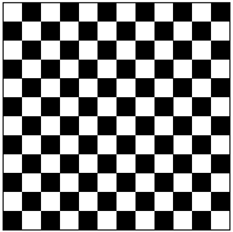
- **Example** : *Checkerboard*





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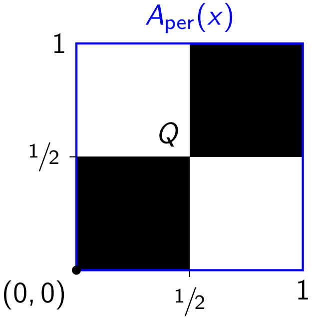
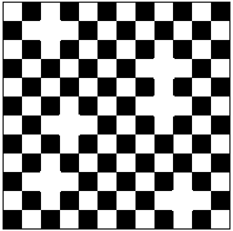
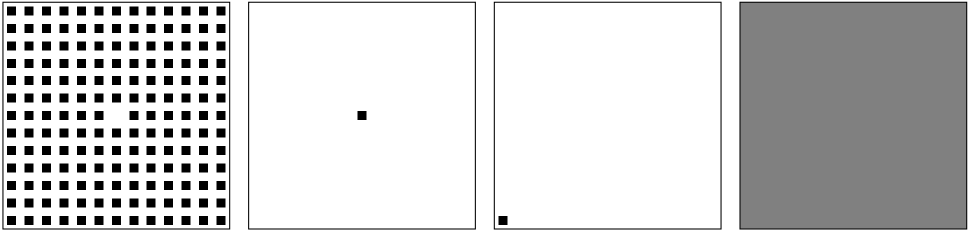




Examples of RHS configurations

⚠ *No random defects*

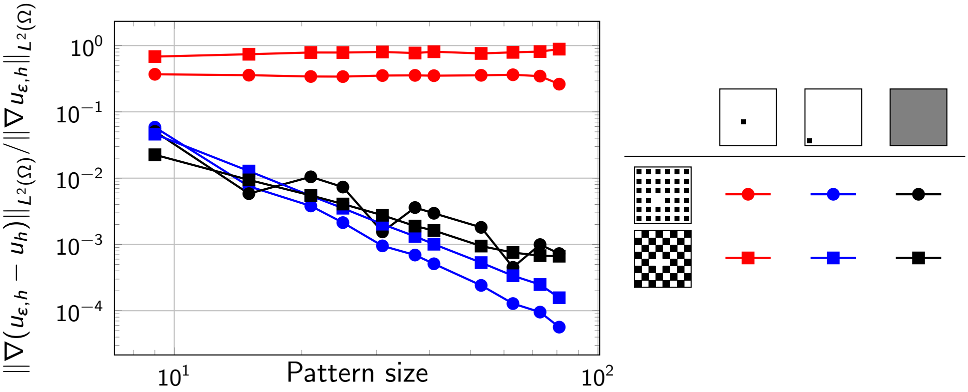


Perturbed coefficient (*sponge*) | RHS **exactly in** the defect block | RHS **far away** from the defect block | Global RHS

Questions

- $\exists$ RHS s.t. $\|\nabla(u_\varepsilon - u)\|_{L^2(\Omega)}$ is **big** ?
- **Global** RHS $\Longrightarrow$ **small** solution differences ?
- Dependence **diameter**/**number** of defects, **contrast** and **FEM mesh size**

A single non-random defect ($\mathbb{P}_1$ FEM)



$\alpha = 1$, $\beta = 10$, FEM mesh size : 243

Observations

- f exactly in : the **worst error**, as expected
- $f \equiv 1$: in-between the two other configurations
- f exactly in & f far away : errors for ***checkerboard*** > errors for ***sponge***

Random defects

Goal

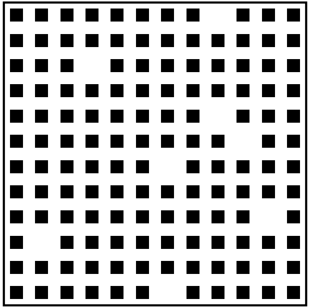
Efficient computation of solution for **many** different realizations A

⚠ $\mathbb{P}_1$ *FEM, no multiscale method*

1. Subspace decomposition **preconditioner** & Convergence analysis
2. Multipoint **inversion formula**
3. **Offline-online** strategy

Subspace decomposition preconditioner

[Kornhuber & Yserentant, 2016]



- **Decomposition** $V = V_0 + V_1 + \cdots + V_n$

$$\underbrace{V_0 = V_H}_{\text{coarse space}}, \qquad \underbrace{V_i = \left\{ v \in V \;\middle|\; \mathrm{supp}(v) \subset \omega_i \right\}}_{\text{local spaces}}.$$

- **Projections** $P_i : V \to V_i$, such that

$$(A\nabla P_i v, \nabla w) = (A\nabla v, \nabla w) \quad w \in V_i$$

Preconditioner

$$P = \underbrace{P_0}_{\text{coarse}} + \underbrace{P_1 + \cdots + P_n}_{\text{decoupled \& local}}$$

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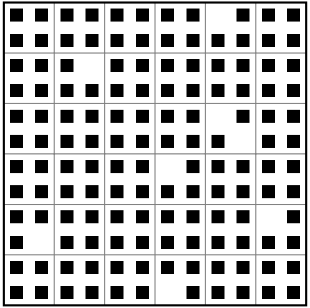

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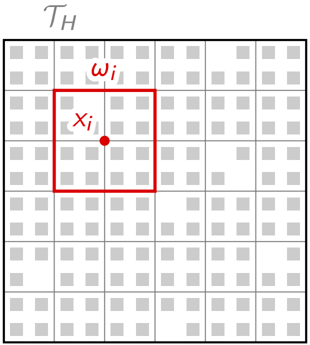

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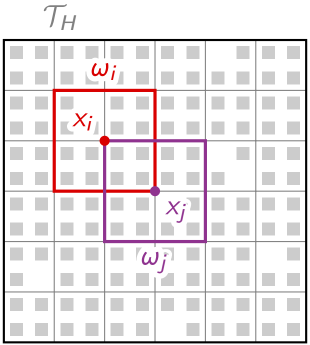

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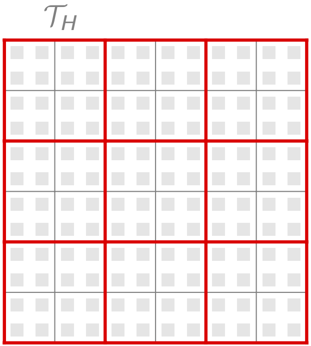

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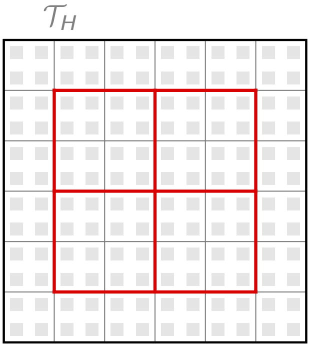

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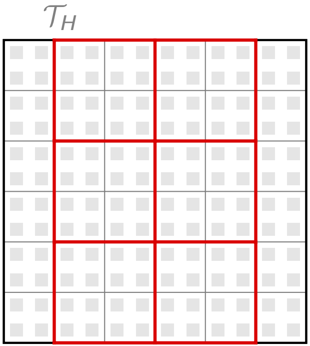

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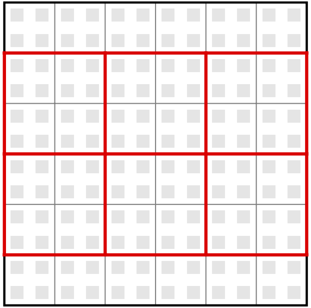

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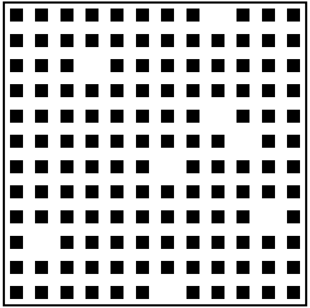

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▶ **Preconditioned conjugate gradient method** (PCG method)

Convergence analysis [Kornhuber & Yserentant, 2016]

- Any function $v \in V$ **can be decomposed** into $v = v_0 + v_1 + \cdots + v_n$, where $v_i \in V_i$ so that
$$\sum_{i=0}^{n} \|v_i\|_A^2 \leqslant K_1 \|v\|_A^2.$$
Achieved with $v_0 = \mathcal{I}_H v$ and $v_j = \varphi_j(v - \mathcal{I}_H v)$ where $\mathcal{I}_H \colon H_0^1(\Omega) \to V_H$ is an interpolation operator and $\sum_{i=1}^{n} \varphi_i = 1$.
- **For any decomposition** $v = v_0 + v_1 + \cdots + v_n$:
$$\|v\|_A^2 \leqslant K_2 \sum_{i=0}^{n} \|v_i\|_A^2.$$
K_1 and K_2 are independant of h and H and only depend on the contrast β/α.

Bound for the error of the PCG algorithm after i iterations

$$\left\|u_h - u_h^{(i)}\right\|_A \leqslant 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^i \left\|u_h - u_h^{(0)}\right\|_A,$$

where $\kappa = K_1 K_2$

Multipoint inversion formula [Dusson, Garrigue & Stamm, 2023]

- **Idea** : Assuming that we know the inverses $\left(A_i^{-1}\right)_{i=1,\dots,N}$ and that

$$A = \sum_{i=1}^{N} \alpha_i A_i,$$

under which conditions is the *same* **linear combination** of inverses

$$\widetilde{A} := \sum_{i=1}^{N} \alpha_i A_i^{-1}$$

a **good approximation** for A^{-1} ?

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- **Numerical experiments**

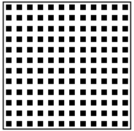
$$\text{Find } u^{(i)} : \Omega \to \mathbf{R} \text{ such that}$$

$$\begin{cases} -\operatorname{div}\left(A_i \nabla u^{(i)}\right) = f & \text{in } \Omega \\ u^{(i)} = 0 & \text{on } \partial\Omega \end{cases}$$

$$\frac{\|\nabla(u - \widetilde{u})\|_{L^2(\Omega)}}{\|\nabla u\|_{L^2(\Omega)}} \quad \text{where} \quad \widetilde{u} := \sum_{i=0}^{N} \alpha_i u^{(i)}.$$

Offline-online strategy **Inspired by** [Målqvist & Verfürth, 2022]

A_ε



Input : Problem data A_ε, B_ε, Q, f

Fix $k \in \{1, \dots, n\}$, Precompute and save offline coefficients $\{A_\ell\}_{\ell=0}^{N}$

for $\ell = 0, \dots, N$ **do**

  Precompute $P_k^{(\ell)} : V \to V_k$ defined by $(A_\ell \nabla P_k^{(\ell)} v, \nabla w) = (A_\ell \nabla v, \nabla w) \quad \forall w \in V_k$

end

for all sample coefficients A **do**

  for $i = 1, \dots, n$ **do**

    Compute $\{\mu_\ell\}_{\ell=0}^{N}$ such that $A|_{\omega_i} = \sum_{\ell=0}^{N} \mu_\ell A_\ell$

    Assemble $\widetilde{P}_i := \sum_{\ell=0}^{N} \mu_\ell P_k^{(\ell)}$

  end

  $\widetilde{P} := \widetilde{P_0} + \sum_{i=1}^{n} \widetilde{P}_i$ and Solve PCG system

end

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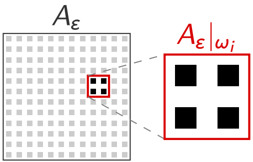

Input : Problem data A_ε, B_ε, Q, f

Fix $k \in \{1, \dots, n\}$, Precompute and save offline coefficients $\{A_\ell\}_{\ell=0}^N$ **Offline phase**

for $\ell = 0, \dots, N$ **do**

  Precompute $P_k^{(\ell)} : V \to V_k$ defined by $(A_\ell \nabla P_k^{(\ell)} v, \nabla w) = (A_\ell \nabla v, \nabla w) \quad \forall w \in V_k$

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for all sample coefficients A **do**

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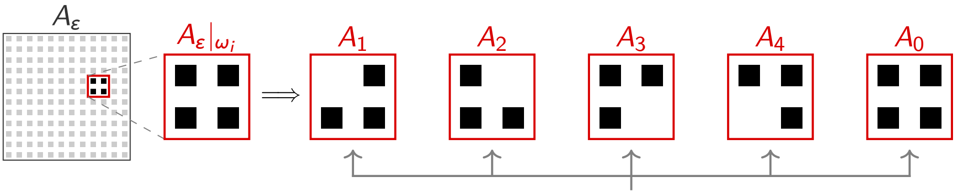

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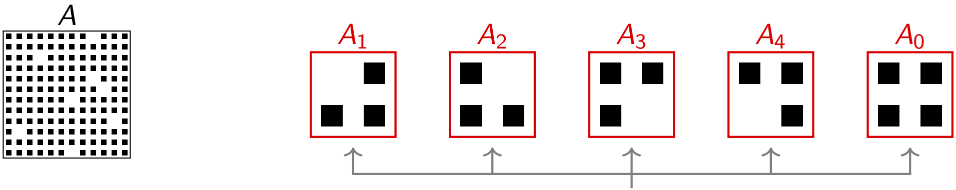

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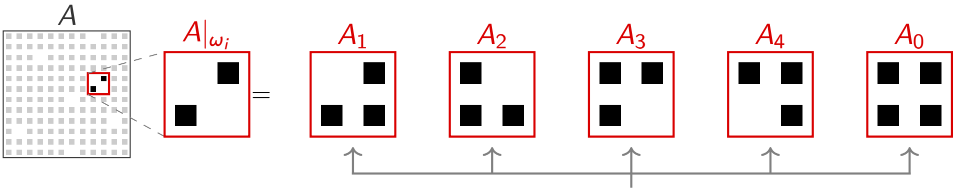

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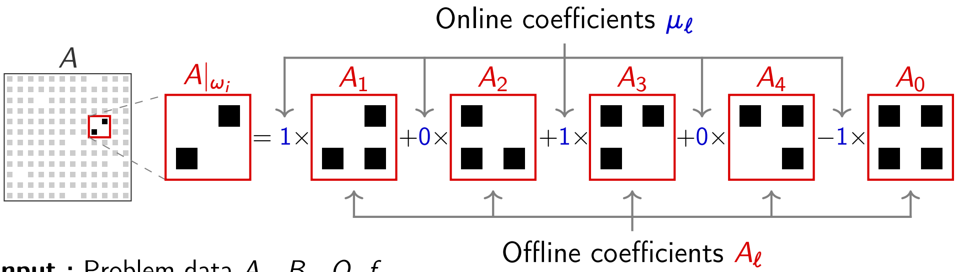

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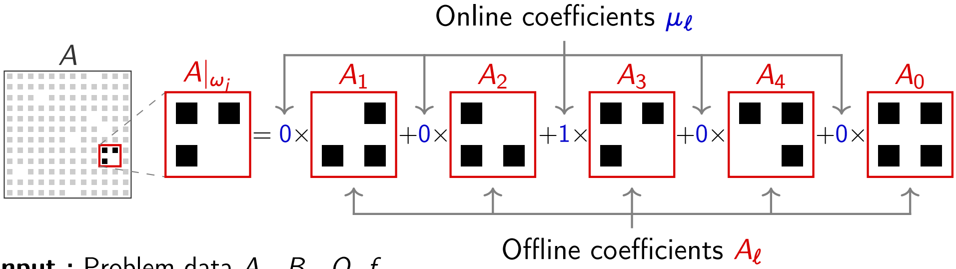

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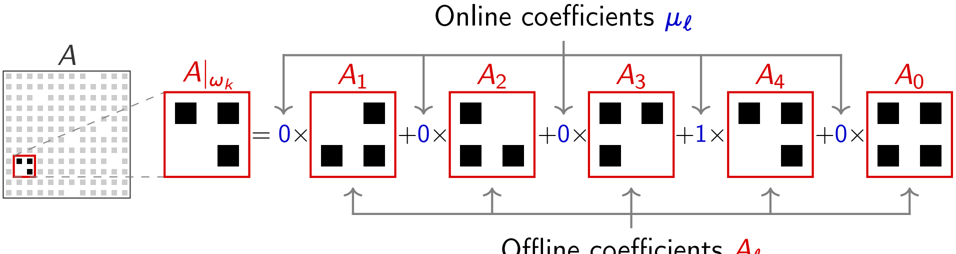

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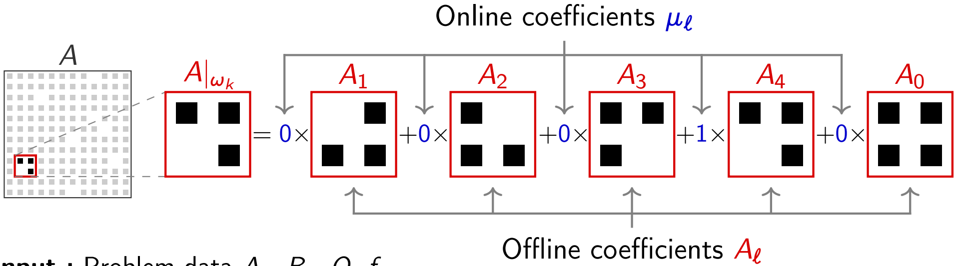

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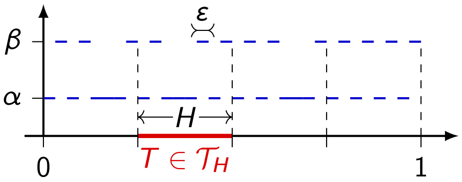
Three strategies

- ✗ Solving directly with $A(x, \omega)$ defined on a ε-scale
- ✓ **Piecewise constant coefficient** defined on a coarse mesh $H \gg \varepsilon$
- Standard FEM on $\mathcal{T}_H$



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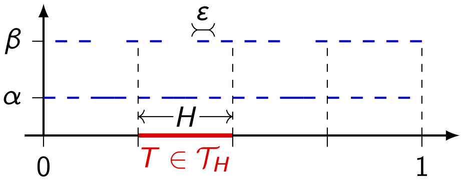

Offline-online	$A^{\circ}\|_T(\omega) := \mu_0\, \bar{A}_{\text{per}} + \sum_{i=1}^{N} \mu_i \bar{A}_i$ with $\bar{A}_i$ offline coefficients
Expansion [Anantharaman & Le Bris, 2010]	$A^* := \bar{A}_{\text{per}} + p\, A^{\text{e}}$, with $A^{\text{e}} = \bar{A}_{\text{per}} - \dfrac{\bar{A}_{\text{per}}{}^2}{\bar{A}}$
1D LOD	$\widehat{A}\|_T(\omega) := \bar{A}_{\text{per}} \fint_T \dfrac{A(x,\omega)}{A_{\text{per}}(x)}\,\mathrm{d}x$

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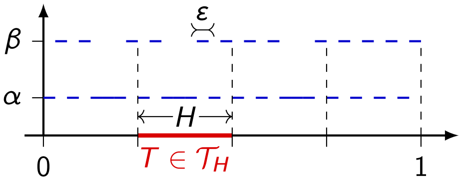

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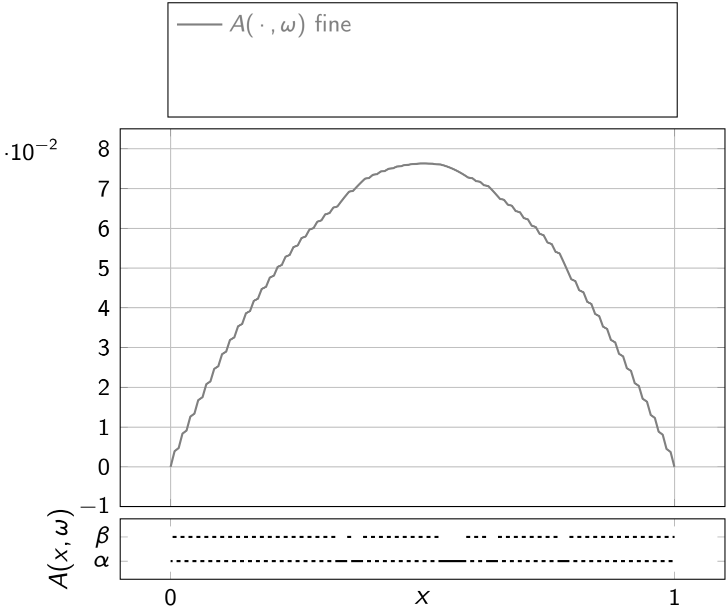
Remark : $N_{\text{def}} = 0 \implies$ standard periodic homogenization

Three strategies



$H = 2^{-3}$, $h = 10^{-3}$, $\varepsilon = 2^{-7}$, $\alpha = 1$, $\beta = 5$

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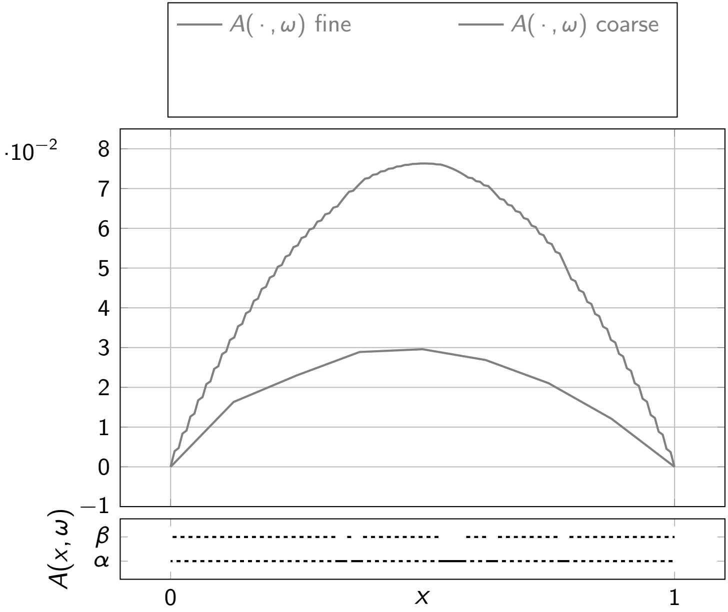

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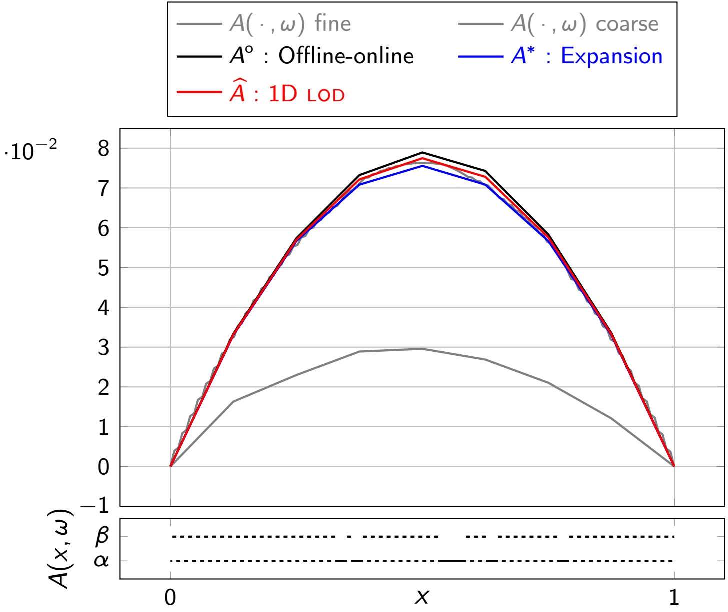

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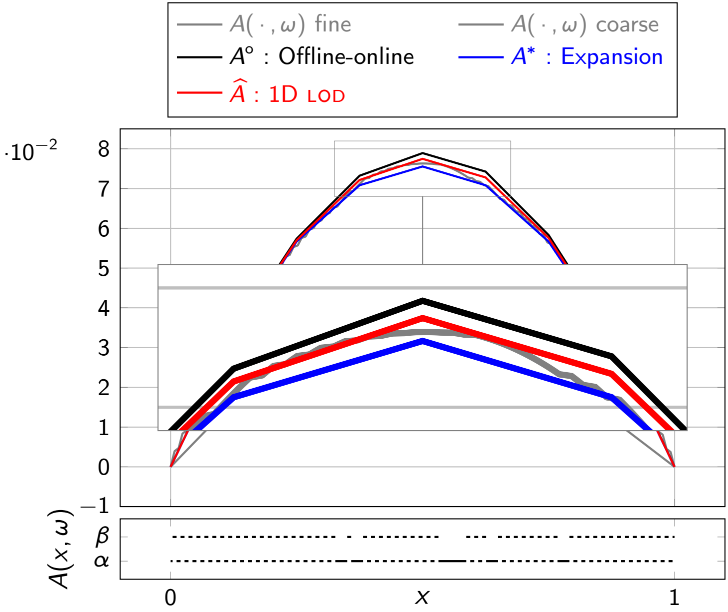

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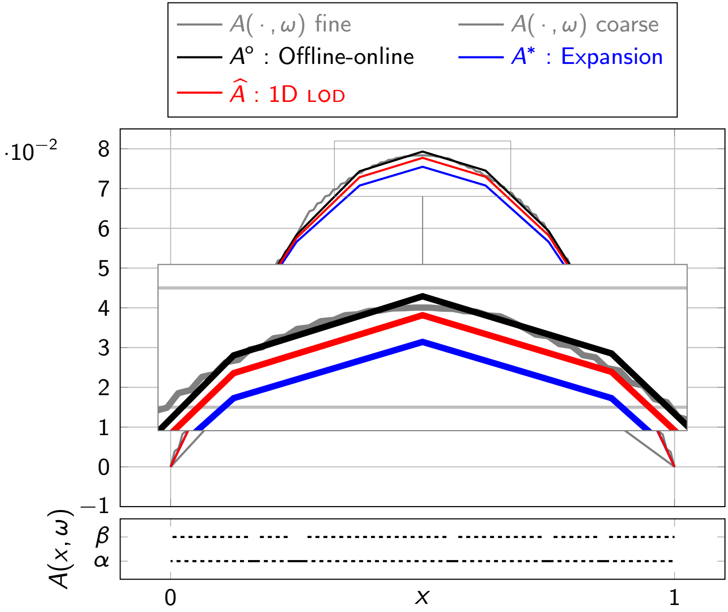

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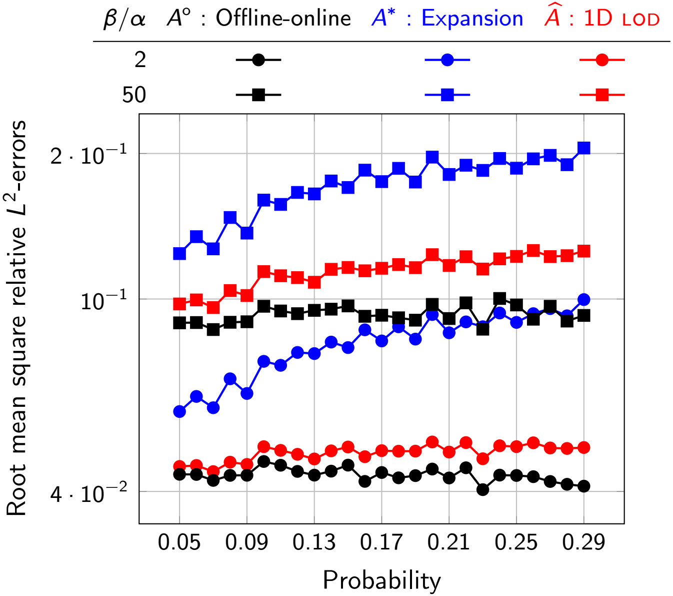
Monte-Carlo simulations



$H = 2^{-3}, \; h = 2^{-11}, \; N_{\text{samples}} = 100, \; \varepsilon = 2^{-5}$

Conclusion

What we did

1. **Implementation** of **1D** and **2D** experiments
2. **Adaptation** of the **offline-online** alg. to a subspace correction method
3. **Comparison** of strategies in **1D**

Future work

- Estimate the error $\|P - \widetilde{P}\|$ $\leftrightsquigarrow$ **Inexact** PCG method
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Thank you for your attention !