Generalised Multiscale FEs:
Efficient Offline/Online HPC Implementation

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Outline

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Multiscale problems

Many scientific/engineering problems involve multiscale phenomena:

- Flow and transport in **porous media**,
- Turbulent flows at **high Reynolds numbers**,
- Physical processes in **composite materials**.

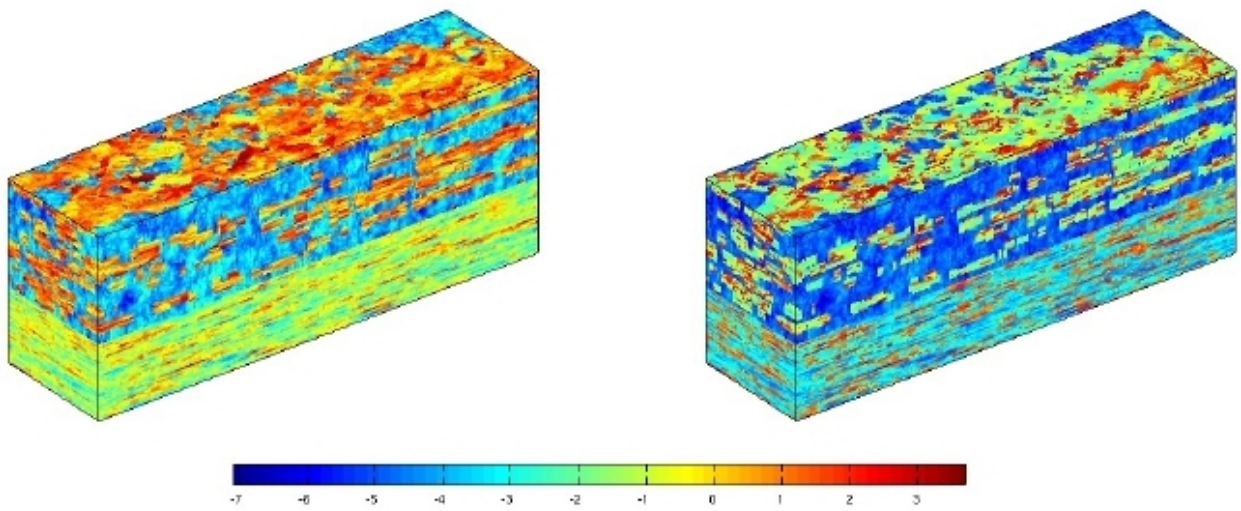

Figure: Oil reservoir exploration (SPE10 benchmark)

Structural Engineering (composites & additive manufacturing)

Linear elasticity equations:

$$a(\mathbf{u},\mathbf{v}) := \int_\Omega C(\mathbf{x})\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v})\,\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{f}\cdot\mathbf{v}\,\mathrm{d}\mathbf{x} + \int_\Gamma (\sigma\cdot\mathbf{n})\cdot\mathbf{v}\;d\mathbf{x} \quad \forall \mathbf{v}\in V$$

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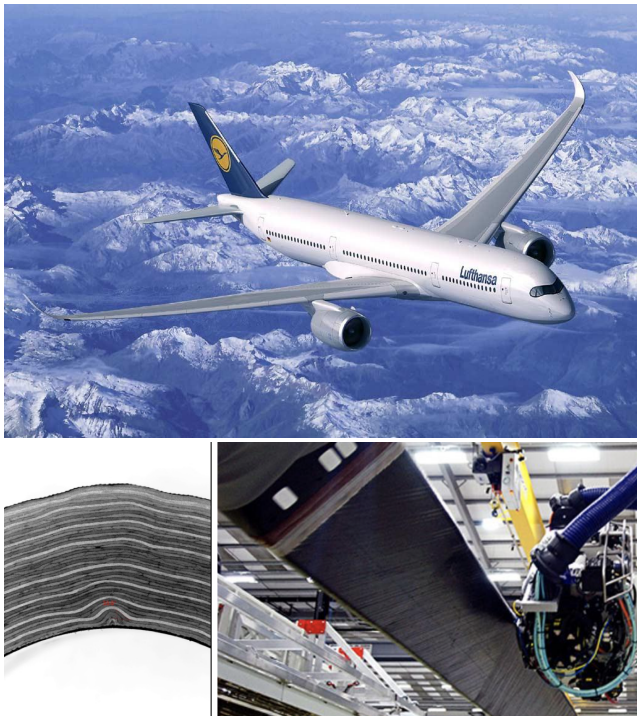
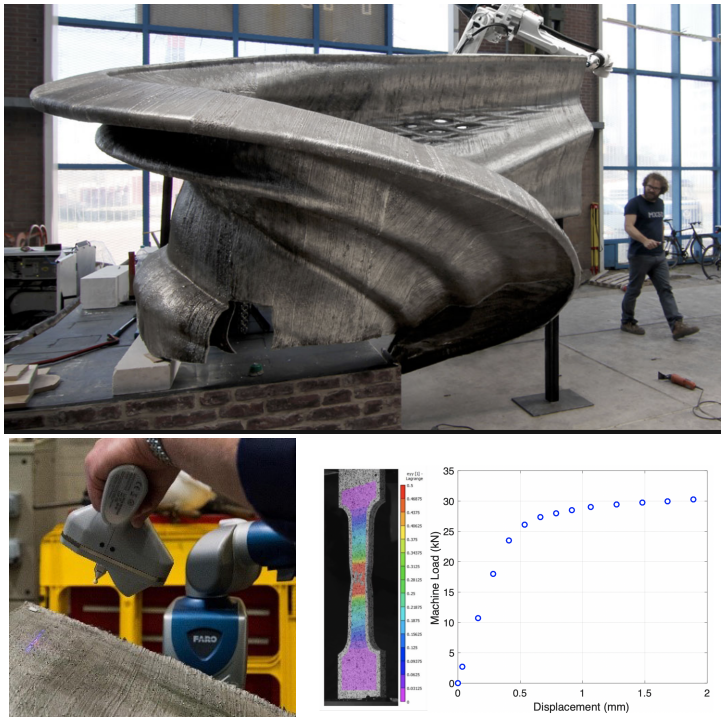
small length scales (<mm), **high contrast** and **strongly anisotropic**



CERTEST (EPSRC Project, UK)



STEAM (Turing/Royce Project)

Why not use standard FEMs for such problems?

Illustrating Example: Steady-state diffusion in heterogeneous medium

$$-\mathrm{div}(A\nabla u) = f \qquad \text{in} \quad \Omega \qquad + \text{BCs},$$

By Cea's lemma, for classical, conforming FEs, we have

$$\|u - u_h\|_{H^1(\Omega)} \leq C \inf_{v \in V_h} \|u - v\|_{H^1(\Omega)}.$$

Accuracy depends solely on the approximation properties of the FE space.

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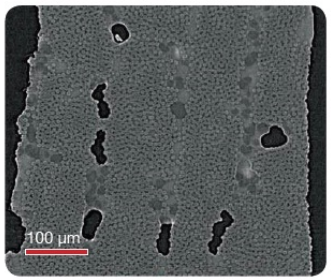
Accuracy depends solely on the approximation properties of the FE space.

If the coefficient $A \in L^\infty(\Omega)$ is strongly varying on fine scale, then

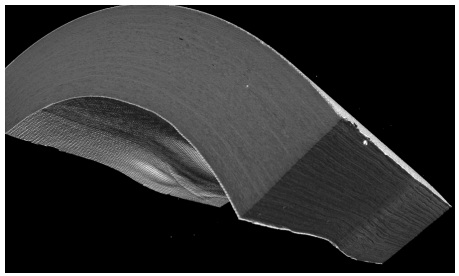
- **theoretically:** $u \notin H^2(\Omega)$ (in general) and it is difficult to obtain an explicit convergence rate for classical FEs;
- **numerically:** a sufficiently small h is required to achieve an acceptable accuracy, leading to **huge computational cost**.

Two Possible Aims

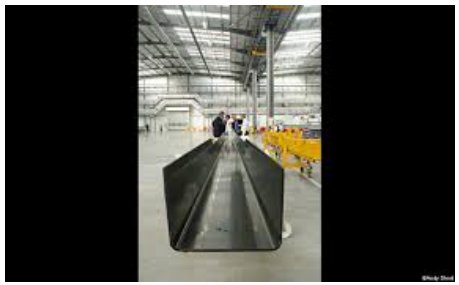
- Complicated variation of $A(x)$ on many scales ($h \ll \mathrm{diam}(\Omega)$)
  Hard to **resolve** by "geometric" **coarse** mesh, e.g.



Ply with individual fibres



Coupon with defect



whole wing spar

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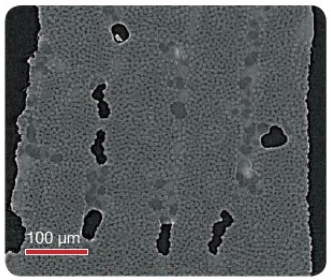

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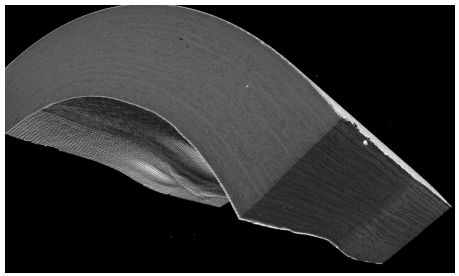

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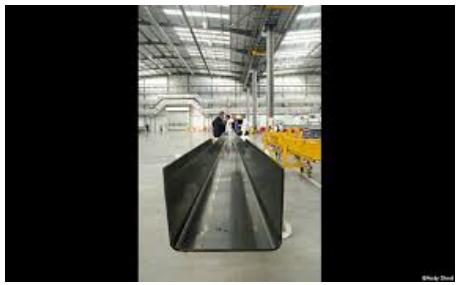

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- **Goal A:** Efficient, scalable multilevel parallel solver Peter's Talk
  - **robust** w.r.t. mesh size h + coefficient variation $A(x)$ **!**

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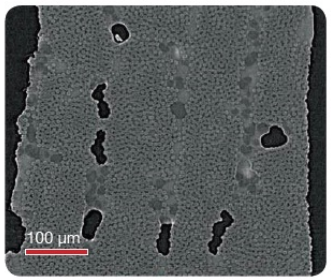

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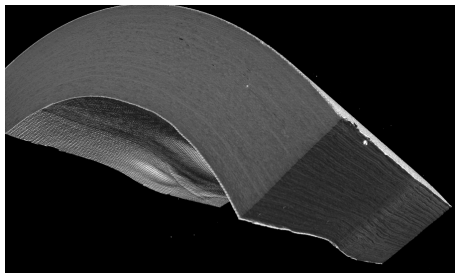

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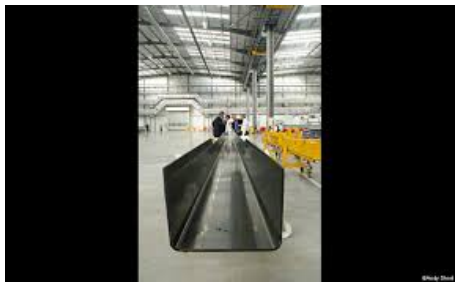

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  - Discretisation in **bespoke** (adapted) A-dependent space V^H

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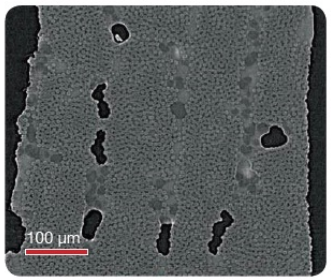

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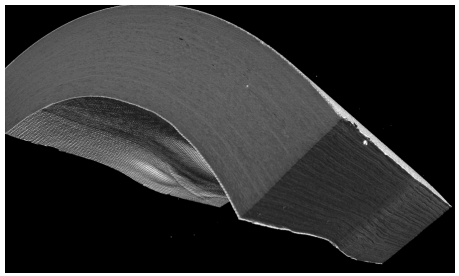

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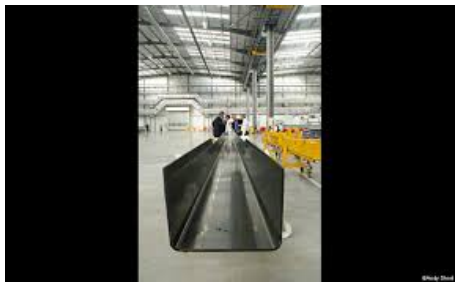

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- **Goal B:** Simulate on coarse mesh where $A(x)$ is **not resolved !**
  - Discretisation in **bespoke** (adapted) A-dependent space V^H
- **Key Question** (for both): **Robust coarse space**

(coefficient-robust theory for **Goal B** much less well developed)

Multiscale methods

Multiscale methods are effective techniques to reduce computational cost by incorporating fine-scale information into coarse-scale models.

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Traditionally: Asymptotic homogenization (Lions, Olenik, Allaire,...)

Various multiscale methods (initially focussing only on related ones):

1. Multiscale Finite Element Method (MsFEM) (Hou, Wu, Efendiev,...)
2. Generalized Multiscale FE Method (GMsFEM) (Hou, Efendiev,...)
3. Localized Orthogonal Decomposition (LOD) (Peterseim, Malqvist,...)
4. *Multiscale Spectral Generalized FE Method (MS-GFEM)*
   [**Babuska & Lipton**, *Multiscale Model Sim (SIAM)* **9**, 2011], ...

All these are based on enriching FE space with pre-computed multiscale basis functions containing fine-scale information of the solution.

Other Types of Multiscale Methods

- Adaptive FEs ..., [Babuska, Rheinboldt, 1978]
- Generalised FEs [Babuska, Osborn, 1983]
- Numerical Upscaling ..., [Durlofsky, 1991]
- Variational Multiscale Method [Hughes et al, 1998]
- Multigrid Based Upscaling [Moulton, Dendy, Hyman, 1998]
- Multiscale Finite Volume Methods [Jenny, Lee, Tchelepi, 2003]
- Heterogeneous Multiscale Method [E, Engquist, 2003]
- Multiscale Mortar Spaces [Arbogast, Wheeler et al, 2007]
- Adaptive Multiscale FVMs/FEs [Durlovsky, Efendiev, Ginting, 2007]
- Energy minimising bases [Dubois, Mishev, Zikatanov, 2009]
- ... etc ...

Some Context

- Construction of robust multiscale FE spaces is **very expensive** for **general** coefficients!
- Unless we can **reuse** (most parts of) the space **multiple times** (particular structure, multiple RHS, optimisation, uncertainty quantif.,...) **no clear gains** over efficient, scalable multilevel parallel solver!
- **Important** to define **context** and to embed it in an **efficient** offline/online, adaptive, multi-level scheme!
- Also strong links to **local model order reduction methods** [Smetana, Patera, 2016], [Buhr, Smetana, 2018],...

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TODAY: Novel spectral GFEM, novel analysis & implementation

Coefficient-robust theory for **multiscale approximation** without periodicity or scale separation & links to **multilevel domain decomposition preconditioners**.

Problem formulation

Find $u \in H^1_{qD}(\Omega)$ such that $(\Omega \subset \mathbb{R}^d,\ d = 2, 3,$ bdd. with $\partial\Omega$ Lipschitz$)$

$$a(u, v) = F(v), \quad \forall v \in H^1_{0D}(\Omega),$$

where

$$H^1_{qD}(\Omega) = \{v \in H^1(\Omega) \ : \ v = q(\boldsymbol{x}) \ \text{ on } \ \partial\Omega_D\},$$

and the bilinear form $a(\cdot, \cdot)$ and the functional F are defined by

$$a(u, v) = \int_\Omega A(\boldsymbol{x}) \nabla u \cdot \nabla v \, d\boldsymbol{x}, \quad F(v) = \int_{\partial\Omega_N} g v \, d\boldsymbol{s} + \int_\Omega f v \, d\boldsymbol{x}.$$

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Coefficient $A(\boldsymbol{x}) \in L^\infty(\Omega)^{d\times d}$ assumed SPD w. $0 < a_{\min} < a_{\max} < \infty$ s.t.

$$a_{\min}|\boldsymbol{\xi}|^2 \leq A(\boldsymbol{x})\boldsymbol{\xi} \cdot \boldsymbol{\xi} \leq a_{\max}|\boldsymbol{\xi}|^2 \quad \forall \boldsymbol{\xi} \in \mathbb{R}^d, \quad \boldsymbol{x} \in \Omega.$$

No a priori regularity, periodicity or scale separation of A assumed!

Outline

Generalized Finite Element Method (GFEM)

Key features

- Extension of the FEM based on domain decomposition and a partition of unity (PoU) approach.
- GFEMs consist of three steps:
  1. Construct local spaces with good approximation properties;
  2. Glue together local spaces by PoU to form global approximation;
  3. Solve the problem over the global approximation space.
- Global error fully determined by local approximation errors.
- Allows design of **special approximation spaces** tailored to particular problem.

Generalized Finite Element Method (GFEM)

Partition of Unity

- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and $\{\omega_i\}_{i=1}^M$ be an open cover of Ω satisfying a pointwise overlap condition, i.e.

$$\text{each } x \in \Omega \text{ is in } \textbf{at most } \kappa \text{ subdomains } \omega_i .$$

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Definition (Partition of Unity)

A set of functions $\{\chi_i\}_{i=1}^M$ is called a (sufficiently smooth) **partition of unity** subordinate to the open cover $\{\omega_i\}_{i=1}^M$ w. $H_i = \text{diam}(\omega_i)$ if

$$0 \leq \chi_i(\boldsymbol{x}) \leq 1, \quad \sum_{i=1}^{M} \chi_i(\boldsymbol{x}) = 1, \quad \forall\, \boldsymbol{x} \in \Omega,$$

$$\chi_i(\boldsymbol{x}) = 0, \quad \forall\, \boldsymbol{x} \notin \omega_i, \ i = 1, \cdots, M,$$

$$\chi_i \in C^1(\omega_i), \quad \max_{i=1,\ldots,M} \left(H_i \|\nabla \chi_i\|_\infty\right) \leq C_1$$

Local and global approximation spaces

Given an open cover $\{\omega_i\}_{i=1}^M$ of Ω with partition of unity $\{\chi_i\}_{i=1}^M$:

each $\boldsymbol{x}$ in $\leq \kappa$ subdomains ω_i $\qquad$ $\sum_i \chi_i(\boldsymbol{x}) = 1$ and $\max_i H_i \|\nabla \chi_i\|_\infty \leq C_\chi$

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- Choose local particular solutions $u_i^p \in H^1(\omega_i)$ to satisfy $u_i^p = q$ on $\partial\omega_i^* \cap \partial\Omega_D$ and $u_i^p = 0$ otherwise on $\partial\omega_i^*$
  (for an oversampling domain $\omega_i^* \supseteq \omega_i$ defined below)
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Global particular function u^p and trial space $S_n(\Omega)$ then defined as:

$$u^p := \sum_{i=1}^M \chi_i u_i^p \in H^1_{qD}(\Omega), \quad S_n(\Omega) := \left\{ \sum_{i=1}^M \chi_i \phi_i \ : \ \phi_i \in S_{n_i}(\omega_i) \right\}.$$

The approximate (Galerkin) solution $u^G = u^p + u^s$ is then sought such that $u^s \in S_n(\Omega) \subset H^1_{0D}(\Omega)$ (n-dimensional).

New Global Approximation Theorem

Theorem (Ma, **RS**, Dodwell, 2021)

Assume that there exists $\phi_i \in S_{n_i}(\omega_i)$, $i = 1, \cdots, M$, *such that*

$$\|\chi_i(u - u_i^p - \phi_i)\|_{a,\omega_i} \leq \varepsilon_i \|u\|_{a,\omega_i^*},$$

where $\omega_i \subset \omega_i^* \subset \Omega$ *and* $\|v\|_a := \sqrt{a(v,v)}$. *Let* $u^F = u^p + \sum_{i=1}^{M} \chi_i \phi_i$.

Then $u^F \in H^1_{qD}(\Omega)$ *and*

$$\|u - u^F\|_a \leq \sqrt{\kappa\kappa^*} \left(\max_{i=1,\cdots,M} \varepsilon_i \right) \|u\|_a.$$

Here we assume that each point $\boldsymbol{x} \in \Omega$ *belongs to at most* κ^* *subdomains* ω_i^*.

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Traditional GFEM [Melenk, Babuska, 1996], [Babuska, Lipton, 2011]:

- Exact solution u and **not** $\chi_i u$ is approximated in each subdomain ω_i.
- Need to have bounds on local L^2- and H^1-error.

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Roadmap for local approximation

- Introduce oversampling domain ω_i^* s.t. $\omega_i \subseteq \omega_i^* \subset \Omega$
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- Decompose u into two orthogonal parts w.r.t. $a(\cdot,\cdot)$:
  1. Particular solution ψ_i that satisfies the PDE locally
     (subject to homogeneous Dirichlet BCs $\psi_i(\boldsymbol{x}) = 0$ on $\partial\omega_i^*$):
     $$-\mathrm{div}(A(\boldsymbol{x})\nabla\psi_i(\boldsymbol{x})) = f(\boldsymbol{x}), \quad \text{for } \boldsymbol{x} \in \omega_i^* .$$
  2. Locally a-harmonic part in
     $$H_A(\omega_i^*) = \left\{ v \in H^1(\omega_i^*) \,:\, a_{\omega_i^*}(v,\varphi) = 0 \;\; \forall \varphi \in H_0^1(\omega_i^*) \right\}.$$

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- To **approximate optimally** the a-harmonic part:
  1. associate this with a **compact operator** related to the PoU function and finding its Kolmogorov n-width;
  2. construct an optimal approximation space based on its SVD.

The compact operator

- We introduce the operator $P : H_{A,0}(\omega_i^*) \to H_0^1(\omega_i)$ such that

$$Pv(\boldsymbol{x}) = \chi_i(\boldsymbol{x})v(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \omega_i, \quad \forall v \in H_{A,0}(\omega_i^*)\,,$$

  where χ_i is the PoU function supported on ω_i and

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$$Pv(x) = \chi_i(x)v(x), \quad \forall x \in \omega_i, \quad \forall v \in H_{A,0}(\omega_i^*),$$

where χ_i is the PoU function supported on ω_i and

$$H_{A,0}(\omega_i^*) = \{v \in H_A(\omega_i^*) \,:\, a_{\omega_i}(\chi_i v, \chi_i) = 0\}.$$

- Since $H^1(\omega_i^*) \subset\subset L^2(\omega_i^*)$, it follows from the following Caccioppoli-type inequality that P is a compact operator:

Lemma (Caccioppoli-type inequality)

Assume that $\eta \in W^{1,\infty}(\omega_i^*) \cap H_0^1(\omega_i^*)$ *and* $v \in H_A(\omega_i^*)$. *Then*

$$\|\eta v\|_{a,\omega_i^*}^2 = \int_{\omega_i^*} (A\nabla\eta \cdot \nabla\eta) v^2 \, dx \;\leq\; a_{\max} \|\nabla\eta\|_{L^\infty(\omega_i^*)}^2 \|v\|_{L^2(\omega_i^*)}^2 .$$

Recall: $a_{\max}$ = spectral upper bound of A and $\|\nabla\chi_i\|_{L^\infty} \leq C_\chi H_i^{-1}$

Kolmogorov n-width

Finding the optimal n-dim'l subspace $\widehat{Q}(n)$ to approximate the range $PH_{A,0}(\omega_i^*)$ in $H_0^1(\omega_i)$ is equivalent to finding the **Kolmogorov n-width d_n** of the compact operator P, i.e.

$$d_n := \inf_{Q(n)} \sup_{u \in H_A(\omega_i^*)/\mathbb{R}} \inf_{v \in Q(n)} \frac{\|Pu - v\|_{a,\omega_i}}{\|u\|_{a,\omega_i^*}}.$$

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Theorem (A. Pinkus, 1985)

The optimal approximation space associated with the Kolmogorov n-width is given by $\widehat{Q}(n) = \operatorname{span}\{Pv_1, \cdots, Pv_n\}$ and $d_n = \sqrt{\mu_{n+1}}$, where $\{v_k\}$ and $\{\mu_k\}$ denote the eigenfunctions and eigenvalues of the problem

$$P^*Pv = \mu v\,.$$

Local particular sol'n & optimal approxim'n space

Theorem

Let the local particular solution & the local approximation space on ω_i *for the GFEM be defined as*

$$u_i^p := \psi_i|_{\omega_i}, \quad S_n(\omega_i) := \operatorname{span}\{v_1|_{\omega_i}, \cdots, v_n|_{\omega_i}\},$$

where v_k *denotes the* k*-th eigenfunction of the (***GenEO-type***) eigenproblem* **[Spillane et al, 2014]**

$$a_{\omega_i^*}(v, \varphi) = \lambda\, a_{\omega_i}(\chi_i v, \chi_i \varphi), \quad \forall \varphi \in H_A(\omega_i^*).$$

Then, there exists a $\phi_i \in S_n(\omega_i)$ *such that*

$$\|\chi_i(u - u_i^p - \phi_i)\|_{a,\omega_i} \leq d_n \|u\|_{a,\omega_i^*},$$

where u *is the exact solution of the elliptic equation and* $d_n = \lambda_{n+1}^{-1/2}$.

Bounding the local error

By assuming that ω_i and ω_i^* are concentric cubes of side lengths H_i and H_i^* ($H_i^* > H_i$), respectively, we have

Theorem (Ma, **RS**, Dodwell, 2021)

For $\epsilon \in (0, \frac{1}{d+1})$, there exists an $N_\epsilon > 0$, such that for any $n > N_\epsilon$

$$d_n = \lambda_{n+1}^{1/2} \leq \underbrace{\left(C_\chi e^2 e^{-n^{(\frac{1}{d+1}-\epsilon)} h(H_i/H_i^*)} \right)}_{} \underbrace{\left(e^{-n^{(\frac{1}{d+1}-\epsilon)}} \right)}_{},$$

where we recall that $H_i \|\nabla \chi_i\|_\infty \leq C_\chi$

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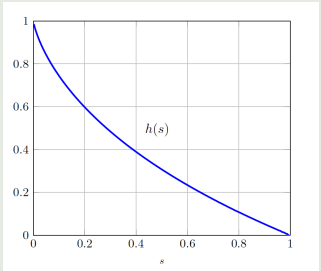

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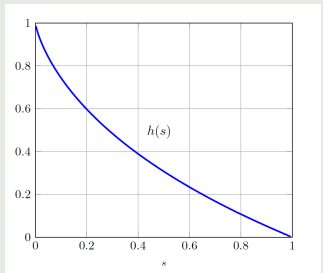

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With γ_d denoting the volume of the unit ball in $\mathbb{R}^d$, we explicitly have

$$N_\epsilon \leq \left(3e \frac{\gamma_d^{1/d}}{\sqrt{\pi}} \left(\frac{a_{\max}}{a_{\min}} \right)^{1/2} \frac{H_i^*}{H_i^* - H_i} \right)^{\frac{d}{\epsilon(1+d)}} + 1.$$

Remarks on new error bound

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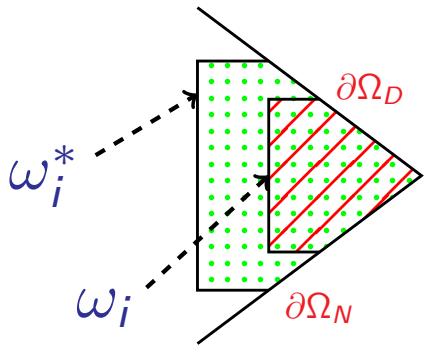
- **Ongoing work:** Reduce dependence on $a_{\max}/a_{\min}$ in N_ϵ.

Boundary subdomains

- **Same results** for subdomains ω_i that intersect the (global) boundary $\partial\Omega$, but this requires additional work. I will **skip this!**
- Again an oversampling domain is introduced s.t. $\omega_i \subseteq \omega_i^* \subset \Omega$:



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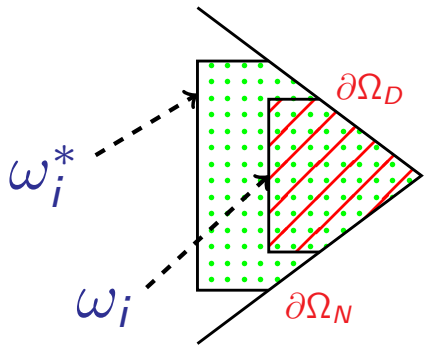

- We **only** require $\partial\Omega$ to be **Lipschitz**. For **mixed BCs**, we need to compute **two** local particular solutions.

The **analysis** in [Babuska, Lipton, 2011] does not extend to mixed BCs!

Due to harmonic extension [Babuska, Lipton '11] need to assume $\partial\Omega \in C^1$

Outline

Finite element (FE) discretisation

- Take a conforming FE space V_h in $H^1(\Omega)$ w.r.t. a mesh $\mathcal{T}_h$ with mesh size h small enough to resolve all fine-scale details of $A(\boldsymbol{x})$.

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- The local approximation space (again interior only) is defined as

$$S_{h,n_i}(\omega_i) = \operatorname{span}\{\phi^i_{h,1}|_{\omega_i}, \cdots, \phi^i_{h,n_i}|_{\omega_i}\},$$

where $\{\phi^i_{h,j}\}_{j=1}^{n_i}$ are the eigenfcts. of the **GenEO-type** problem

$$a_{\omega_i^*}(\phi, v) = \lambda \, a_{\omega_i}(\chi_i \phi, \chi_i v), \quad \forall \, v \in W_h(\omega_i^*).$$

and

$$W_h(\omega_i^*) = \{u \in V_{h,0}(\omega_i^*) : a_{\omega_i^*}(u, v) = 0, \, \forall v \in V_{h,0}(\omega_i^*)\}.$$

Discrete MS-GFEM

- Define the global particular function and the trial space as

$$u_h^p := \sum_{i=1}^{M} \chi_i u_{h,i}^p \quad , \quad S_h(\Omega) := \left\{ \sum_{i=1}^{M} \chi_i v_i : \ v_i \in S_{h,n_i}(\omega_i) \right\}.$$

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$$a(u_h^s, \, v) = F(v) - a(u_h^p, v), \quad \forall v \in S_h(\Omega).$$

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- Discrete local orthogonal decomposition:

$$u_h^e|_{\omega_i^*} - \psi_{h,i} \in W_h(\omega_i^*), \quad a_{\omega_i^*}(u_h^e|_{\omega_i^*} - \psi_{h,i}, \, \psi_{h,i}) = 0.$$

u_h^e is fine-scale solution; $W_h(\omega_i^*)$ is **discrete** a-**harmonic** space.

Optimal local approximation spaces (discrete version)

Theorem

Let $\lambda_{h,k}$ and $\phi_{h,k}$ be the k-th eigenvalue and eigenfunction of the discrete GenEO-type eigenproblem. The n-width $d_n(\omega_i, \omega_i^*) = \lambda_{h,n+1}^{-1/2}$ and the optimal approximation space is given by

$$\hat{Q}(n) = \operatorname{span}\{\chi_i \phi_{h,1}, \cdots, \chi_i \phi_{h,n}\} = \chi_i \, S_{h,n}(\omega_i).$$

In addition, there exists a $\xi_i \in S_{h,n}(\omega_i)$ such that

$$\|\chi_i(u_h^e - u_{h,i}^p - \xi_i)\|_{a,\omega_i} \leq d_n(\omega_i, \omega_i^*) \, \|u_h^e\|_{a,\omega_i^*}.$$

Equivalently, $\|\chi_i(u_h^e - u_{h,i}^p - \xi_i)\|_{a,\omega_i} \leq \lambda_{h,n+1}^{-1/2} \, \|u_h^e\|_{a,\omega_i^*}.$

$$P_{h,i}^* P_{h,i} \, \phi_h = \mu_h \phi_h \quad \overset{\lambda_h = \mu_h^{-1}}{\Longleftrightarrow} \quad a_{\omega_i^*}(\phi_h, v) = \lambda_h \, a_{\omega_i}(\chi_i \phi_h, \chi_i v).$$

Error bound of the discrete MS-GFEM

Theorem

Let u^e and u_h^e be the weak solution and fine-scale FE approximation of the model problem, resp, and let u_h^G be the discrete MS-GFEM approximation. Then,

$$\left\| u^e - u_h^G \right\|_a \leq \| u^e - u_h^e \|_a + \sqrt{\kappa \kappa^*} \Big(\max_{i=1,\cdots,M} \lambda_{h,n_i+1}^{-1/2} \Big) \| u_h^e \|_a,$$

where λ_{h,n_i+1} is the (n_i+1)-th eigenvalue of the discrete eigenproblem.

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- An equivalent error bound is

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- By implementing the method on a sufficiently fine mesh, we only need focus on the local approximation errors.

Roadmap for convergence analysis

- The local approximation errors in the discrete MS-GFEM are bounded by $\lambda_{h,n_i+1}^{-1/2}$, or the n-widths $d_n(\omega_i, \omega_i^*)$.

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  1. We prove that

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  2. We prove **directly** that the n-width $d_n(\omega_i, \omega_i^*)$ decays nearly exponentially with respect to n if h is sufficiently small.

Continuous and discrete operators

- Define the operator $T = P^*P : H_{A,D}(\omega^*) \to H_{A,D}(\omega^*)$ such that for each $u \in H_{A,D}(\omega^*)$, $Tu \in H_{A,D}(\omega^*)$ satisfies

$$a_{\omega^*}(Tu, v) = a_\omega(\chi u, \chi v), \quad \forall v \in H_{A,D}(\omega^*).$$

$P : H_{A,D}(\omega^*) \to H^1_{D,I}(\omega^*)$ is defined as $Pv = \chi v$.

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- T, T_h $(0 < h \leq 1)$ are positive, self-adjoint, compact operators.

Convergence of the eigenvalues

The convergence analysis is **challenging**:

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Theorem

Let $\mu_{h,k}$ and μ_k be the eigenvalues of the operators T_h and T, resp. For each $k \in \mathbb{N}$,

$$\mu_{h,k} \to \mu_k, \quad \text{as} \quad h \to 0.$$

Explicit convergence rate (under some further assumptions):

$$|\mu_k - \mu_{h,k}| \leq Ch.$$

- Proof is based on abstract theoretical framework developed in the context of homogenization theory [Jikov, Kozlov, Olenik 2012].

Upper bound for the n-width

- We assume that ω and ω^* are (truncated) concentric cubes with side lengths H and H^*, respectively.

Theorem (Nearly exponential decay)

For $\epsilon \in (0, \frac{1}{d+1})$, there exists an $n_\epsilon > 0$, such that for any $n > n_\epsilon$, if h is sufficiently small, then

$$d_n(\omega, \omega^*) \leq \left(e^3 n^{\frac{1}{2}(\frac{1}{d+1}-\epsilon)} + C_p e^2\right) e^{-n^{(\frac{1}{d+1}-\epsilon)}} e^{-R(H/H^*)\, n^{(\frac{1}{d+1}-\epsilon)}},$$

where $R(s) = 1 + s\log(s)/(1-s)$.

Outline

Practical Algorithm – Main Steps

1. Discretise PDE in conforming FE space $V_h \subset H^1(\Omega)$ w.r.t. $\mathcal{T}_h$:
   Mesh size h small enough to resolve fine-scale details of $A(\boldsymbol{x})$.

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See below!

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   c. Solve the GenEO-type eigenproblem over the discrete a-harmonic space to build the local approximation space on ω_i^*.
3. Build the global particular solution and trial space and then solve the coarse problem to get the approximate solution.

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3. Build the global particular solution and trial space and then solve the coarse problem to get the approximate solution.

Steps 1a-c can be carried out **in parallel** and we can **reuse** precomputed bases (offline/online). Part 2

Discrete a-harmonic spaces

Main computational cost: Building the discrete a-harmonic spaces

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Idea 1: Instead, we can generate (approximate) $W_h(\omega_i^*)$ by using eigenfunctions of Steklov (DtN) eigenproblem [Dolean et al, 2012]

$$a_{\omega_j^*}(\zeta, v) = \lambda \int_{\partial\omega_j^*} \zeta v \, ds, \quad \forall v \in V_{h,0}(\omega_j^*),$$

For n_i-dimensional local approximation space, it is **sufficient** to approximate $W_h(\omega_i^*)$ using the first $s_i \approx 5n_i$ functions $\{\zeta_j^i\}_{j=1}^{s_i}$.

Easy to implement, error under control & much lower cost!

Idea 2: Eigensolver based on mixed formulation

- Find $\lambda_h \in \mathbb{R}$, $\phi_h \in V_{h,D}(\omega^*)$, and $\overbrace{p_h \in V_{h,DI}(\omega^*)}^{\text{Lagrange multiplier}}$ such that

$$\begin{aligned} a_{\omega^*}(\phi_h, v) + a_{\omega^*}(v, p_h) &= \lambda_h a_\omega(\chi\phi_h, \chi v) && \forall v \in V_{h,D}(\omega^*), \\ a_{\omega^*}(\phi_h, \xi) &= 0 && \forall \xi \in V_{h,DI}(\omega^*). \end{aligned}$$

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Note. The a-harmonic constraint is incorporated into the eigenproblem.

- Matrix eigenvalue problem: find $\lambda \in \mathbb{R}$, $\boldsymbol{\phi} = (\boldsymbol{\phi}_1, \boldsymbol{\phi}_2) \in \mathbb{R}^{n_1+n_2}$, and $\boldsymbol{p} \in \mathbb{R}^{n_1}$ such that

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{A}_{11} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{A}_{21} \\ \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \\ \boldsymbol{p} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{B}_{11} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\phi}_1 \\ \boldsymbol{\phi}_2 \\ \boldsymbol{p} \end{pmatrix},$$

$\boldsymbol{\phi}_1$: DOFs in the interior; $\boldsymbol{\phi}_2$: DOFs on the boundary.

Efficient and accurate eigensolver

- By block-elimination, it follows that

$$\mathbf{B}_{11}\boldsymbol{\phi}_1 = \lambda^{-1}\mathbf{A}_{11}\boldsymbol{p}, \qquad \mathbf{A}_{11} \text{ is SPD} \tag{2}$$

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- Together (2) & (3) form the reduced eigenproblem to be solved.

  Note. Original eigenproblem is solved accurately instead of approximately.

Two favourable features

1. **A posteriori** error bound:
   - We have a sharp, computable upper bound on the local approximation error, i.e., $\lambda_{h,n_i+1}^{-\frac{1}{2}}$, from computed eigenvalues.
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2. **Large relative gap** between eigenvalues:
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     This property doesn't hold for general PDE eigenproblems.
   - Classical iterative methods work very well for solving the eigenvalue problem under these circumstances.

Summary of the algorithm

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Main features:

1. **Step 1** can be carried out fully in parallel (**no** communication!).
2. The coarse problem is **small** (nearly exponential error bound).
3. The precomputed local approximation spaces can be **reused**.

Outline

Problem setting

Consider the steady-state heat conduction (or Darcy) problem:

$$\begin{aligned} -\mathrm{div}(A(\boldsymbol{x})\nabla u(\boldsymbol{x})) &= f(\boldsymbol{x}), && \text{in } \Omega = (0,1)^2, \\ \boldsymbol{n} \cdot A(\boldsymbol{x})\nabla u(\boldsymbol{x}) &= 1, && \text{for } x_2 = 0 \text{ or } 1, \\ u(\boldsymbol{x}) &= 1, && \text{for } x_1 = 0 \text{ or } 1, \end{aligned}$$

with the source term

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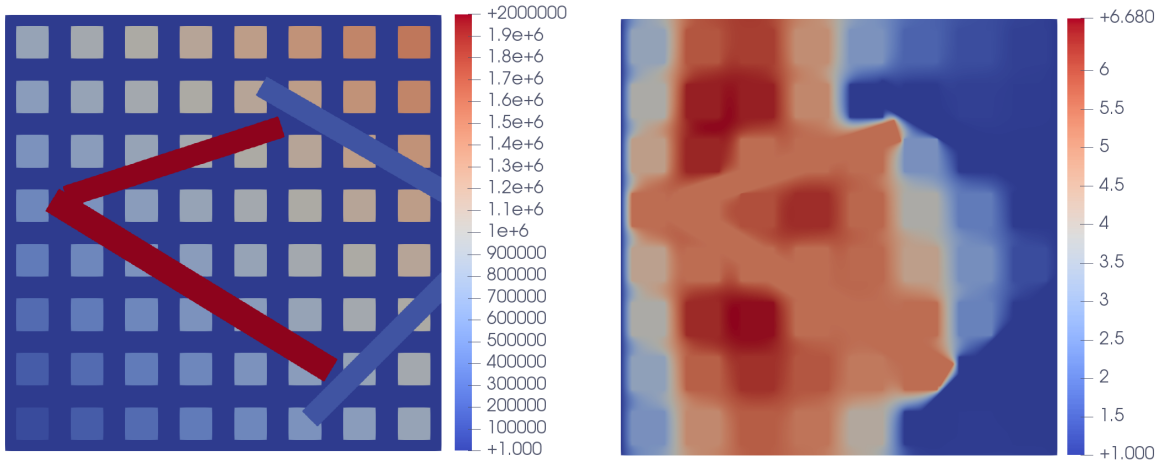
and **high-contrast** heterogeneous thermal conductivity (permeability)



The coefficient $A(\boldsymbol{x}) = a(\boldsymbol{x})\mathbf{I}$ (left) and the fine-scale solution u_h^e (right).

Computational settings

- Local computations are performed on a uniform Cartesian grid τ_h with piecewise bilinear FEs and $h = 1/500$.
- $M = m^2$ overlapping subdomains ω_i (overlap $2h$), extended by ℓ layers of fine mesh elements to create oversampling domains ω_i^*.
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- Dimension of each local approximation space is n_{loc}.
- Define the (relative) error

$$\textbf{error} := \|u_h^e - u_h^G\|_a \,/\, \|u_h^e\|_a.$$

between the GFEM solution u_h^G and the fine-scale solution u_h^e.

Numerical results (error vs. local dimension)

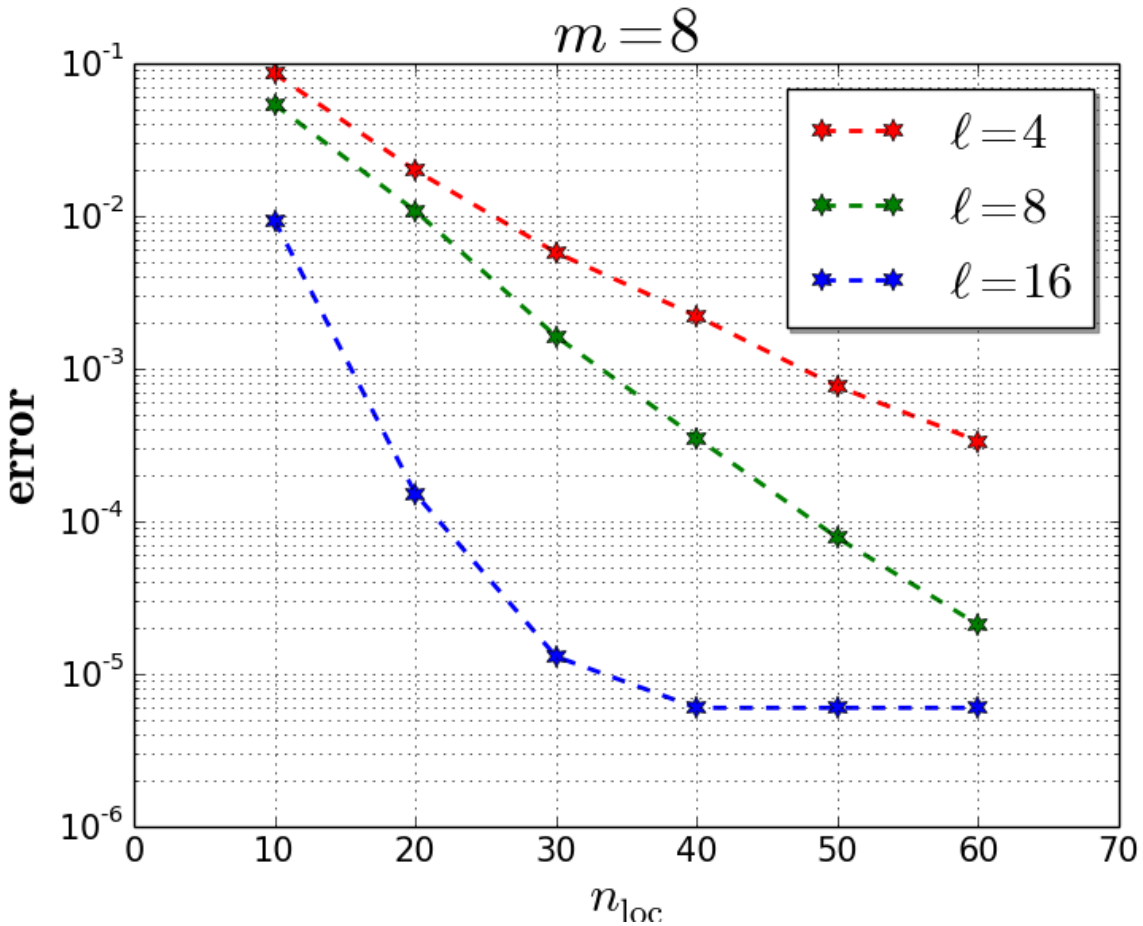

Figure: n_{loc} is the dimension of the local approximation space.

Numerical results (error vs. oversampling size)

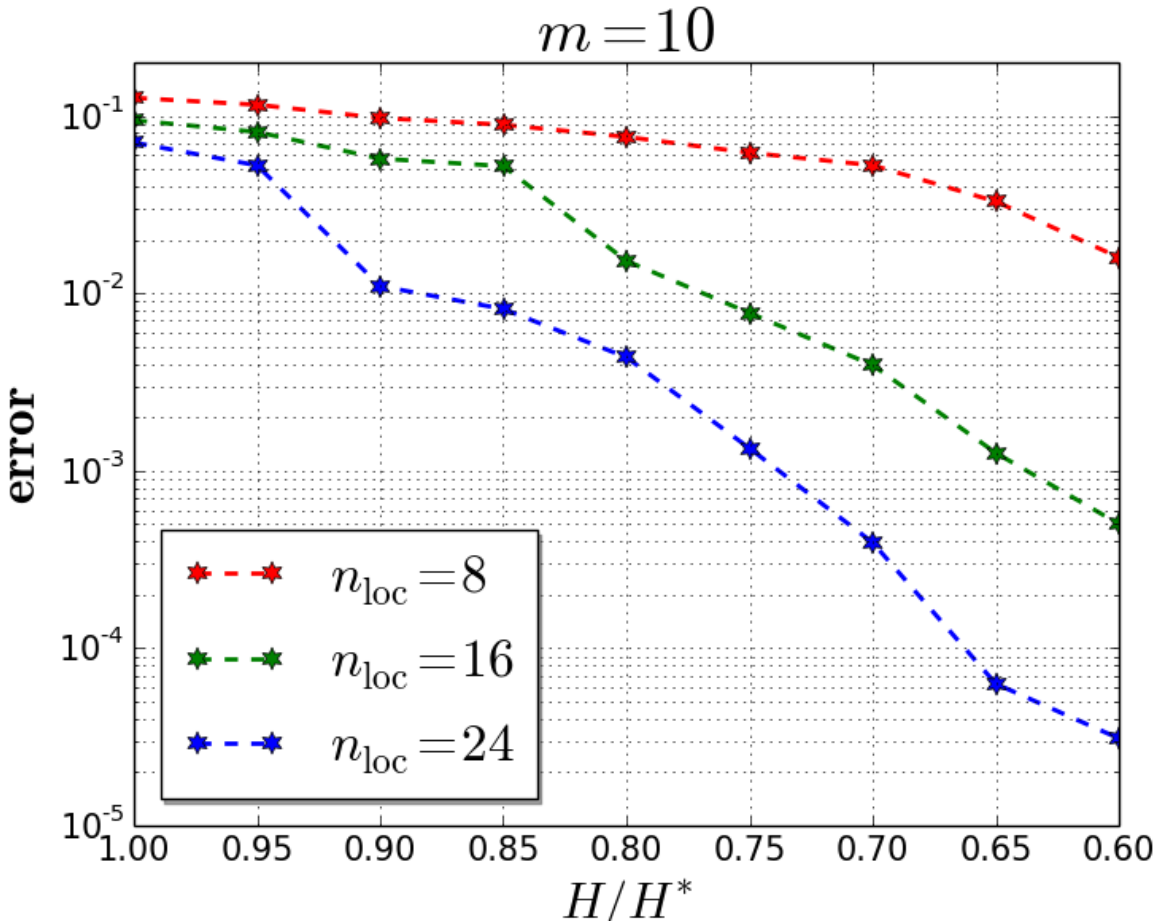

Figure: H and H^* are subdomain and oversampling domain sizes, resp.

Numerical results ($\lambda_{h,k}^{-1}$ vs. k)

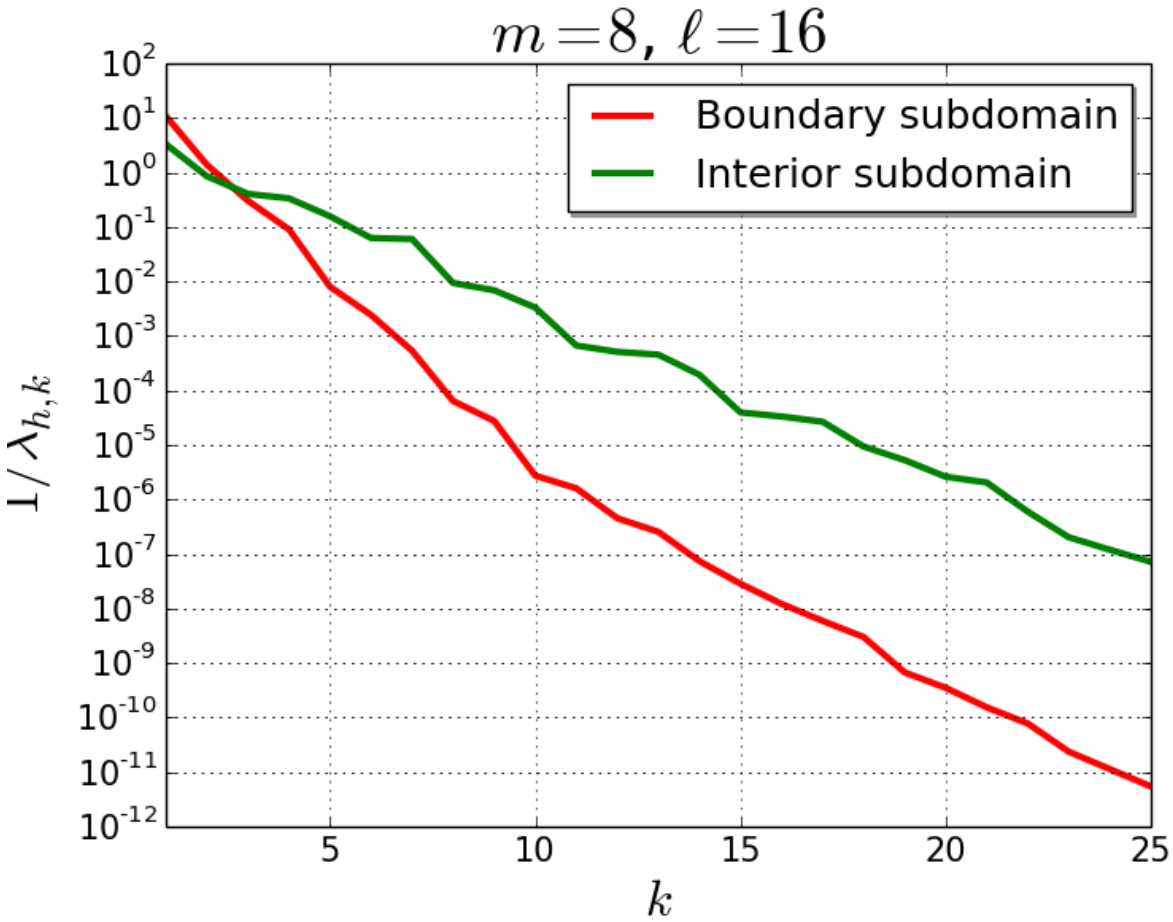

Figure: **Eigenvalues** of the local eigenproblems in an interior subdomain and a boundary subdomain.

Outline

HPC Implementation: Offline/Online Approach

Presentation of Postdoc **Jean Benezech** (Bath) at

VIII ECCOMAS Thematic Conference on the Mechanical Response ofComposites, Sep '21, Gteborg

"Scalable Localized Model Order Reduction Applied to Composite Aero-Structures"

Outline

Conclusions

- **GenEO-type eigenproblems** to construct **new** optimal local spaces for GFEM to approximate $\chi_i u$ instead of u on each ω_i.
- **Sharper bound** for local approximation error: nearly exponential decay with the local dimension and the amount of oversampling.
- **Two ideas** for efficient approaches to solve the eigenproblems with discrete a-harmonic constraint.
- First **fully discrete analysis** of MS-GFEM.
- Efficient **offline/online** implementation.
- Application to **aerospace composites**.

Outlook & Hardware-Awareness

- Theory for **linear elasticity**.
- **Cruder approximation** and iteration (like iterative refinement).
- Extend approach to other PDEs (**even indefinite**. ones**!**): Helmholtz (**done!**), Maxwell, Darcy in mixed form, ...
- Extension to **nonlinear** problems.
- **More robust** error estimates depending only on $\log(a_{\max}/a_{\min})$

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- **More robust** error estimates depending only on $\log(a_{\max}/a_{\min})$

- Ideally suited for **communication-avoidance** and **asynchrony**.
- **Exploit parallelism** at all levels to optimise components (eigensolver, Galerkin projection, local factorisations, global solve,...)
- Implement full adaptive scheme $\rightarrow$ **load balancing**
- Extend the approach to **multilevel** scheme Peter's lecture

References

- I Babuska, R Lipton, Optimal local approximation spaces for GFEM with application to multiscale problems, *MMS (SIAM)* **9**, 373–406, 2011
- Y Efendiev, J Galvis, TY Hou, Generalized multiscale finite element methods (GMsFEM), *J Comput Phys* **251**, 116–135, 2013
- N Spillane, V Dolean, P Hauret, F Nataf, C Pechstein, **RS**, Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps, *Numer Math* **126**, 741–770, 2014
- K Smetana, AT Patera, Optimal local approximation spaces for component-based static condensation procedures, *SISC* **38**, A3318–A3356, 2016
- I Babuska, R Lipton, P Sinz, M Stuebner, Multiscale-Spectral GFEM and optimal oversampling *CMAME* **364**, 112960, 2020
- R Butler, T Dodwell, A Reinarz, A Sandhu, **RS**, L Seelinger, High-perform. dune modules for solving large-scale, strongly anisotropic elliptic problems with applications to aerospace composites, *CPC* **249**, 106997, 2020
- C Ma, **RS**, T Dodwell, Novel design and analysis of generalized FE methods based on locally optimal spectral approximations, *arXiv:2103.09545*, 2021
- C Ma, **RS**, Error estimates for fully discrete generalized FEMs with locally optimal spectral approximations, arXiv:2107.09988, 2021