Non-intrusive implementation of multiscale finite element methods

CANUM 2020(+2), Evian-les-Bains

Rutger Biezemans

Joint work with Claude Le Bris, Frédéric Legoll and Alexei Lozinski

14 June, 2022

Multiscale diffusion problem

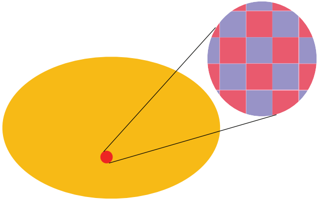
Boundary-value problem

Find $u^\varepsilon \in H^1(\Omega)$ s.t.

$$\begin{cases} -\mathrm{div}(A^\varepsilon \nabla u^\varepsilon) = f & \text{in } \Omega, \\ u^\varepsilon = 0 & \text{on } \partial\Omega, \end{cases}$$

$\Omega \subset \mathbb{R}^d$ bounded, $f \in L^2(\Omega)$

ε represents one or multiple small scales ($\ll \mathrm{diam}(\Omega)$)



Conduction/flow in heterogeneous media, composite materials, porous media

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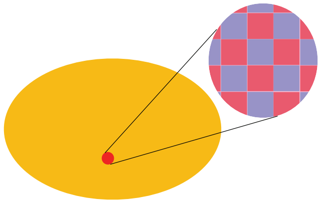
Variational formulation

Find $u^\varepsilon \in H^1_0(\Omega)$ s.t.

$$\forall\, v \in H^1_0(\Omega) \;:\quad \underbrace{\int_\Omega \nabla v \cdot A^\varepsilon \nabla u^\varepsilon}_{a^\varepsilon(u^\varepsilon, v)} = \underbrace{\int_\Omega f\, v,}_{F(v)}$$



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Multiscale problems and Finite Elements

$\mathbb{P}_1$ finite element method

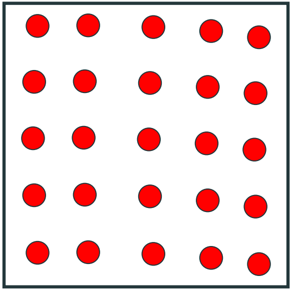
- Build a mesh $\mathscr{T}_H$ of Ω of size H
- Let V_H = continuous piecewise $\mathbb{P}_1$ functions on $\mathscr{T}_H$
- *Galerkin approximation:* find $u_H \in V_H$ s.t.

$$\forall v_H \in V_H \;: \quad a^\varepsilon(u_H, v_H) = F(v_H)$$

Example

$$-\operatorname{div}(A^\varepsilon \nabla u^\varepsilon) = 500$$

○ $A^\varepsilon = 1$
● $A^\varepsilon = 10$



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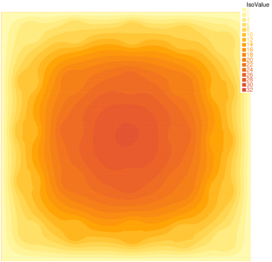
u_H with 10^6 degrees of freedom



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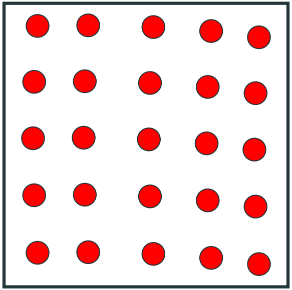

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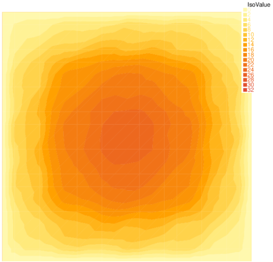
u_H with 441 degrees of freedom



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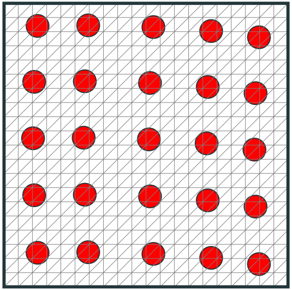

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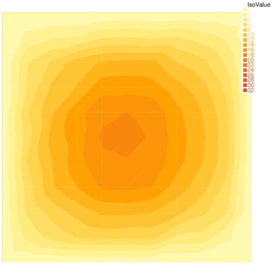
u_H with 121 degrees of freedom



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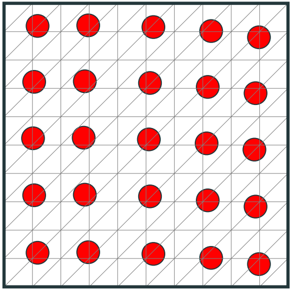

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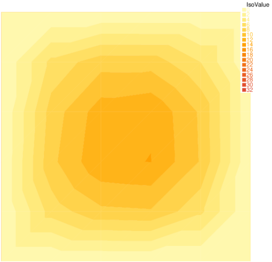
u_H with 36 degrees of freedom



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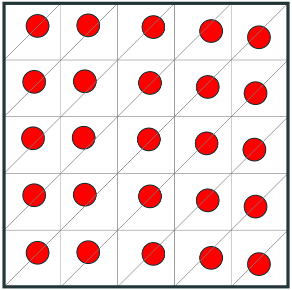

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Macroscopic properties are lost if the microstructure is not resolved.

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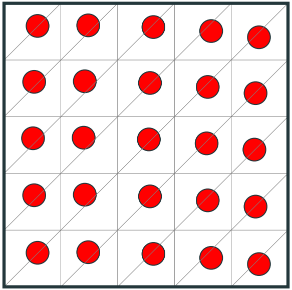

Numerical homogenization

Heterogeneous Multiscale Method (E and Engquist 2003), Local Orthogonal Decomposition (Målqvist and Peterseim 2014), we focus on the Multiscale Finite Element Method (MsFEM) (Hou and Wu 1997)

1. Offline stage: resolve the microstructure locally

2. Online stage: solve a coarse global problem

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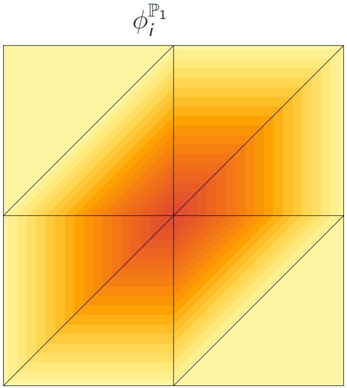

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Multiscale basis functions:

$$\forall K \in \mathscr{T}_H, \quad \begin{cases} -\mathrm{div}(A^\varepsilon \nabla \phi_i^\varepsilon) = 0 & \text{in } K, \\ \phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} & \text{on } \partial K. \end{cases}$$

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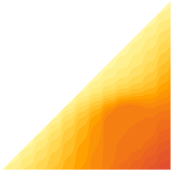

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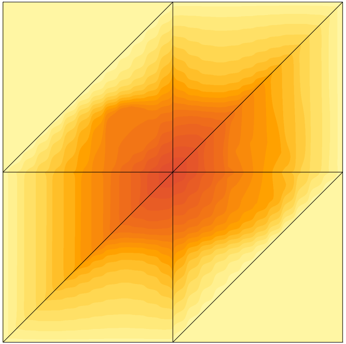

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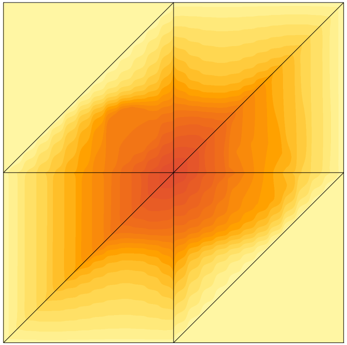

2. Online stage: solve a coarse global problem

Find $u_H^\varepsilon \in V_H^\varepsilon = \mathrm{span}\,\{\phi_i^\varepsilon\}$ s.t.

$$\forall\, v_H^\varepsilon \in V_H^\varepsilon : \quad a^\varepsilon\left(u_H^\varepsilon, v_H^\varepsilon\right) = F(v_H^\varepsilon)$$

MsFEM workflow

Discrete problem

Set $\mathbb{A}^\varepsilon_{j,i} = a^\varepsilon\left(\phi^\varepsilon_i, \phi^\varepsilon_j\right)$, $\mathbb{F}^\varepsilon_j = F\left(\phi^\varepsilon_j\right)$. Then $u^\varepsilon_H = \sum_{i=1}^{N} U^\varepsilon_i \phi^\varepsilon_i$ where $\mathbb{A}^\varepsilon U^\varepsilon = \mathbb{F}^\varepsilon$.

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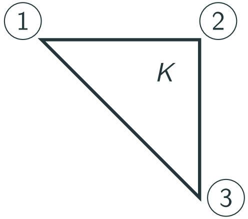

Algorithm (MsFEM)

for all mesh elements $K \in \mathscr{T}_H$ **do**

  for $1 \leq m \leq 3$ **do**

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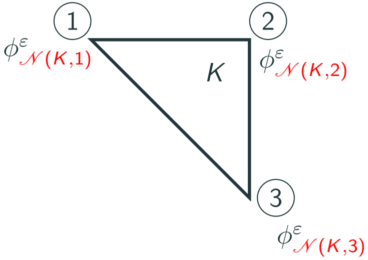

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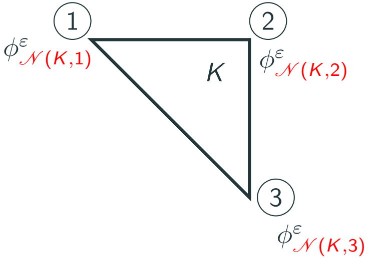

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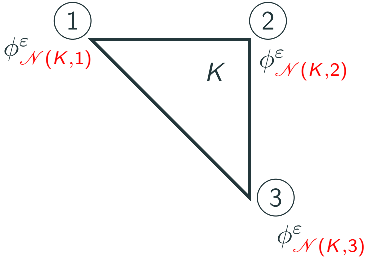

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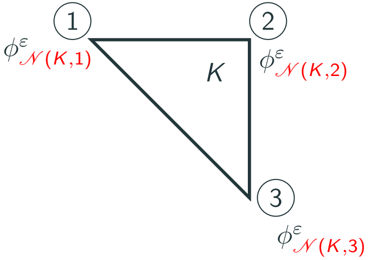

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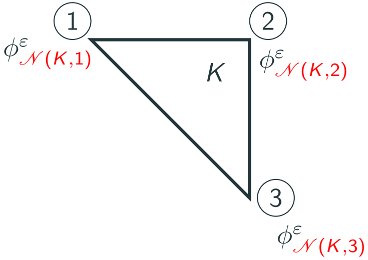

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$\mathcal{N}(K,n)$ inaccessible from a black box code

Decoupling macro and microscales

ϕ_i^ε: microstructure is coupled to macroscopic model

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$\to$ Numerical correctors ($\alpha = 1, 2$)

$$\forall\, K \in \mathscr{T}_H, \quad \begin{cases} -\mathrm{div}(A^\varepsilon \nabla \chi_K^{\varepsilon,\alpha}) = \mathrm{div}\left(A^\varepsilon \nabla e_\alpha\right) & \text{in } K, \\ \chi_K^{\varepsilon,\alpha} = 0 & \text{on } \partial K, \end{cases}$$

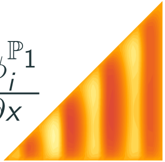
$\chi_K^{\varepsilon,\alpha} = 0$ outside K. Then

$$\phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} + \sum_{K \in \mathscr{T}_H} \sum_{\alpha=1,2} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\right)\Big|_K \chi_K^{\varepsilon,\alpha}$$

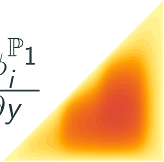
Decoupling macro and microscales

$=$

$+ \dfrac{\partial \phi_i^{\mathbb{P}1}}{\partial x}$



$+ \dfrac{\partial \phi_i^{\mathbb{P}1}}{\partial y}$



Linear system revisited

Decoupling: $$\phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} + \sum_{K \in \mathscr{T}_H} \sum_{\alpha=1,2} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\right)\Big|_K \chi_K^{\varepsilon,\alpha}$$

$$\mathbb{A}_{j,i}^\varepsilon = \int_\Omega \nabla \phi_j^\varepsilon \cdot A^\varepsilon \nabla \phi_i^\varepsilon = \sum_{K \in \mathscr{T}_H} \int_K \nabla \phi_j^\varepsilon \cdot A^\varepsilon \nabla \phi_i^\varepsilon$$

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$$= \sum_{K\in\mathcal{T}_H}\sum_{\alpha,\beta=1,2}\int_K \partial_\beta\phi_j^{\mathbb{P}_1}\left(e_\beta + \nabla\chi_K^{\varepsilon,\beta}\right)\cdot A^\varepsilon\left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)\partial_\alpha\phi_i^{\mathbb{P}_1}$$

$$= \sum_{K\in\mathcal{T}_H}\sum_{\alpha,\beta=1,2}\partial_\beta\phi_j^{\mathbb{P}_1}\Big|_K\left(\int_K\left(e_\beta + \nabla\chi_K^{\varepsilon,\beta}\right)\cdot A^\varepsilon\left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)\right)\partial_\alpha\phi_i^{\mathbb{P}_1}\Big|_K$$

Effective matrix $\overline{A}_{\beta,\alpha}\Big|_K = \frac{1}{|K|}\int_K\left(e_\beta + \nabla\chi_K^{\varepsilon,\beta}\right)\cdot A^\varepsilon\left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)$

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$$= \sum_{K\in\mathscr{T}_H} \sum_{\alpha,\beta=1,2} \partial_\beta \phi_j^{\mathbb{P}_1}\Big|_K \left(\int_K \left(e_\beta + \nabla\chi_K^{\varepsilon,\beta}\right) \cdot A^\varepsilon \left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)\right) \partial_\alpha \phi_i^{\mathbb{P}_1}\Big|_K$$

$$= \sum_{K\in\mathscr{T}_H} |K| \left(\nabla\phi_j^{\mathbb{P}_1} \cdot \overline{A}\, \nabla\phi_i^{\mathbb{P}_1}\right)\Big|_K$$

Effective matrix $\overline{A}_{\beta,\alpha}\Big|_K = \dfrac{1}{|K|} \displaystyle\int_K \left(e_\beta + \nabla\chi_K^{\varepsilon,\beta}\right) \cdot A^\varepsilon \left(e_\alpha + \nabla\chi_K^{\varepsilon,\alpha}\right)$

Linear system revisited

Decoupling: $\phi_i^\varepsilon = \phi_i^{\mathbb{P}_1} + \sum_{K \in \mathcal{T}_H} \sum_{\alpha=1,2} \left(\partial_\alpha \phi_i^{\mathbb{P}_1}\right)\Big|_K \chi_K^{\varepsilon,\alpha}$

$\mathbb{A}_{j,i}^\varepsilon =$

$$= \int_\Omega \nabla \phi_j^{\mathbb{P}_1} \, \overline{A} \, \nabla \phi_i^{\mathbb{P}_1}$$

Effective matrix $\overline{A}_{\beta,\alpha}\big|_K = \frac{1}{|K|} \int_K \left(e_\beta + \nabla \chi_K^{\varepsilon,\beta}\right) \cdot A^\varepsilon \left(e_\alpha + \nabla \chi_K^{\varepsilon,\alpha}\right)$

Effective PDE

The $\mathbb{P}_1$ FEM applied to

$$\begin{cases} -\mathrm{div}(\overline{A}\nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

yields the matrix

$$\mathbb{A}^{\mathbb{P}_1}_{j,i} = \int_\Omega \nabla \phi^{\mathbb{P}_1}_j \cdot \overline{A}\, \nabla \phi^{\mathbb{P}_1}_i$$

Testing the RHS yields $\mathbb{F}^{\mathbb{P}_1}_j = F\left(\phi^{\mathbb{P}_1}_j\right)$

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So, a legacy FEM code can compute

$$u_H = \sum_{i=1}^{N} U^{\mathbb{P}_1}_i \phi^{\mathbb{P}_1}_i, \qquad \text{with } \mathbb{A}^{\varepsilon} U^{\mathbb{P}_1} = \mathbb{F}^{\mathbb{P}_1}$$

Effective PDE

The $\mathbb{P}_1$ FEM applied to

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So, a legacy FEM code can compute

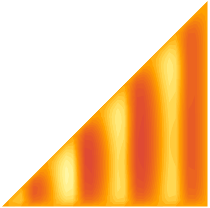
$$u_H = \sum_{i=1}^{N} U^{\mathbb{P}_1}_i \phi^{\mathbb{P}_1}_i, \qquad \text{with } \mathbb{A}^{\varepsilon} U^{\mathbb{P}_1} = \mathbb{F}^{\mathbb{P}_1},$$

from which we construct

$$u_H^{\varepsilon,\text{non-in}} = \sum_{i=1}^{N} U^{\mathbb{P}_1}_i \phi^{\varepsilon}_i = u_H + \sum_{K\in\mathcal{T}_H} \sum_{\alpha=1,2} (\partial_\alpha u_H)|_K\, \chi^{\varepsilon,\alpha}_K.$$

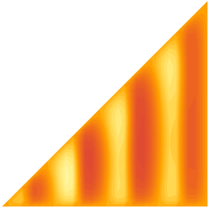
Non-intrusive MsFEM

$\chi_K^{\varepsilon,\alpha}$

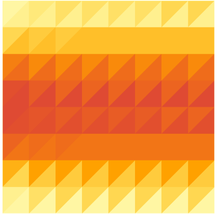


Non-intrusive MsFEM

$\chi_K^{\varepsilon,\alpha}$

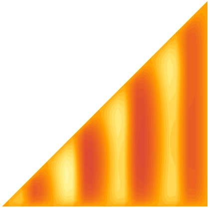


$\overline{A}$

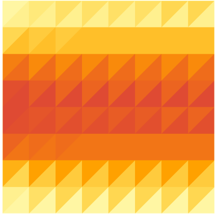


Non-intrusive MsFEM

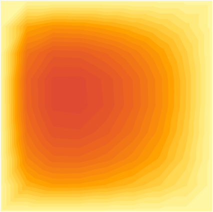
$\chi_K^{\varepsilon,\alpha}$



$\overline{A}$

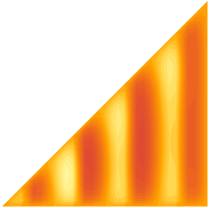


u_H



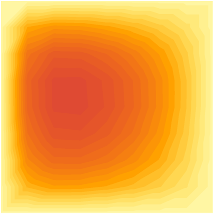
Non-intrusive MsFEM

$\chi_K^{\varepsilon,\alpha}$

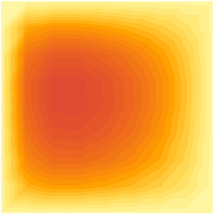


$\overline{A}$

u_H



$u_H^{\varepsilon,\text{non-in}}$



Non-intrusive MsFEM

Algorithm (Biezemans et al. 2022)

for all mesh elements $K \in \mathscr{T}_H$ **do**

  for $\alpha = 1, 2$ **do**

    Compute $\chi_K^{\varepsilon,\alpha}$ on K // *microscale code*

  for $\alpha,\ \beta = 1, 2$ **do**

    Compute $\left.\overline{A}_{\beta,\alpha}\right|_K$ // *microscale code*

Solve $\mathbb{A}^\varepsilon U^{\mathbb{P}_1} = \mathbb{F}^{\mathbb{P}_1}$ // *legacy code*

Set $u_H = \sum_{i=1}^{N} U_i^{\mathbb{P}_1} \phi_i^{\mathbb{P}_1}$ // *legacy code*

for all mesh elements $K \in \mathscr{T}_H$ **do**

  Compute $\left. u_H^{\varepsilon,\text{non-in}} \right|_K = u_H|_K + \sum_{K \in \mathscr{T}_H} \sum_{\alpha=1,2} (\partial_\alpha u_H)|_K \, \chi_K^{\varepsilon,\alpha}$ // *microscale code*

Interpretation

Non-intrusive MsFEM: find $u_H^{\varepsilon,\text{non-in}} \in V_H^\varepsilon$ s.t.

$$a^\varepsilon\left(u_H^{\varepsilon,\text{non-in}}, \phi_j^\varepsilon\right) = F\left(\phi_j^{\mathbb{P}_1}\right) \quad \text{for all } 1 \leq j \leq N$$

Interpretation

Non-intrusive MsFEM: find $u_H^{\varepsilon,\text{non-in}} \in V_H^\varepsilon$ s.t.

$$a^\varepsilon\left(u_H^{\varepsilon,\text{non-in}}, \phi_j^\varepsilon\right) = F\left(\phi_j^{\mathbb{P}_1}\right) \quad \text{for all } 1 \leq j \leq N$$

For each $\beta = 1, 2$ and any ϕ_i^ε:

$$\begin{aligned} a^\varepsilon\left(\phi_i^\varepsilon, \chi_K^{\varepsilon,\beta}\right) &= \int_K \nabla \chi_K^{\varepsilon,\beta} \cdot A^\varepsilon \nabla \phi_i^\varepsilon \\ &= \int_K -\text{div}\,(A^\varepsilon \nabla \phi_i^\varepsilon)\, \chi_K^{\varepsilon,\beta} + \int_{\partial K} \chi_K^{\varepsilon,\beta}\, n \cdot A^\varepsilon \nabla \phi_i^\varepsilon = 0 \end{aligned}$$

Interpretation

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Thus

$$a^\varepsilon\left(\phi_i^\varepsilon, \phi_j^\varepsilon\right) = a^\varepsilon\left(\phi_i^\varepsilon, \phi_j^{\mathbb{P}_1}\right)$$

Interpretation

Non-intrusive MsFEM: find $u_H^{\varepsilon,\text{non-in}} \in V_H^\varepsilon$ s.t.

$$a^\varepsilon\left(u_H^{\varepsilon,\text{non-in}}, \phi_j^\varepsilon\right) = F\left(\phi_j^{\mathbb{P}_1}\right) \quad \text{for all } 1 \le j \le N$$

For each $\beta = 1, 2$ and any ϕ_i^ε:

$$a^\varepsilon\left(\phi_i^\varepsilon, \chi_K^{\varepsilon,\beta}\right) = \int_K \nabla \chi_K^{\varepsilon,\beta} \cdot A^\varepsilon \nabla \phi_i^\varepsilon$$

$$= \int_K -\text{div}\left(A^\varepsilon \nabla \phi_i^\varepsilon\right) \chi_K^{\varepsilon,\beta} + \int_{\partial K} \chi_K^{\varepsilon,\beta}\, n \cdot A^\varepsilon \nabla \phi_i^\varepsilon = 0$$

Thus

$$a^\varepsilon\left(\phi_i^\varepsilon, \phi_j^\varepsilon\right) = a^\varepsilon\left(\phi_i^\varepsilon, \phi_j^{\mathbb{P}_1}\right)$$

Petrov-Galerkin MsFEM: find $u_H^{\varepsilon,\text{non-in}} \in V_H^\varepsilon$ s.t.

$$a^\varepsilon\left(u_H^{\varepsilon,\text{non-in}}, \phi_j^{\mathbb{P}_1}\right) = F\left(\phi_j^{\mathbb{P}_1}\right) \quad \text{for all } 1 \le j \le N$$

Comparison

Lemma 1 (Biezemans et al. 2022)

There exists $C > 0$ indepdent of ε, H and f such that

$$\|u_H^\varepsilon - u_H^{\varepsilon,\text{non-in}}\|_{H^1(\Omega)} \leq C\, H\, \|f\|_{L^2(\Omega)}.$$

Classical error estimate when $A^\varepsilon(\bullet) = A^{\text{per}}(\bullet/\varepsilon)$, under some technical assumptions (Efendiev and Hou 2009):

$$\|u^\varepsilon - u_H^\varepsilon\|_{H^1(\Omega)} \leq C\left(H + \sqrt{\varepsilon} + \sqrt{\frac{\varepsilon}{H}}\right)$$

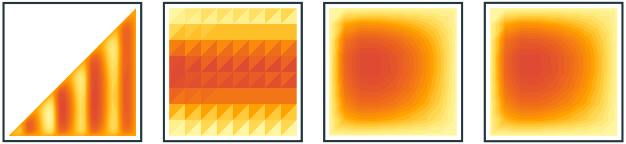
$\rightarrow$ same estimate for $\|u^\varepsilon - u_H^{\varepsilon,\text{non-in}}\|_{H^1(\Omega)}$

Numerical comparison

H/ε	$\|u_h^\varepsilon - u_H^\varepsilon\|_{H^1(\Omega)}$	$\|u_H^\varepsilon - u_H^{\varepsilon,\text{non-in}}\|_{H^1(\Omega)}$
16.88	5.6×10^{-3}	1.5×10^{-5}
8.44	4.8×10^{-3}	1.3×10^{-5}
4.22	6.3×10^{-3}	8.5×10^{-6}
2.11	8.0×10^{-3}	1.1×10^{-5}
1.06	9.5×10^{-3}	9.9×10^{-6}
0.53	8.6×10^{-3}	6.6×10^{-6}
0.26	6.6×10^{-3}	3.5×10^{-6}

$A^\varepsilon = \nu^\varepsilon \,\mathrm{Id}$,
$\nu^\varepsilon(x,y) = 1+100\cos\left(\frac{\pi x}{\varepsilon}\right)^2 \sin\left(\frac{\pi y}{\varepsilon}\right)^2$,
$f(x,y) = \sin(x)\,\sin(y)$,
$\varepsilon = \frac{\pi}{150} \approx 0.02$

Conclusion

Non-intrusive MsFEM: 

Allows to exploit a legacy code by pre- and postprocessing the microscale

Change of test functions, with identical accuracy

Extensions

Modifications possible for more general PDEs, different MsFEM variants,...