

Coefficient perturbations in diffusion equations

Internship project

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Motivation & Goal

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

Coefficient
perturbations

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Introduction

Motivation & Goal

Problem
formulation

Notations

Construction of
randomly perturbed
coefficient A

Single defect

Random
defects

Comparison of
strategies in 1D

Conclusion

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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

Coefficient
perturbations

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Introduction

Motivation & Goal

Problem
formulation

Notations

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Random
defects

Comparison of
strategies in 1D

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Problem formulation

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

Perfect coefficient

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

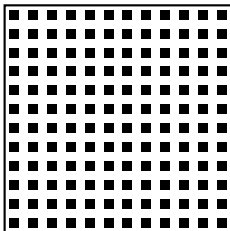
Perturbed coefficient

$$(\mathcal{P}) \left| \begin{array}{l} \text{Find } u: \Omega \rightarrow \mathbf{R} \text{ s.t.} \\ -\operatorname{div}(\mathbf{A} \nabla u) = f \quad \text{in } \Omega \\ u = 0 \quad \text{on } \partial\Omega \end{array} \right.$$

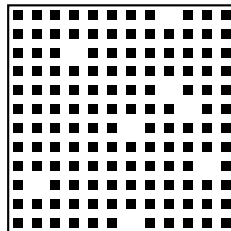
- Setting

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

- Example



\mathbf{A}_ε , perfect coefficient

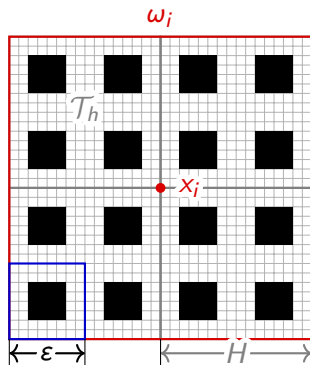


\mathbf{A} , perturbed coefficient

Notations

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

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



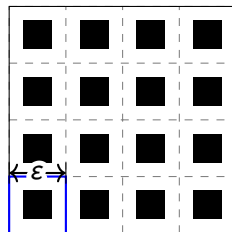
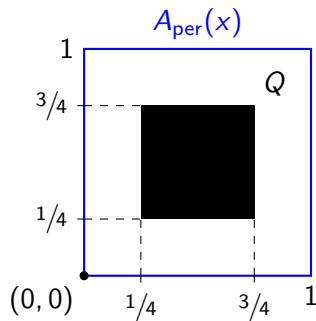
Construction of randomly perturbed coefficient A

■ Randomly perturbed coefficient

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

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

■ Example : *Sponge*



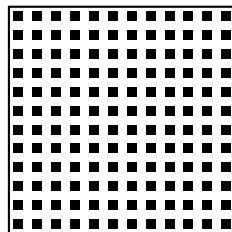
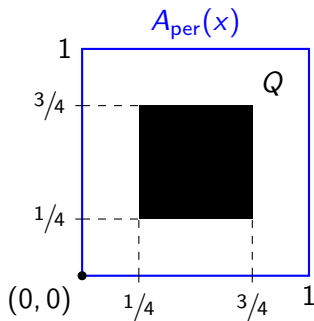
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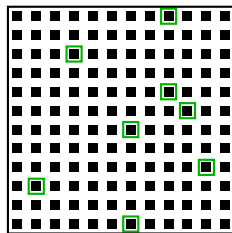
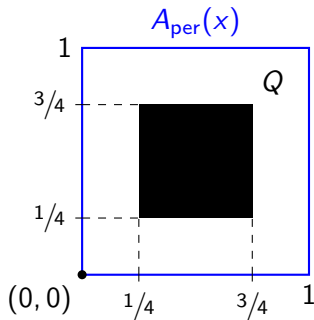
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■ Random character

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

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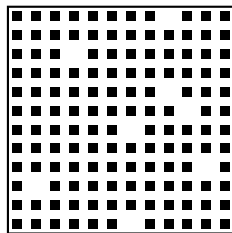
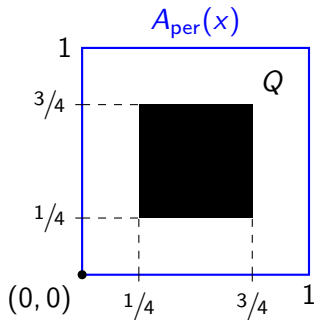
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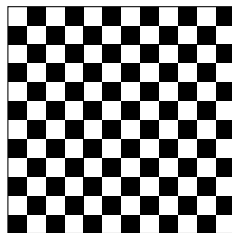
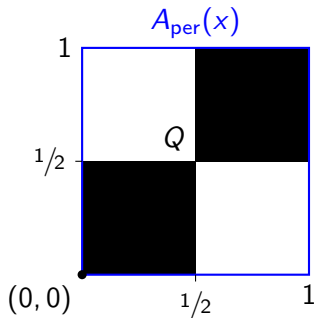
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■ Example : Checkerboard



Construction of randomly perturbed coefficient A

■ Randomly perturbed coefficient

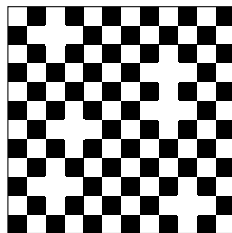
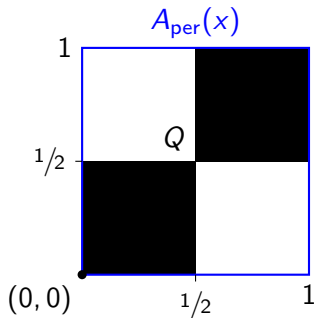
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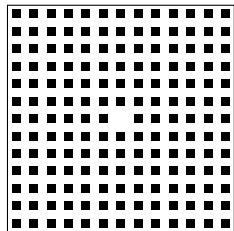
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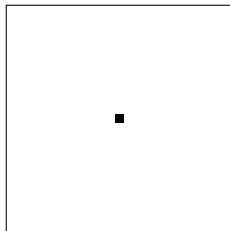


Examples of RHS configurations

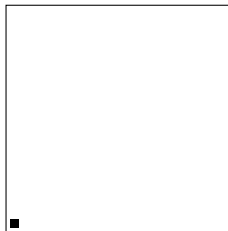
⚠ *No random defects*



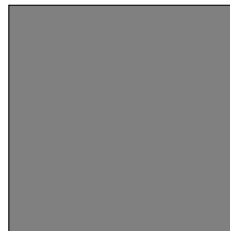
Perturbed coefficient
(sponge)



RHS **exactly in**
the defect block



RHS **far away**
from the defect block



Global RHS

Questions

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

Coefficient
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Introduction

Single defect

Examples of RHS
configurations

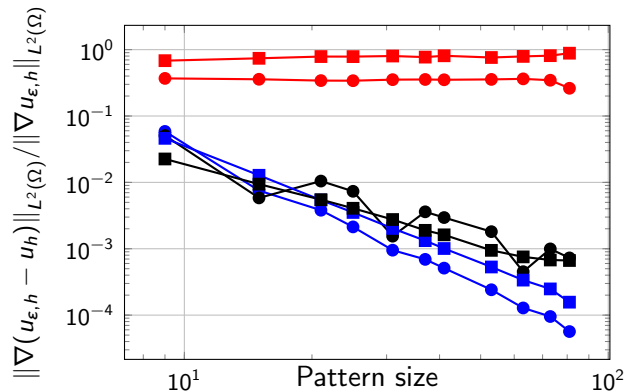
A single
non-random defect
(\mathbb{P}_1 FEM)

Random
defects

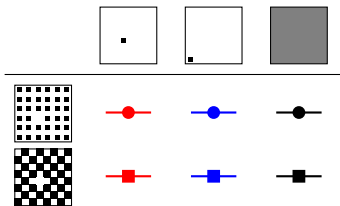
Comparison of
strategies in 1D

Conclusion

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



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



Coefficient perturbations

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Introduction

Single defect

Examples of RHS configurations

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

Random defects

Comparison of strategies in 1D

Conclusion

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**

Goal

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

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

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

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

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

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

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

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

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

Coefficient
perturbations

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Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

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

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Coefficient
perturbations

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Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

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a **good approximation** for A^{-1} ? \implies **Multipoint perturbation formula**

- Numerical experiments

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

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

$$\frac{\|\nabla(u - \tilde{u})\|_{L^2(\Omega)}}{\|\nabla u\|_{L^2(\Omega)}} \quad \text{where} \quad \tilde{u} := \sum_{i=1}^N \alpha_i u^{(i)}.$$

Coefficient
perturbations

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Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Subspace decomposition preconditioner

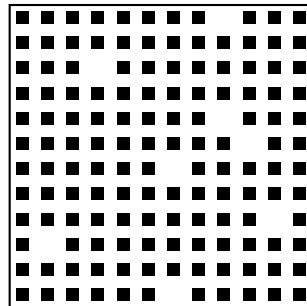
[Kornhuber & Yserentant, 2016]

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

$$\underbrace{V_0 = V_H}_{\text{coarse space}}, \quad \underbrace{V_i = \{v \in V \mid \text{supp}(v) \subset \omega_i\}}_{\text{local spaces}}.$$

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

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



Preconditioner

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

Coefficient
perturbations

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Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Subspace decomposition preconditioner

[Kornhuber & Yserentant, 2016]

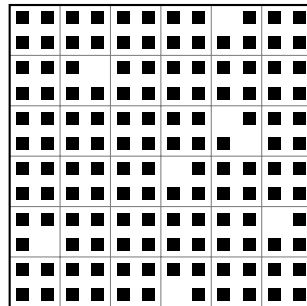
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\mathcal{T}_H



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Coefficient perturbations

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Introduction

Single defect

Random defects

Multipoint inversion formula

Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

Subspace decomposition preconditioner

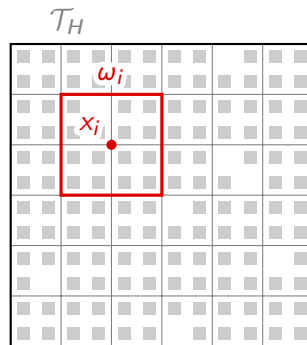
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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

Subspace decomposition preconditioner

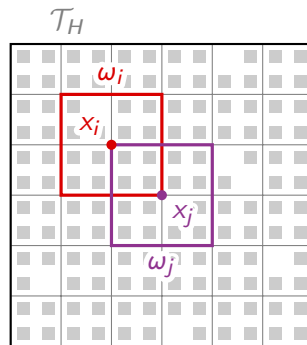
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Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Subspace decomposition preconditioner

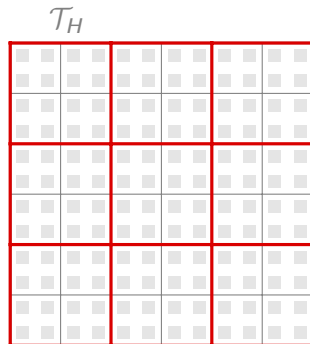
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Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Subspace decomposition preconditioner

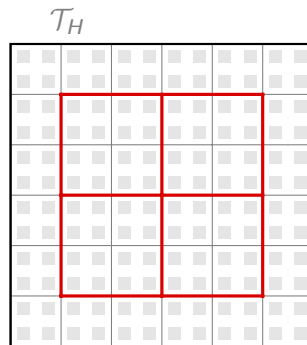
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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

Subspace decomposition preconditioner

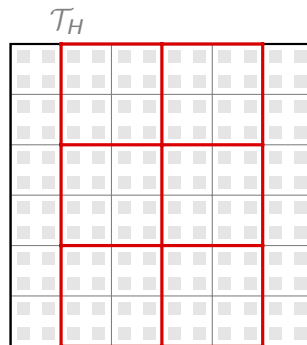
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Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Subspace decomposition preconditioner

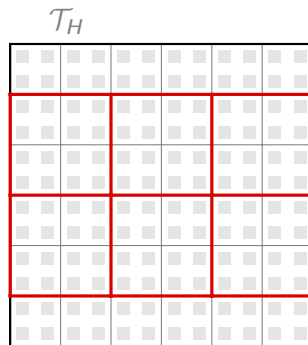
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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

Subspace decomposition preconditioner

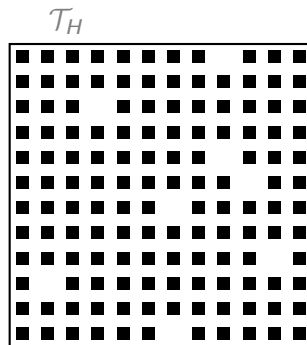
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- **Preconditioned conjugate gradient method** (PCG method)

Coefficient
perturbations

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Introduction

Single defect

Random
defects

Multipoint inversion
formula

Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

Convergence analysis [Kornhuber & Yserentant, 2016]

- Any function $v \in V$ can be decomposed into $v = v_0 + v_1 + \dots + v_n$, where $v_i \in V_i$ so that

$$\sum_{i=0}^n \|v_i\|_A^2 \leq K_1 \|v\|_A^2.$$

Achieved with $v_0 = \mathcal{I}_H v$ and $v_j = \varphi_j(v - \mathcal{I}_H v)$ where $\mathcal{I}_H: H_0^1(\Omega) \rightarrow V_H$ is an interpolation operator and $\sum_{i=1}^n \varphi_i = 1$.

- For any decomposition $v = v_0 + v_1 + \dots + v_n$:

$$\|v\|_A^2 \leq K_2 \sum_{i=0}^n \|v_i\|_A^2.$$

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

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

where $\kappa = K_1 K_2$

Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Multipoint inversion
formula

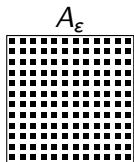
Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

Conclusion

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



Input : Problem data $A_\epsilon, B_\epsilon, Q, f$

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

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

 | Precompute $P_k^{(\ell)} : V \rightarrow V_k$ 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 $\tilde{P}_i := \sum_{\ell=0}^N \mu_\ell P_k^{(\ell)}$

end

$\tilde{P} := \tilde{P}_0 + \sum_{i=1}^n \tilde{P}_i$ and Solve PCG system

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Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Multipoint inversion
formula

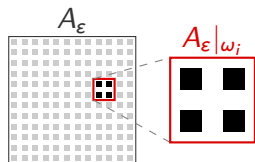
Subspace
decomposition
preconditioner

Offline-online
strategy

Comparison of
strategies in 1D

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

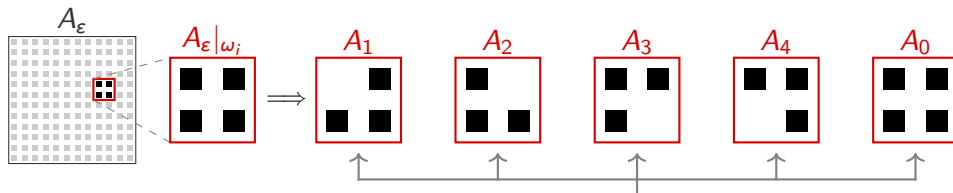
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

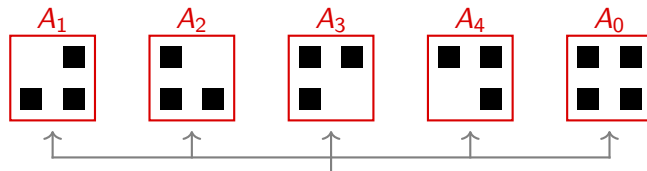
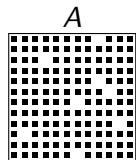
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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



Offline coefficients A_ℓ

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

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

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

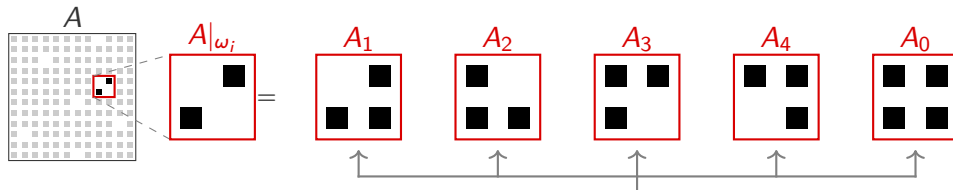
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

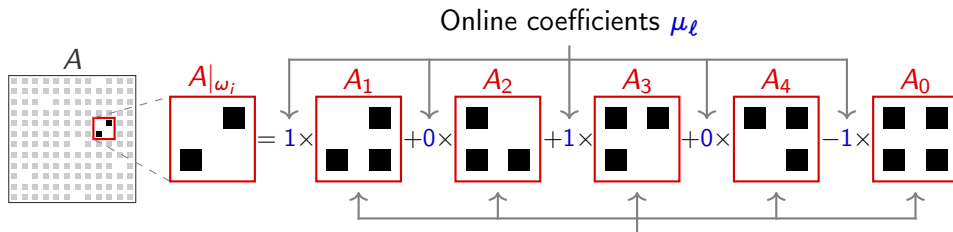
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

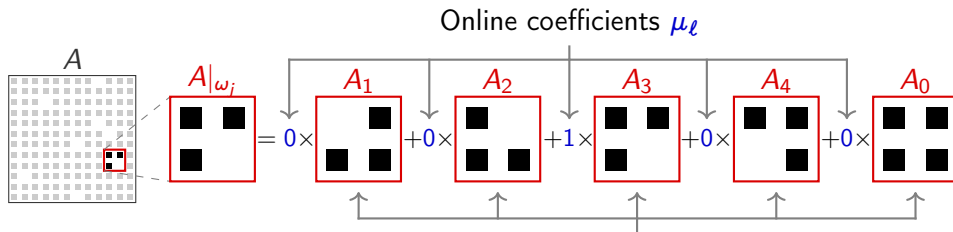
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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Offline phase

Online phase

Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

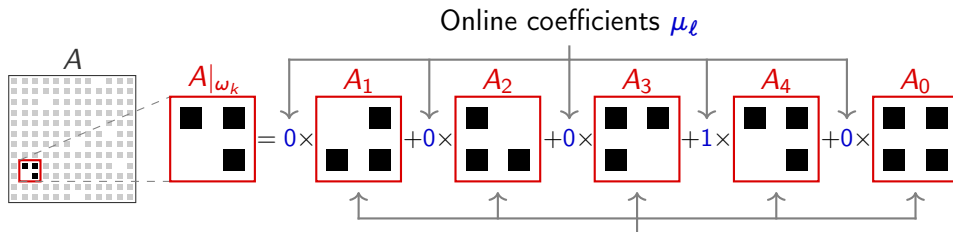
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

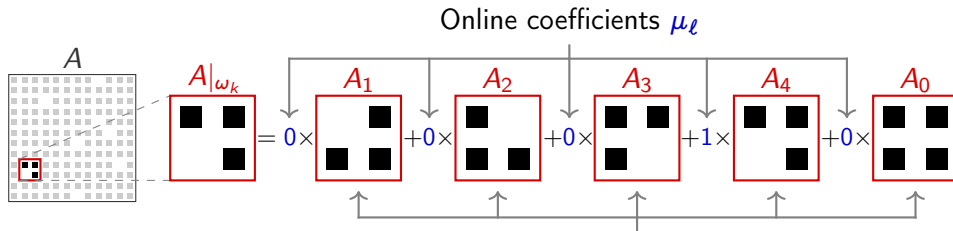
Subspace decomposition preconditioner

Offline-online strategy

Comparison of strategies in 1D

Conclusion

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



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end

for all sample coefficients A **do**

Online phase

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 Assemble $\tilde{P}_i := \sum_{\ell=0}^N \mu_\ell P_k^{(\ell)}$ **Rapid assembly**

end

$\tilde{P} := \tilde{P}_0 + \sum_{i=1}^n \tilde{P}_i$ and Solve PCG system

end

Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Multipoint inversion formula

Subspace decomposition preconditioner

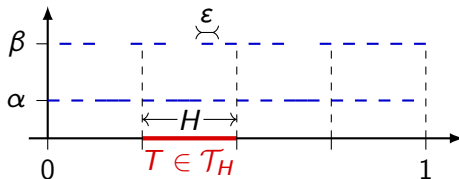
Offline-online strategy

Comparison of strategies in 1D

Conclusion

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



Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Comparison of strategies in 1D

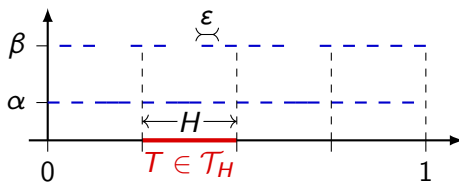
Three strategies

Monte-Carlo simulations

Conclusion

Three strategies

- ✗ Solving directly with $A(x, \omega)$ defined on a ε -scale
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Offline-online	$A^0 _T(\omega) := \mu_0 \bar{A}_{\text{per}} + \sum_{i=1}^N \mu_i \bar{A}_i$ with \bar{A}_i offline coefficients
Expansion [Anantharaman & Le Bris, 2010]	$A^* := \bar{A}_{\text{per}} + p A^e$, with $A^e = \bar{A}_{\text{per}} - \frac{\bar{A}_{\text{per}}^2}{\bar{A}}$
1D LOD	$\hat{A} _T(\omega) := \bar{A}_{\text{per}} \int_T \frac{A(x, \omega)}{A_{\text{per}}(x)} dx$

where \bar{C} is the **harmonic mean** of C

Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Comparison of
strategies in 1D

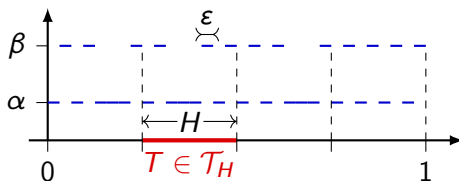
Three strategies

Monte-Carlo
simulations

Conclusion

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where \bar{C} is the **harmonic mean** of C

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

Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

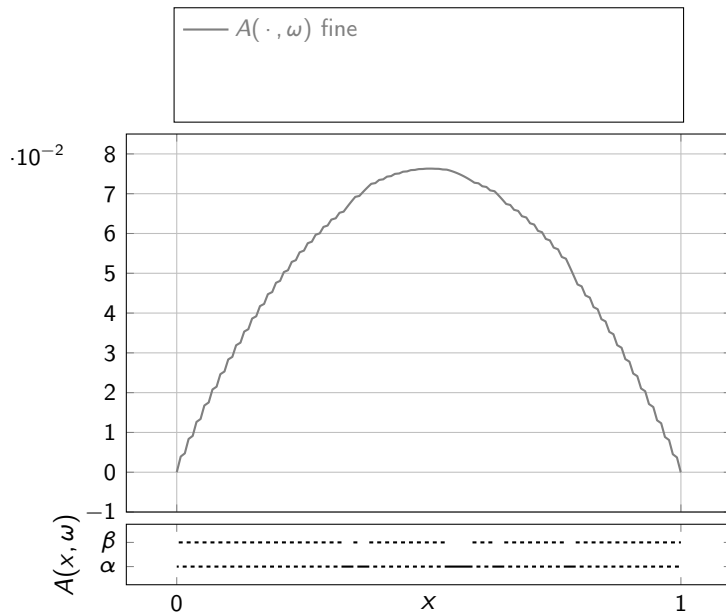
Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Three strategies



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

Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

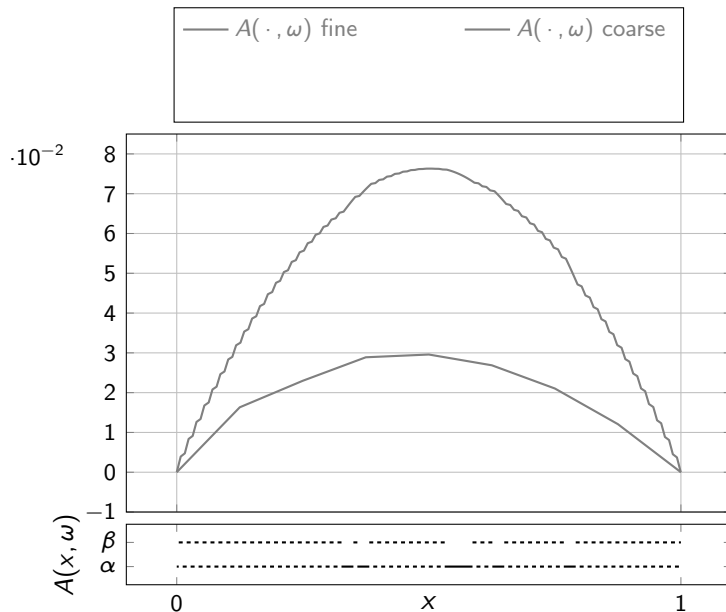
Comparison of
strategies in 1D

Three strategies

Monte-Carlo
simulations

Conclusion

Three strategies



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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

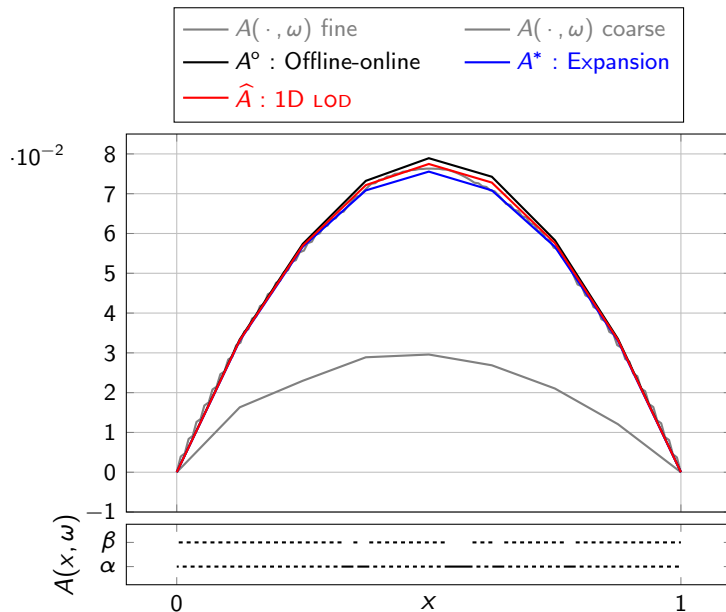
Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Three strategies



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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

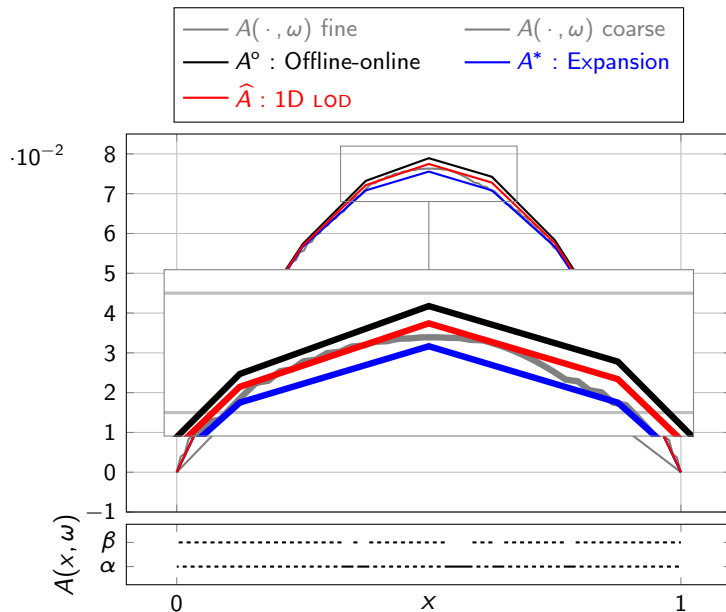
Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Three strategies



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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

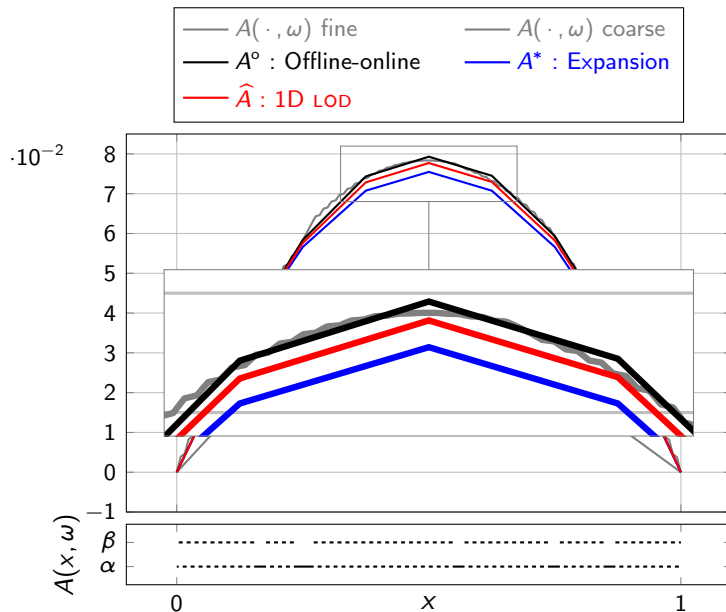
Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Three strategies



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Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

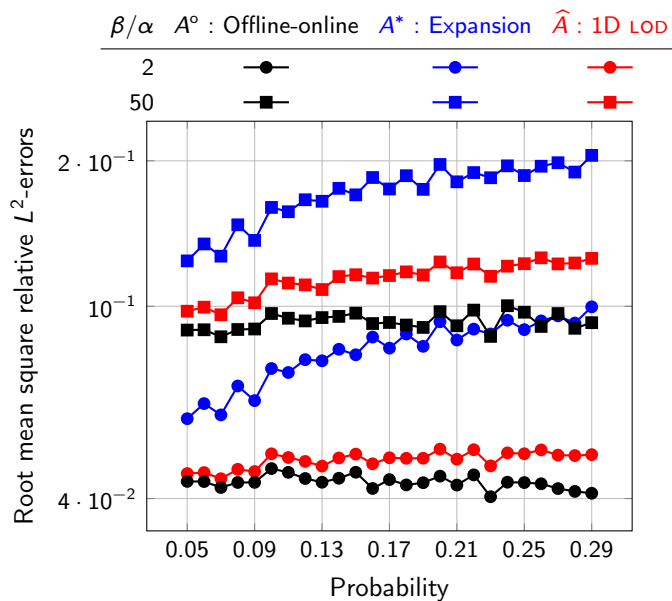
Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Monte-Carlo simulations



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

Coefficient perturbations

A. WAYOFF

Introduction

Single defect

Random defects

Comparison of strategies in 1D

Three strategies

Monte-Carlo simulations

Conclusion

Conclusion

Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Comparison of
strategies in 1D

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 $\|P - \tilde{P}\| \leftrightarrow$ **Inexact** PCG method
- Clarify link with the **Multipoint inversion formula**
- **Implement** the **offline-online** algorithm

Conclusion

Coefficient
perturbations

A. WAYOFF

Introduction

Single defect

Random
defects

Comparison of
strategies in 1D

Conclusion

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Thank you for your attention !