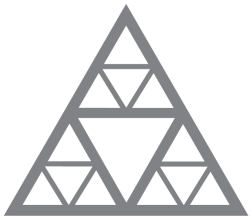
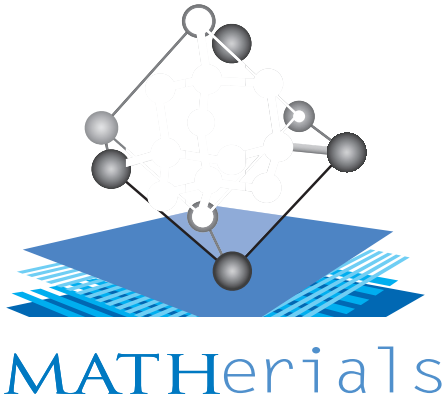




Numerical simulations using the Multiscale Finite Element Method: a posteriori estimates and mesh adaptivity

Frédéric Legoll

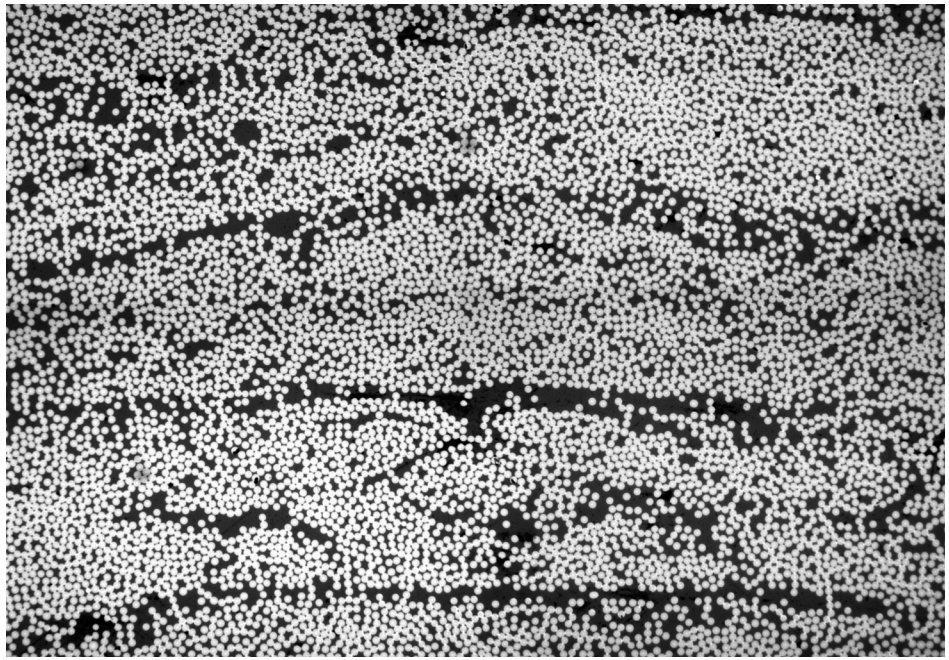
Ecole des Ponts & project-team MATHERIALS, Inria Paris

Joint works with Ludovic Chamoin (ENS Paris-Saclay)

Ecole d'été d'analyse numérique, EDF Lab, 27 juin – 1 juillet 2022

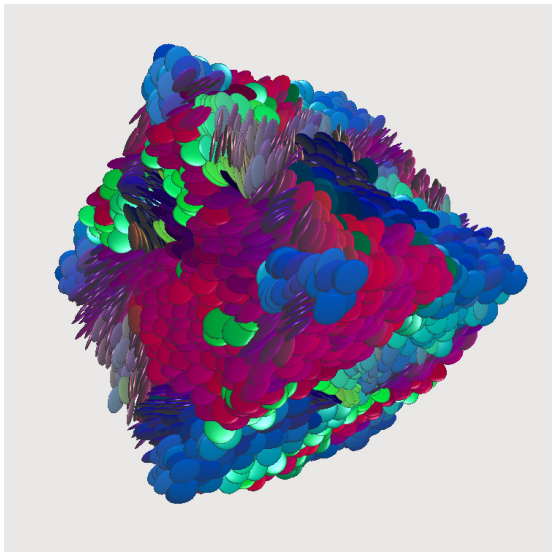
Multiscale problems are ubiquitous

Aircrafts are made of more and more composite materials



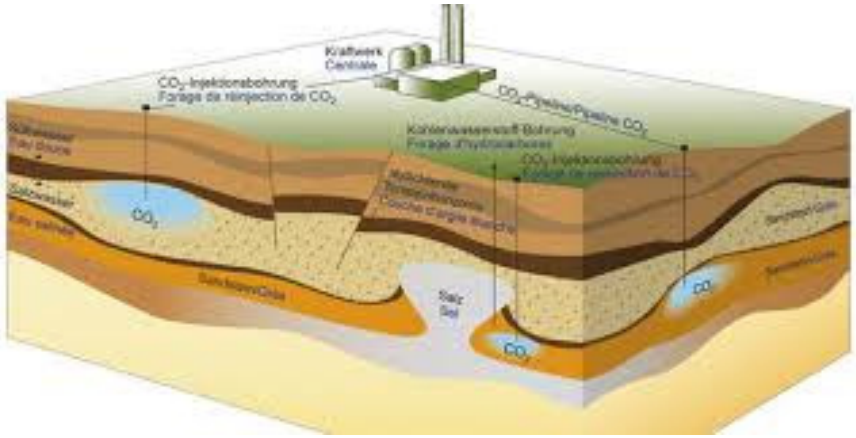
Courtesy M. Thomas (Airbus)

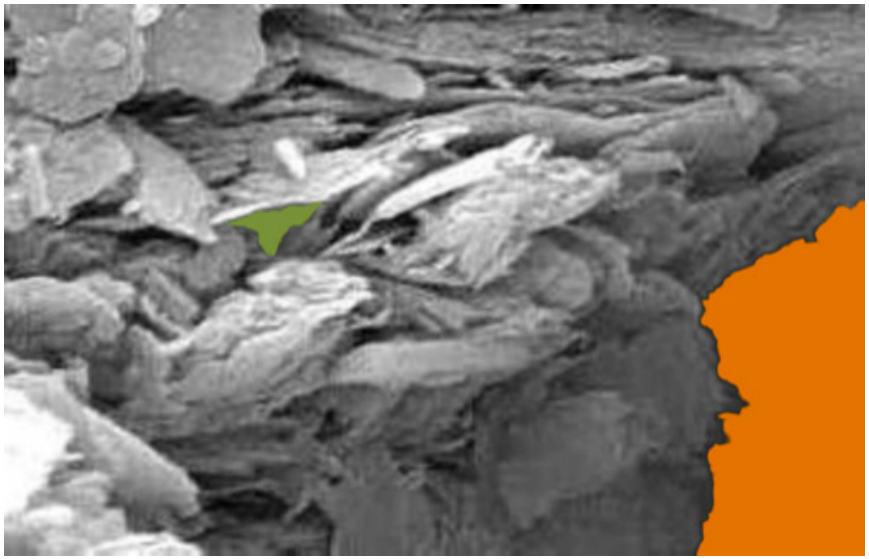
Concrete is a multiscale materials



Courtesy S. Brisard (ENPC)

Modelization of clay in the underground (courtesy Paris 6)

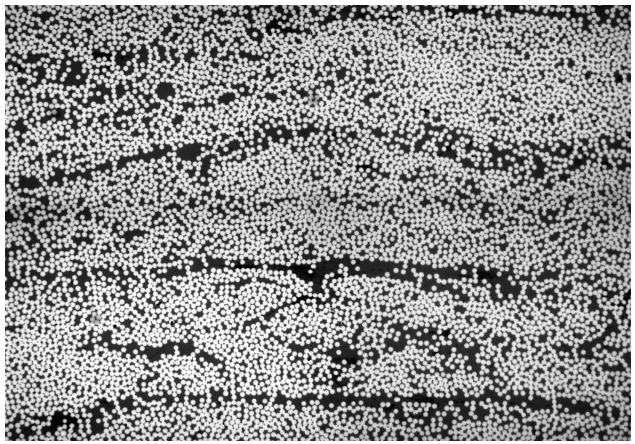


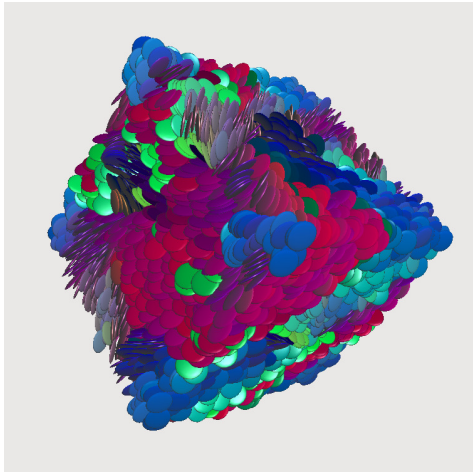


Clay is a complex materials. Channels with random lengths and diameters, according to a complex network.

Very much studied, in order to understand fluid and/or molecular diffusion in clay (e.g. waste storage).

Model problem





Model problem:

$$-\mathrm{div}\left[A_\varepsilon(x)\nabla u^\varepsilon\right] = f \quad \text{in } \Omega, \qquad u^\varepsilon = 0 \quad \text{on } \partial\Omega$$

where the (matrix-valued) diffusion coefficient A_ε

- is bounded from below and above uniformly in ε:

$$0 < m \leq A_\varepsilon(x) \leq M \quad \text{a.e. in } \Omega$$

- varies at the small scale ε

Classical FE approach

Assume we discretize using a P1 approach on a mesh of size H:

$$\|u_\varepsilon - u_\varepsilon^H\|_{H^1(\Omega)} \leq C \inf_{v^H \in V^H} \|u_\varepsilon - v^H\|_{H^1(\Omega)} \leq C\, H\, \|u_\varepsilon\|_{H^2(\Omega)}$$

and since $\|\nabla^2 u_\varepsilon\|_{L^2(\Omega)} \sim 1/\varepsilon$, this leads to requiring $H \ll \varepsilon$: too expensive!

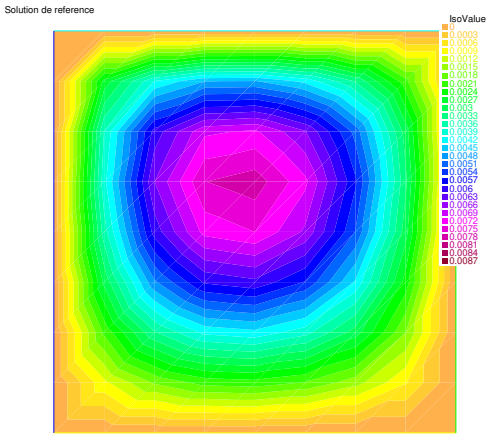
Classical FE approach

Assume we discretize using a P1 approach on a mesh of size H:

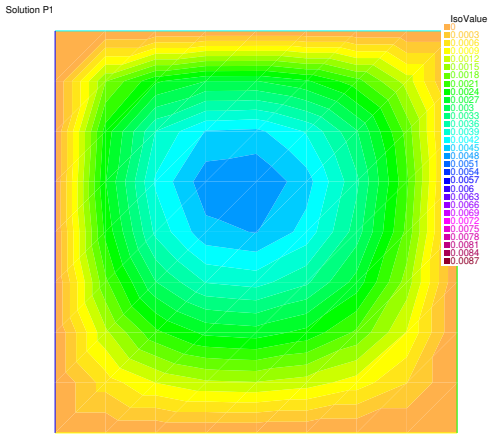
$$\|u_\varepsilon - u_\varepsilon^H\|_{H^1(\Omega)} \leq C \inf_{v^H \in V^H} \|u_\varepsilon - v^H\|_{H^1(\Omega)} \leq C\, H\, \|u_\varepsilon\|_{H^2(\Omega)}$$

and since $\|\nabla^2 u_\varepsilon\|_{L^2(\Omega)} \sim 1/\varepsilon$, this leads to requiring $H \ll \varepsilon$: too expensive!

Typical result ($\Omega = (0,1)^2$, A_ε is ε-periodic with $\varepsilon = 1/64$, $H = 1/8$):



Reference solution



P1 solution

Bad approximation even on the coarse scales ...

Setting

$$-\text{div}\,(A^\varepsilon \nabla u^\varepsilon) = f \quad \text{in } \Omega, \qquad u^\varepsilon = 0 \quad \text{on } \partial\Omega \qquad (\star)$$

- Several numerical multiscale approaches have been proposed to address such problems
- They are particularly worthwile in a multi-query context: need to solve $(\star)$ for several f
- We focus here on one of these, the Multiscale Finite Element Method (MsFEM)

Setting

$$-\text{div}\,(A^\varepsilon \nabla u^\varepsilon) = f \ \text{ in } \Omega, \qquad u^\varepsilon = 0 \ \text{ on } \partial\Omega \qquad (\star)$$

- Several numerical multiscale approaches have been proposed to address such problems
- They are particularly worthwile in a multi-query context: need to solve $(\star)$ for several f
- We focus here on one of these, the Multiscale Finite Element Method (MsFEM)

Basic idea: split the cost into

- offline stage, expensive but independent of f (done one time)
- online stage, to be performed for each new f, but inexpensive

The Multiscale Finite Element Method (MsFEM)

Efendiev, Hou & Wu ($\geq$ 1997)

Many subsequent contributions: Aarnes, Allaire & Brizzi, Brown, Chen et al, Chung et al, Dostert, Ginting, Henning, Ohlberger, ...

Related approaches: Malqvist & Peterseim, Berlyand/Owhadi/Zhang, ...

The Multiscale Finite Element Method (MsFEM)

$$-\text{div}\,(A_\varepsilon \nabla u^\varepsilon) = f \ \text{ in } \Omega, \qquad u^\varepsilon = 0 \ \text{ on } \partial\Omega$$

Variational formulation: find $u^\varepsilon \in H^1_0(\Omega)$ such that

$$\forall v \in H^1_0(\Omega), \qquad \mathcal{A}_\varepsilon(u^\varepsilon, v) = b(v) \qquad (\star)$$

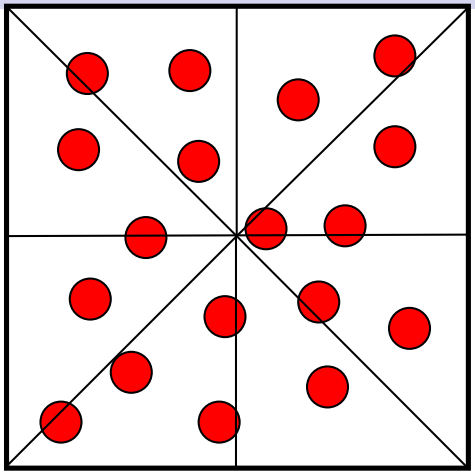
where

$$\mathcal{A}_\varepsilon(u,v) = \int_\Omega (\nabla v)^T A_\varepsilon \nabla u \qquad \text{and} \qquad b(v) = \int_\Omega f\, v.$$

Idea of MsFEM: Galerkin approximation with suitably chosen basis functions:

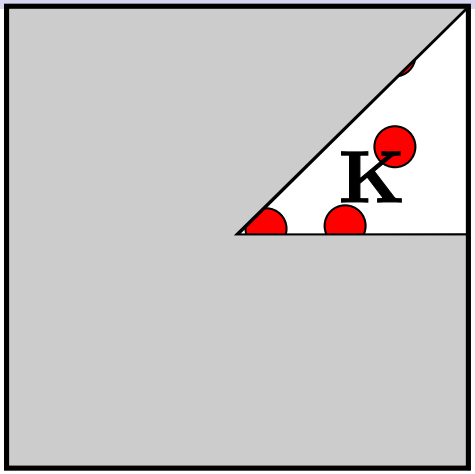
- offline stage: pre-compute the basis functions, that are independent of f
- online stage: for each new f, solve $(\star)$.

Offline stage

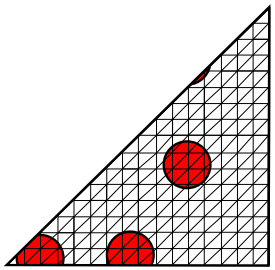


- Coarse mesh with a P1 Finite Element basis functions ϕ_i^0.

Offline stage



- Coarse mesh with a P1 Finite Element basis functions ϕ_i^0.
- MsFEM basis function ϕ_i^ε, associated to node i:

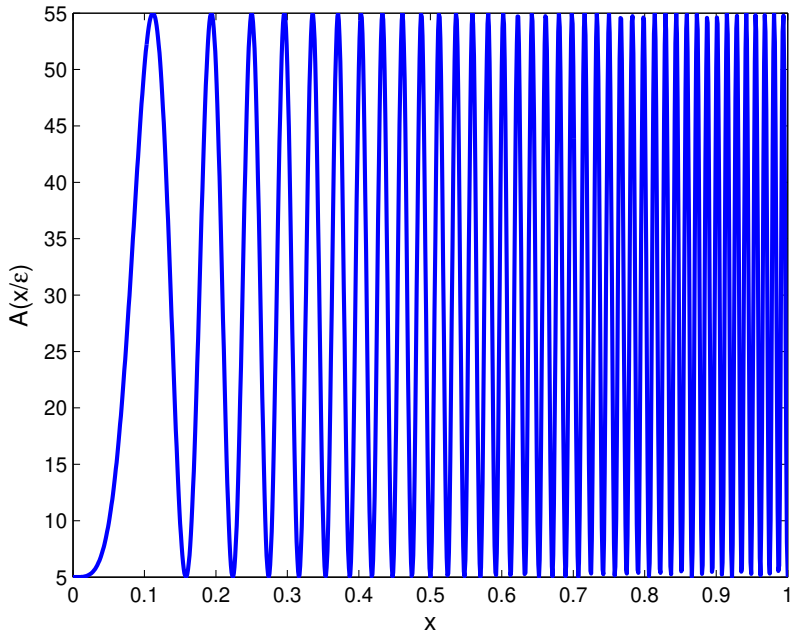


In each element K,

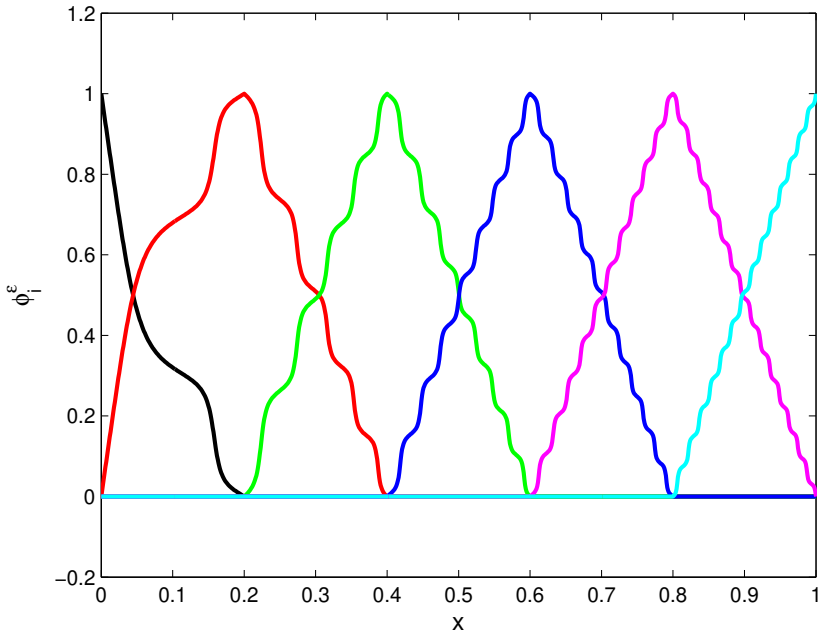
$$\begin{cases} -\text{div}\,(A_\varepsilon \nabla \phi_i^\varepsilon) = 0 & \text{in K} \\ \phi_i^\varepsilon = \phi_i^0 & \text{on } \partial \text{K} \end{cases}$$

The MsFEM basis functions ϕ_i^ε encode the specific fast oscillations (present in A_ε) of the problem. They are independent of f, and can be computed beforehand, in parallel.

Numerical illustration



A^ε

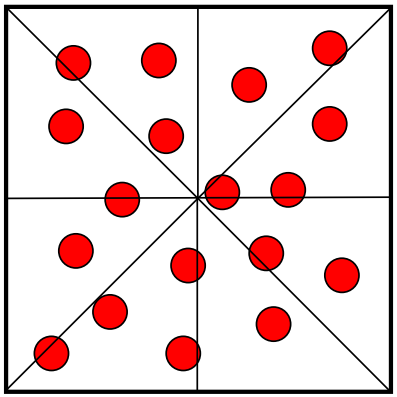


Adapted basis functions

In contrast to the FEM basis functions, the MsFEM basis functions encode the specific fast oscillations of the problem:

$$-\text{div}\,(A^\varepsilon \nabla \phi_i^\varepsilon) = 0 \quad \text{in K}, \qquad \phi_i^\varepsilon = \phi_i^0 \quad \text{on } \partial \text{K}$$

Online stage



$$W_H^\varepsilon = \text{Span}\,\{\phi_i^\varepsilon, \quad 1 \leq i \leq L\}$$

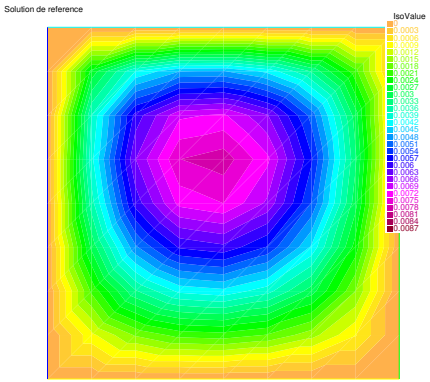
Galerkin approx. on W_H^ε of the original problem: find $u_H^\varepsilon \in W_H^\varepsilon$ s.t.

$$\forall v \in W_H^\varepsilon, \qquad \mathcal{A}_\varepsilon(u_H^\varepsilon, v) = b(v).$$

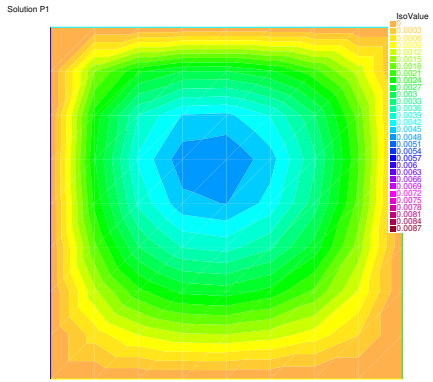
- The macro problem is inexpensive to solve (as many DOFs as in a P1 approach on the same coarse mesh)
- The highly oscillatory basis functions do NOT depend on f (adapted to a multi-query context)

MsFEM accuracy

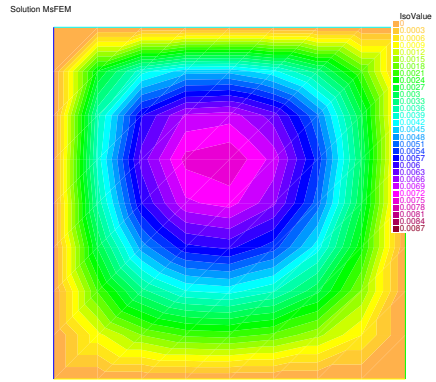
On the same typical problem ($\Omega = (0,1)^2$, A_ε is ε-periodic with $\varepsilon = 1/64$, $H = 1/8$):



Reference solution



P1 solution



MsFEM solution

Theoretical a priori estimate:

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

and thus convergence in the regime $\varepsilon \ll H$.

Oversampling variant

In the definition of the basis functions,

$$-\text{div}\,(A^\varepsilon \nabla \phi_i^\varepsilon) = 0 \ \text{ in K}, \qquad \phi_i^\varepsilon = \phi_i^0 \ \text{ on } \partial\text{K},$$

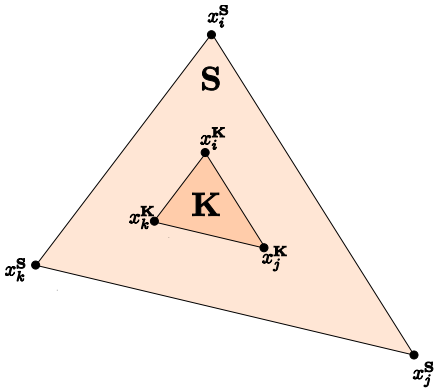
the boundary condition does not seem to be adequate . . .

Oversampling variant

In the definition of the basis functions,

$$-\text{div}\,(A^\varepsilon \nabla \phi_i^\varepsilon) = 0 \ \text{ in K}, \qquad \phi_i^\varepsilon = \phi_i^0 \ \text{ on } \partial\text{K},$$

the boundary condition does not seem to be adequate ...



For any element K, consider a larger domain S $\supset$ K and let $\chi_i^{0,\text{S}}$ be the extension of ϕ_i^0 on S

- Basis function associated to node i: solve

$$-\text{div}\,\left[A_\varepsilon\, \nabla \chi_i^{\varepsilon,\text{S}}\right] = 0 \ \text{ in S}, \qquad \chi_i^{\varepsilon,\text{S}} = \chi_i^{0,\text{S}} \ \text{ on } \partial\text{S},$$

  and restrict on K: $\phi_i^\varepsilon = \chi_i^{\varepsilon,\text{S}}\Big|_{\text{K}}$ on K (one DOF per node)
- Non-conforming discretization: $\phi_i^\varepsilon \notin H^1(\Omega)$
- Much more accurate method

A posteriori error estimation

Very few works on multiscale problems: Abdulle et al [2009–], Henning et al [2015], Henning et al [2014].

We have used a method (based on the Constitutive Relation Error) which is classical in computational mechanics for single-scale problems.

Ladevèze et al [1983 and 2004], Destuynder et al [1999], ...

A posteriori estimation

Let $u^\varepsilon \in H^1_0(\Omega)$ be the exact solution and $u^\varepsilon_H \in H^1_0(\Omega)$ be its numerical approximation.
Let $\widehat{\sigma}_H \in H(\mathrm{div}, \Omega)$ be such that $-\mathrm{div}\, \widehat{\sigma}_H = f$ in Ω (many choices here).

Then

$$\|\nabla u^\varepsilon - \nabla u^\varepsilon_H\|^2_{L^2(A_\varepsilon)} + \|A_\varepsilon \nabla u^\varepsilon - \widehat{\sigma}_H\|^2_{L^2(A_\varepsilon^{-1})} = \underbrace{\|A_\varepsilon \nabla u^\varepsilon_H - \widehat{\sigma}_H\|^2_{L^2(A_\varepsilon^{-1})}}_{\text{Const. Rel. Error (CRE)}}$$

Prager-Synge equality (proof by integration by parts)

The above RHS, which can be practically computed, is hence an upper-bound on the error:

$$\|\nabla u^\varepsilon - \nabla u^\varepsilon_H\|_{L^2(A_\varepsilon)} \leq \underbrace{\|A_\varepsilon \nabla u^\varepsilon_H - \widehat{\sigma}_H\|_{L^2(A_\varepsilon^{-1})}}_{\text{Const. Rel. Error (CRE)}}$$

Notation: $\|\nabla u\|^2_{L^2(A_\varepsilon)} = \displaystyle\int_\Omega (\nabla u)^T A_\varepsilon \nabla u$ and $\|\sigma\|^2_{L^2(A_\varepsilon^{-1})} = \displaystyle\int_\Omega \sigma^T (A_\varepsilon)^{-1} \sigma$

Construction of $\widehat{\sigma}_H$ s.t. $-\text{div}\,\widehat{\sigma}_H = f$

In the single scale framework, there are several ways to build such a $\widehat{\sigma}_H$:

- using Raviart-Thomas elements (see lectures of A. Ern)
- by solving local problems posed on patches around each node (the so-called flux-free approach)
- by solving local problems posed on each element (the so-called hybrid-flux approach, aka Element Equilibration Technique – EET)

Construction of $\widehat{\sigma}_H$ s.t. $-\text{div}\,\widehat{\sigma}_H = f$

In the single scale framework, there are several ways to build such a $\widehat{\sigma}_H$:

- using Raviart-Thomas elements (see lectures of A. Ern)
- by solving local problems posed on patches around each node (the so-called flux-free approach)
- by solving local problems posed on each element (the so-called hybrid-flux approach, aka Element Equilibration Technique – EET)

  It can be shown [Ladevèze and Leguillon, 1983] (e.g. for the Laplace equation with piecewise constant f) that

$$C \, \|\nabla u_H - \widehat{\sigma}_H\|_{L^2(\Omega)} \leq \|\nabla u - \nabla u_H\|_{L^2(\Omega)} \leq \|\nabla u_H - \widehat{\sigma}_H\|_{L^2(\Omega)}$$

  for some C independent of H.

In our multiscale context, we follow the EET technique.

Construction of $\widehat{\sigma}_H$ s.t. $-\mathrm{div}\,\widehat{\sigma}_H = f$

We build $\widehat{\sigma}_H$ following the EET technique, as in the single-scale setting:

- determine $\widehat{F} = n^T \widehat{\sigma}_H$ on any edge e by postprocessing $\sigma_H = A_\varepsilon \nabla u_H^\varepsilon$.
  By construction, these $\widehat{F}$ are in local equilibrium:

$$\int_K f + \sum_{e \subset \partial K} \int_e \widehat{F} = 0$$

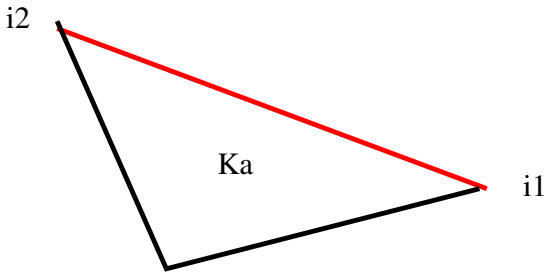
Construction of $\widehat{\sigma}_H$ s.t. $-\text{div}\ \widehat{\sigma}_H = f$

We build $\widehat{\sigma}_H$ following the EET technique, as in the single-scale setting:

- determine $\widehat{F} = n^T \widehat{\sigma}_H$ on any edge e by postprocessing $\sigma_H = A_\varepsilon \nabla u_H^\varepsilon$.
  By construction, these $\widehat{F}$ are in local equilibrium:

$$\int_K f + \sum_{e \subset \partial K} \int_e \widehat{F} = 0$$

- determine $\widehat{\sigma}_H$ in any element K: solve



$$(\star) \quad \begin{cases} -\text{div}\ [A_\varepsilon \nabla \widehat{u}_H] = f & \text{in } K, \\ n^T A_\varepsilon \nabla \widehat{u}_H = \widehat{F}_{ij} & \text{on edge from } i \text{ to } j \end{cases}$$

and set $\widehat{\sigma}_H = A_\varepsilon \nabla \widehat{u}_H$ in K.

At the end of the day, we have a computable upper-bound on the error:

$$\|\nabla u^\varepsilon - \nabla u_H^\varepsilon\|_{L^2(A_\varepsilon)} \leq \|\widehat{\sigma}_H - A_\varepsilon \nabla u_H^\varepsilon\|_{L^2(A_\varepsilon^{-1})}$$

L. Chamoin, F.L., CMAME 2018

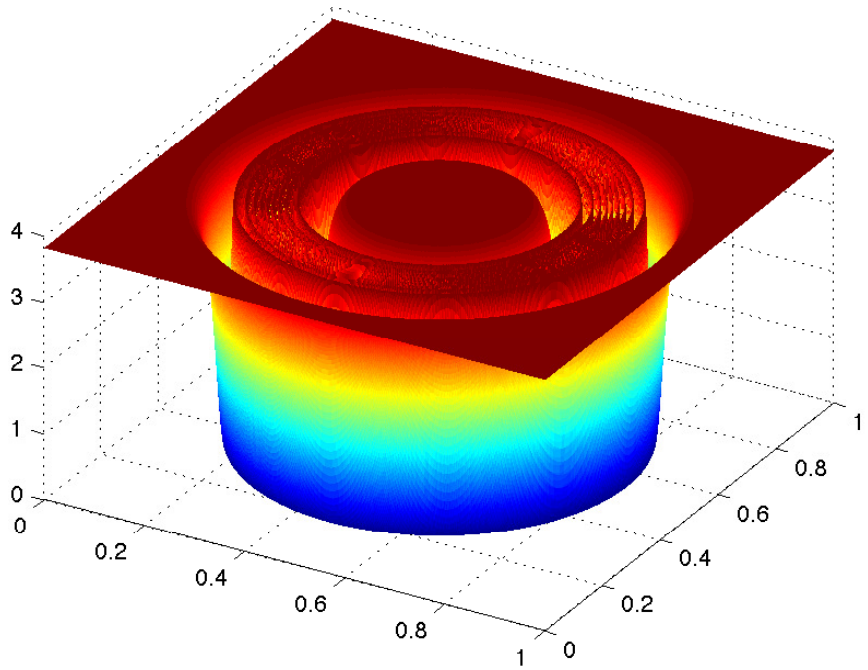
Numerical example: Steady heat conduction in fiber composite

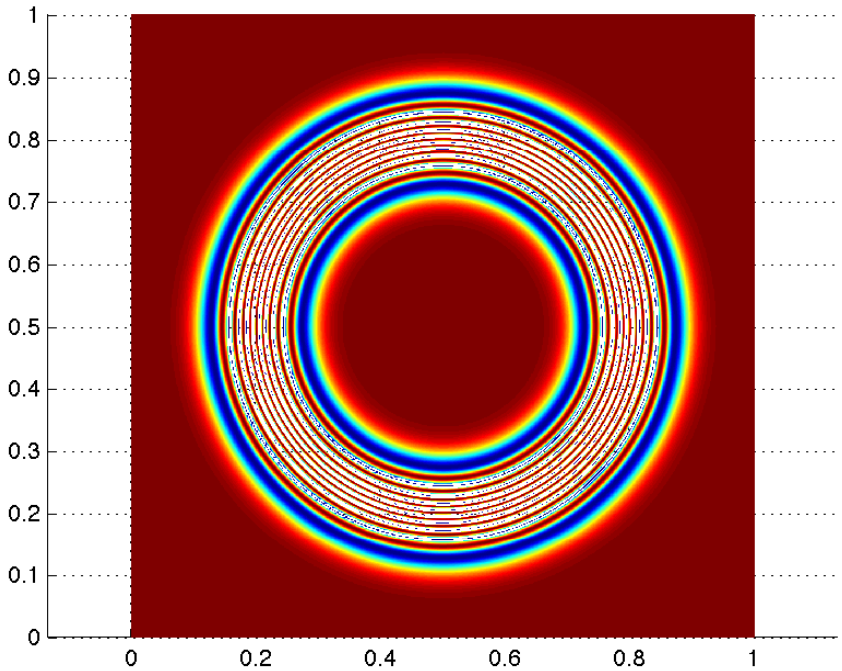
L. Chamoin, F.L., CMAME 2018

Fiber composite (field A_ε)

$$A_\varepsilon(x,y) = A(x/\varepsilon, y/\varepsilon) = \Big(2 + P\cos(2\pi \tanh(w(r-0.3))/\varepsilon)\Big)\ I_2$$

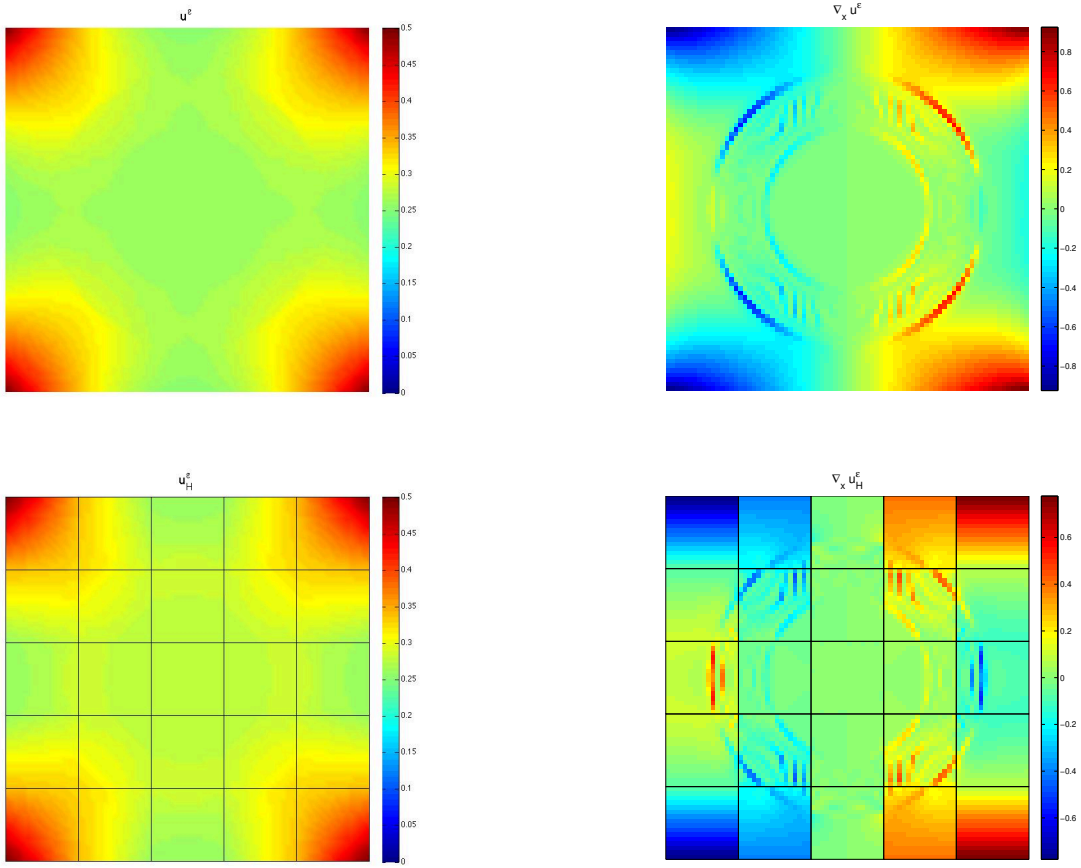
Non-periodic test-case, shortest wavelength in A_ε close to 0.01





Hou & Wu [1997]

Fiber composite (top: exact sol.; bottom: MsFEM sol.)

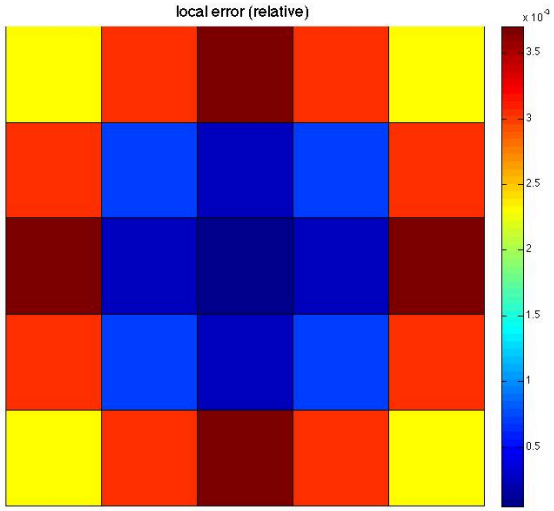


u^ε $\qquad$ $[\nabla u^\varepsilon]_1$

No oversampling, 5×5 macro elements ($H = 0.2$), $h = \dfrac{\varepsilon}{16} \approx 0.0125$.

Error close to 25 % (on purpose, initial computation not so accurate)

Fiber composite (error estimation)



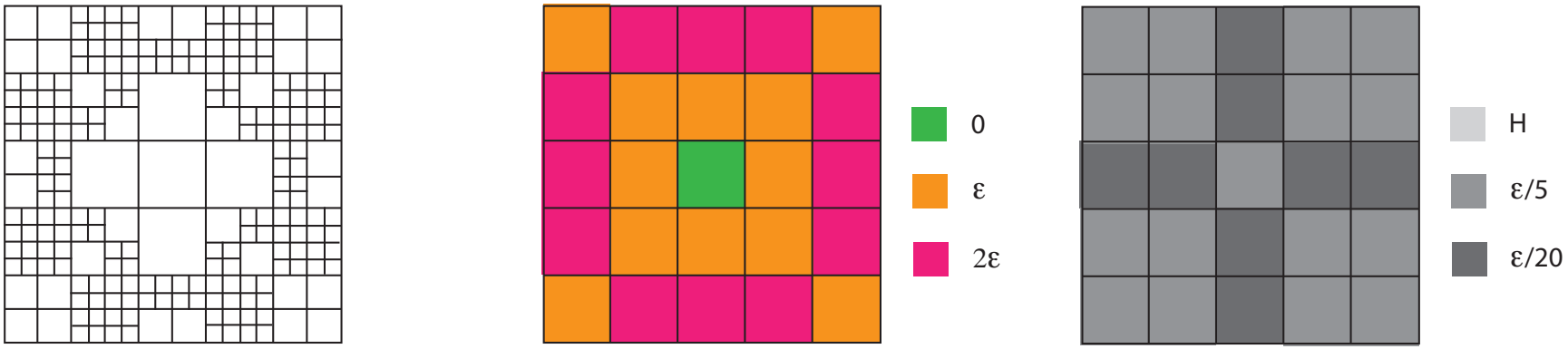
$$E_{CRE|K} = \|\widehat{\sigma}_H - A_\varepsilon \nabla u_H^\varepsilon\|_{L^2(K)}$$

Error distribution $E^2_{CRE|K}$ $(H = 0.2)$

Effectivity index: $$1 \leq \frac{\|\widehat{\sigma}_H - A_\varepsilon \nabla u_H^\varepsilon\|_{L^2(\Omega)}}{\|\nabla u^\varepsilon - \nabla u_H^\varepsilon\|_{L^2(\Omega)}} \approx 1.09$$

Estimated Error $\approx$ True Error!

Fiber composite (adaptive strategy, tolerance 5%)



Adapted macro mesh (left), oversampling size (center), micro mesh (right)

- Split the error into various contributions (associated to H, h, oversampling ratio) in order to adapt the relevant discretization parameters
- Use the Allaire-Brizzi MsFEM variant in order to adapt wrt H, so that no additional fine-scale computations

Goal-oriented error estimation

L. Chamoin and F.L., Comput. Mech. 2021

Goal-oriented analysis

As for many a posteriori methods, our approach can be extended to estimate the error on quantities of interest, e.g. of the form

$$Q(u) = \int_\omega [A_\varepsilon \nabla u]_1 \quad \text{for some } \omega \subset \Omega.$$

The procedure is classical:

- introduce the adjoint problem: let $\widetilde{u}^\varepsilon \in H^1_0(\Omega)$ such that

$$\forall v \in H^1_0(\Omega), \quad \mathcal{A}_\varepsilon(v, \widetilde{u}^\varepsilon) = Q(v).$$

- then

$$\left| Q(u^\varepsilon) - Q(u_H^\varepsilon) - \overline{C}_H^\varepsilon \right| \leq \frac{1}{2} E_{\mathrm{CRE}}(u_H^\varepsilon) \, E_{\mathrm{CRE}}(\widetilde{u}_H^\varepsilon)$$

  where
  - $E_{\mathrm{CRE}}(u_H^\varepsilon)$ (resp. $E_{\mathrm{CRE}}(\widetilde{u}_H^\varepsilon)$) is the constitutive relation error when approximating u^ε (resp. $\widetilde{u}_H^\varepsilon$)
  - $\overline{C}_H^\varepsilon$ is a fully computable quantity (depends on u_H^ε, $\widetilde{u}_H^\varepsilon$, $\widehat{\sigma}_H$ and $\widetilde{\sigma}_H$)

Solving the adjoint problem

Look for $\widetilde{u}^\varepsilon \in H^1_0(\Omega)$ such that

$$\forall v \in H^1_0(\Omega), \quad \mathcal{A}_\varepsilon(v, \widetilde{u}^\varepsilon) = Q(v).$$

In practice:

$$\widetilde{u}^\varepsilon = \widetilde{u}^\varepsilon_{\text{handbook}} + \widetilde{u}^\varepsilon_{\text{res}}$$

where

- $\widetilde{u}^\varepsilon_{\text{handbook}}$ is a localized solution of the adjoint problem, computed using a fine discretization on some $\omega \subset\subset \Omega$
- the remainder $\widetilde{u}^\varepsilon_{\text{res}}$ solves

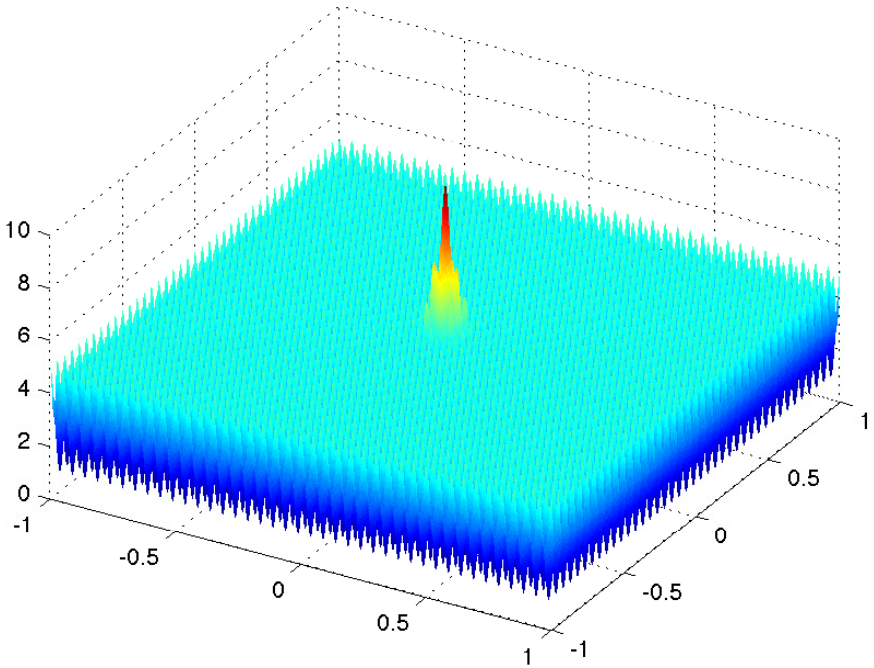
$$\forall v \in H^1_0(\Omega), \quad \mathcal{A}_\varepsilon(v, \widetilde{u}^\varepsilon_{\text{res}}) = Q(v) - \mathcal{A}_\varepsilon(v, \widetilde{u}^\varepsilon_{\text{handbook}})$$

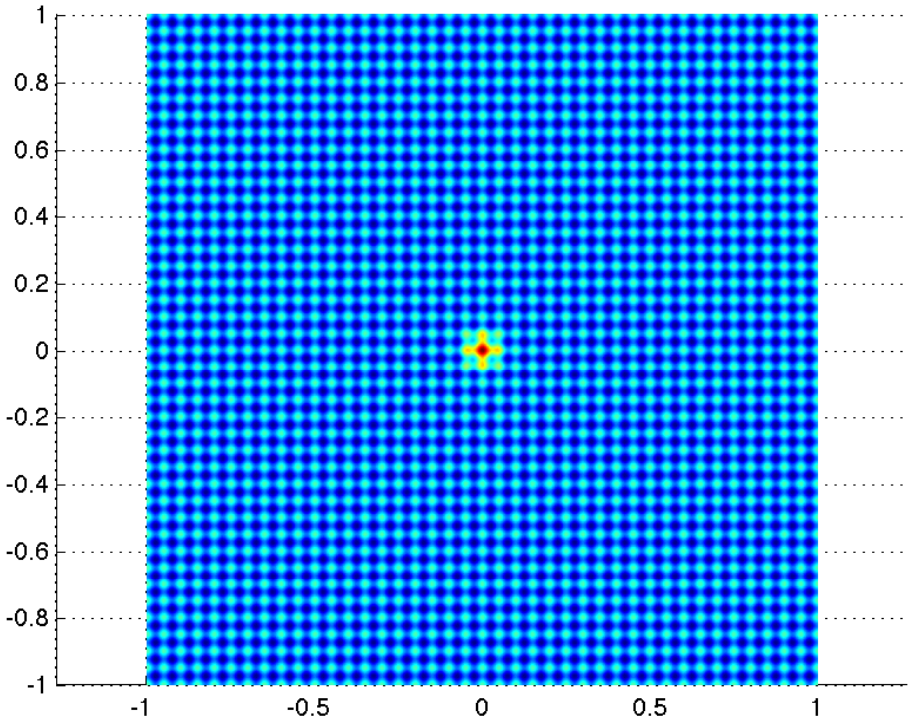
  In practice, MsFEM approximation for $\widetilde{u}^\varepsilon_{\text{res}}$.

No additional offline computation to approximate $\widetilde{u}^\varepsilon$

Material with defect

$$A_\varepsilon(x,y) = \left[A_{\rm per}\left(\frac{x}{\varepsilon},\frac{y}{\varepsilon}\right) + B_{\rm defect}\left(\frac{x}{\varepsilon},\frac{y}{\varepsilon}\right)\right] I_2, \quad B_{\rm defect}(x,y) = 5\exp(-(x^2+y^2))$$

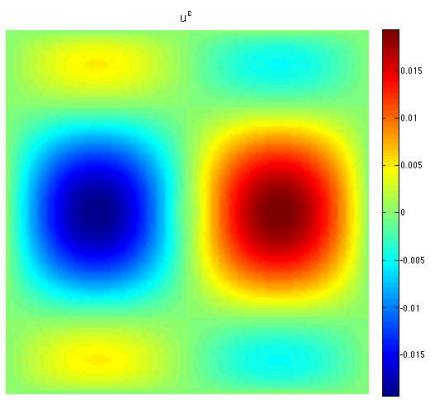


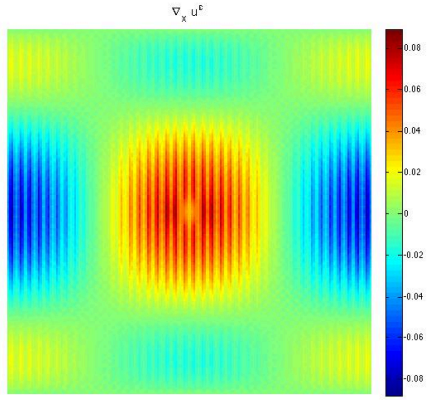


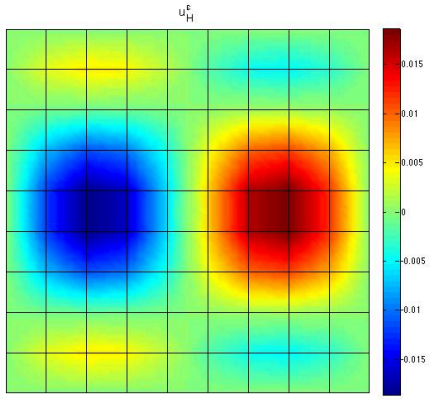
Quantity of interest: $Q(u) = \displaystyle\int_\omega [A_\varepsilon \nabla u^\varepsilon]_1$ with $|\omega| = 4\varepsilon \times 4\varepsilon$. Two cases:

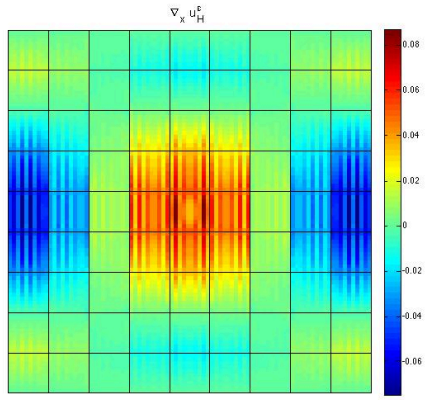
- ω_1 centered on the defect (Q_1)
- ω_2 far from the defect (Q_2)

Material with defect (top: exact; bottom: MsFEM sol.)







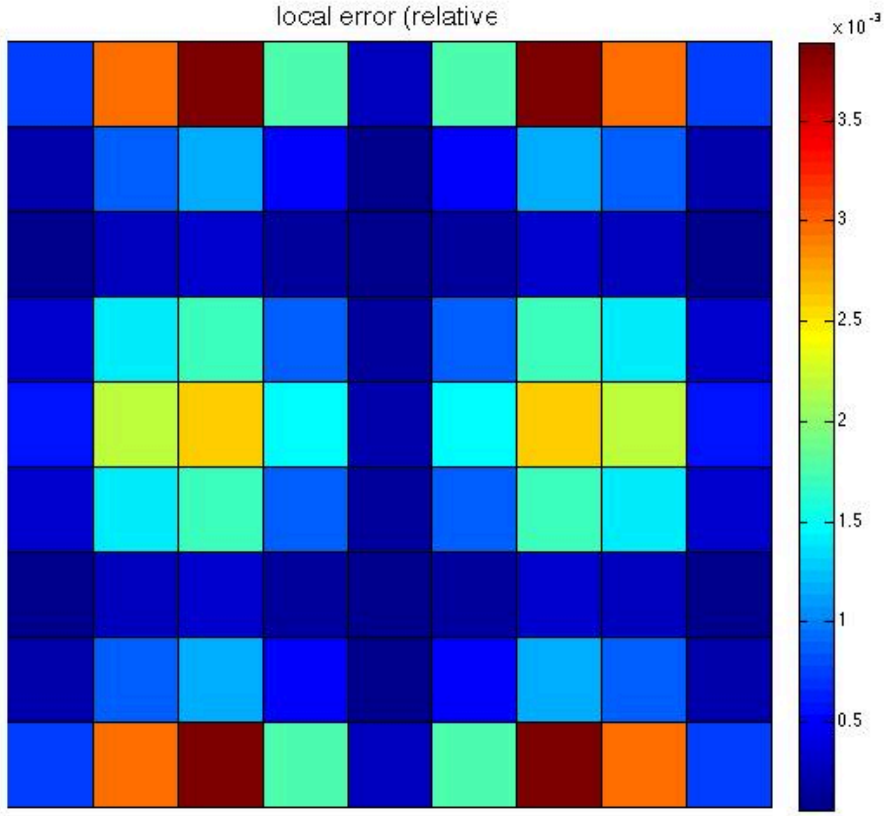


u^ε $\qquad\qquad$ $[\nabla u^\varepsilon]_1$

Crude computation: no oversampling, 9×9 macro elements, $h = \varepsilon/3$.

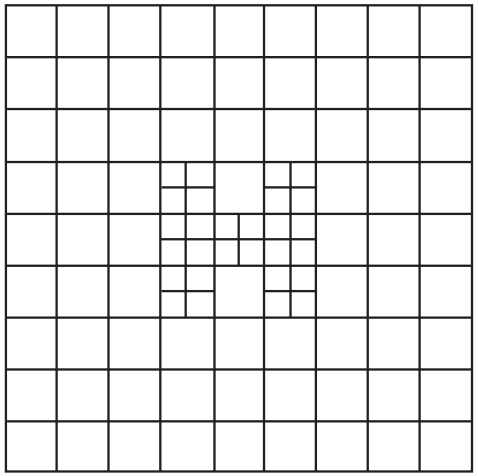
Initial error on the QoI ≈ 25 %.

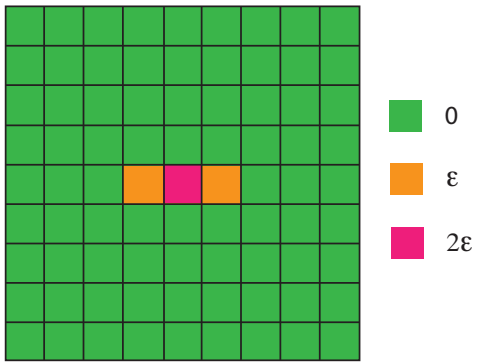
Material with defect (true error)



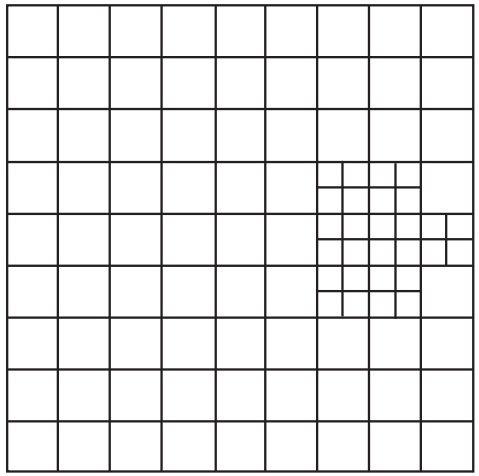
Initial error on the QoI $\approx$ 25 % (on purpose, initial computation not so accurate).

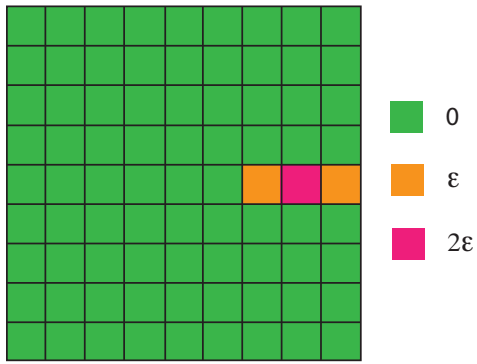
Adapted meshes: QoI Q_1 (left) vs Q_2 (center) vs global (right)



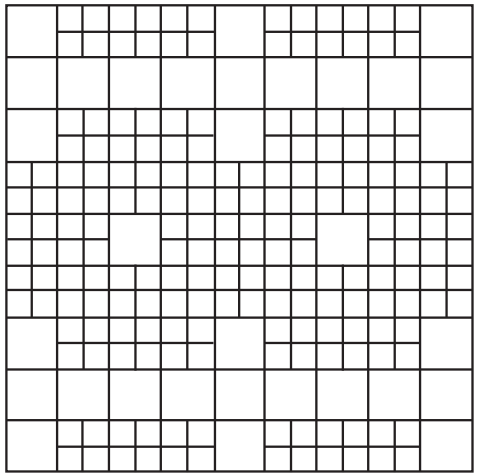


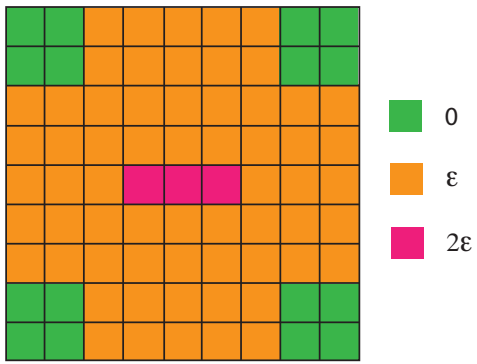
$Q_1(u)$





$Q_2(u)$

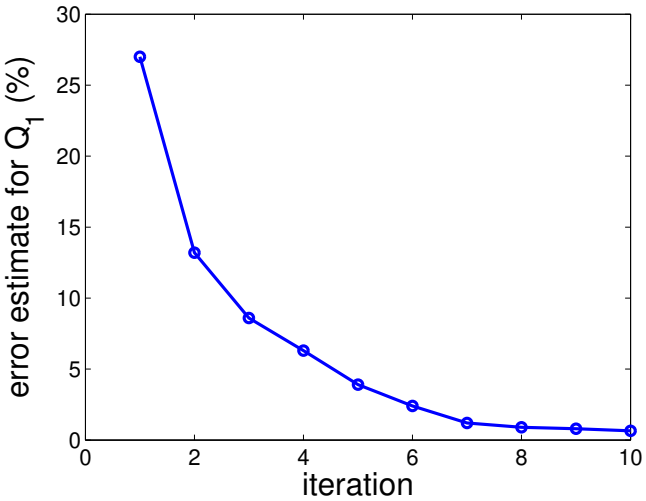


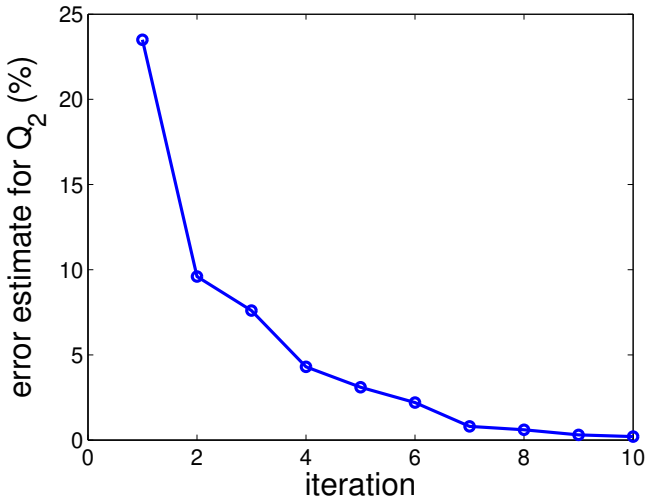


global

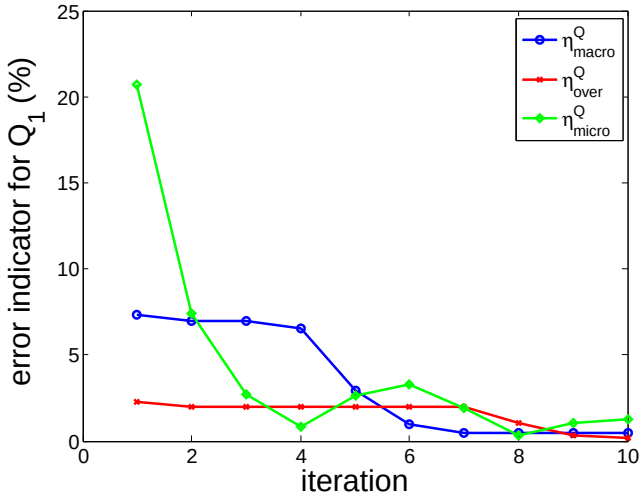
The adapted mesh is much coarser for the QoI.
No systematic need to refine around the defect, only around ω!

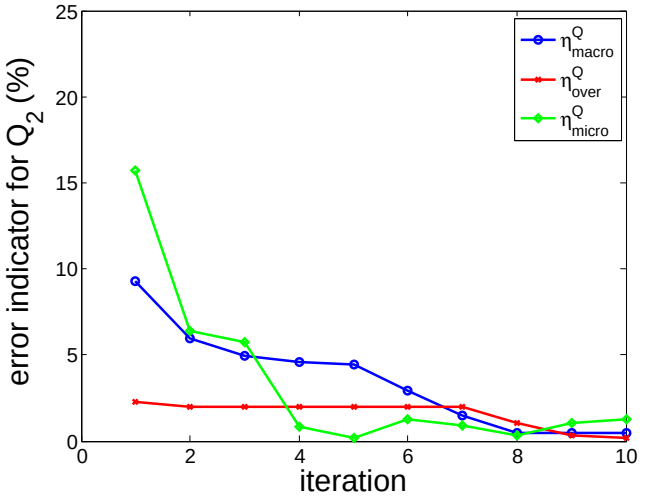
Convergence of the error estimate





Convergence of the error estimate (top) and of the error indicators (bottom) for Q_1 (left) and Q_2 (right)

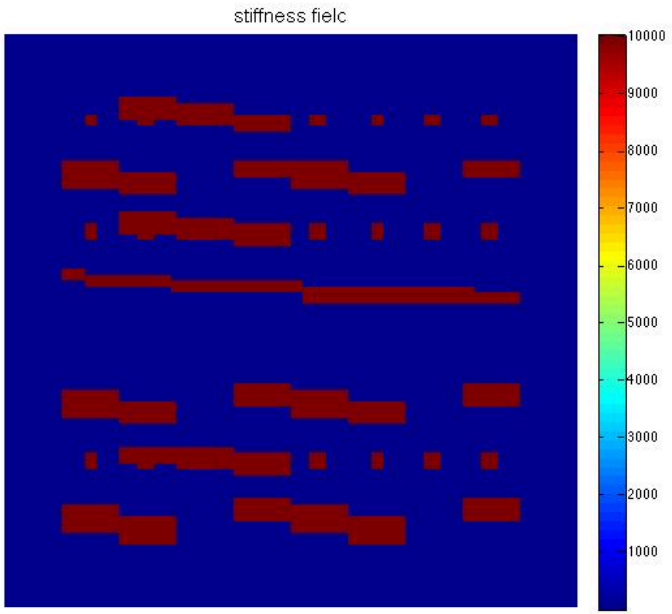




Another illustration: Darcy flow in porous medium

$$-\text{div}\left[A_\varepsilon(x)\nabla u^\varepsilon(x)\right] = f(x) \ \text{ in } \Omega, \qquad u^\varepsilon = 0 \ \text{ on } \partial\Omega$$

Take $f = 1_{K_1} - 1_{K_2}$, where $\begin{cases} K_1 = [0.1, 0.2] \times [0.8, 0.9], \\ K_2 = [0.8, 0.9] \times [0.1, 0.2]. \end{cases}$



Following Chung et al 2016:

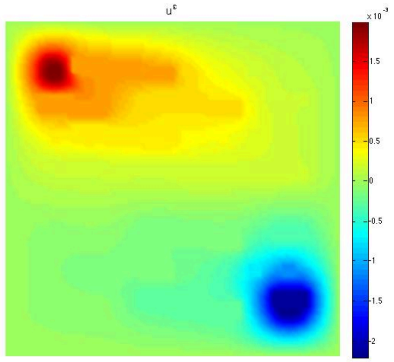
$$A_\varepsilon(x, y) = a_\varepsilon(x, y)\ I_2$$

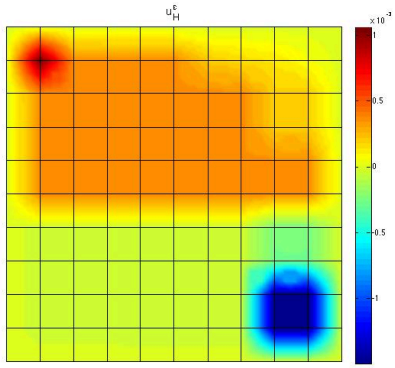
with $a_\varepsilon \equiv 10^4$ in the fractures,
$a_\varepsilon \equiv 1$ elsewhere.

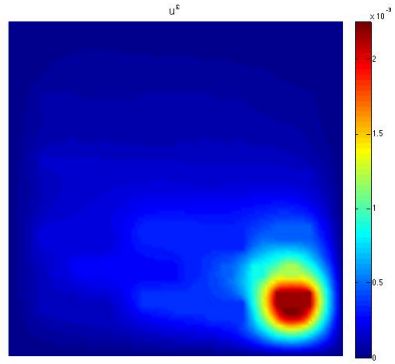
Quantity of interest: $Q(u) = \dfrac{1}{|K_2|} \displaystyle\int_{K_2} u$ (average value of u on the outflow region K_2).

Darcy flow: numerical results

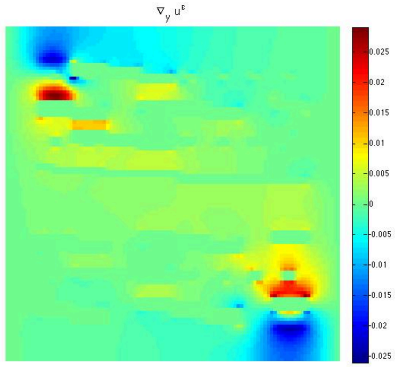
u^ε

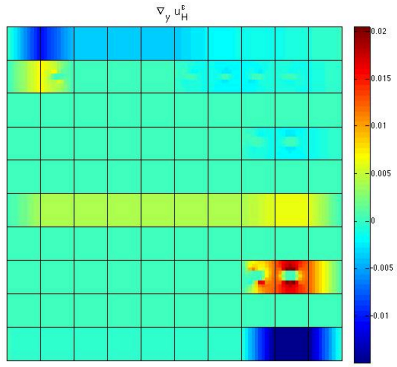


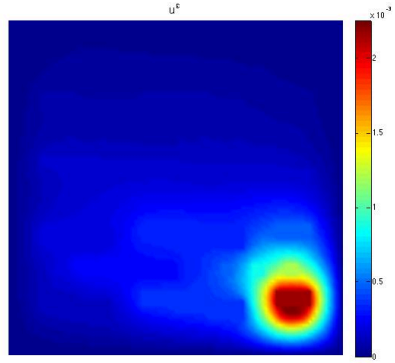




$[\nabla u^\varepsilon]_2$







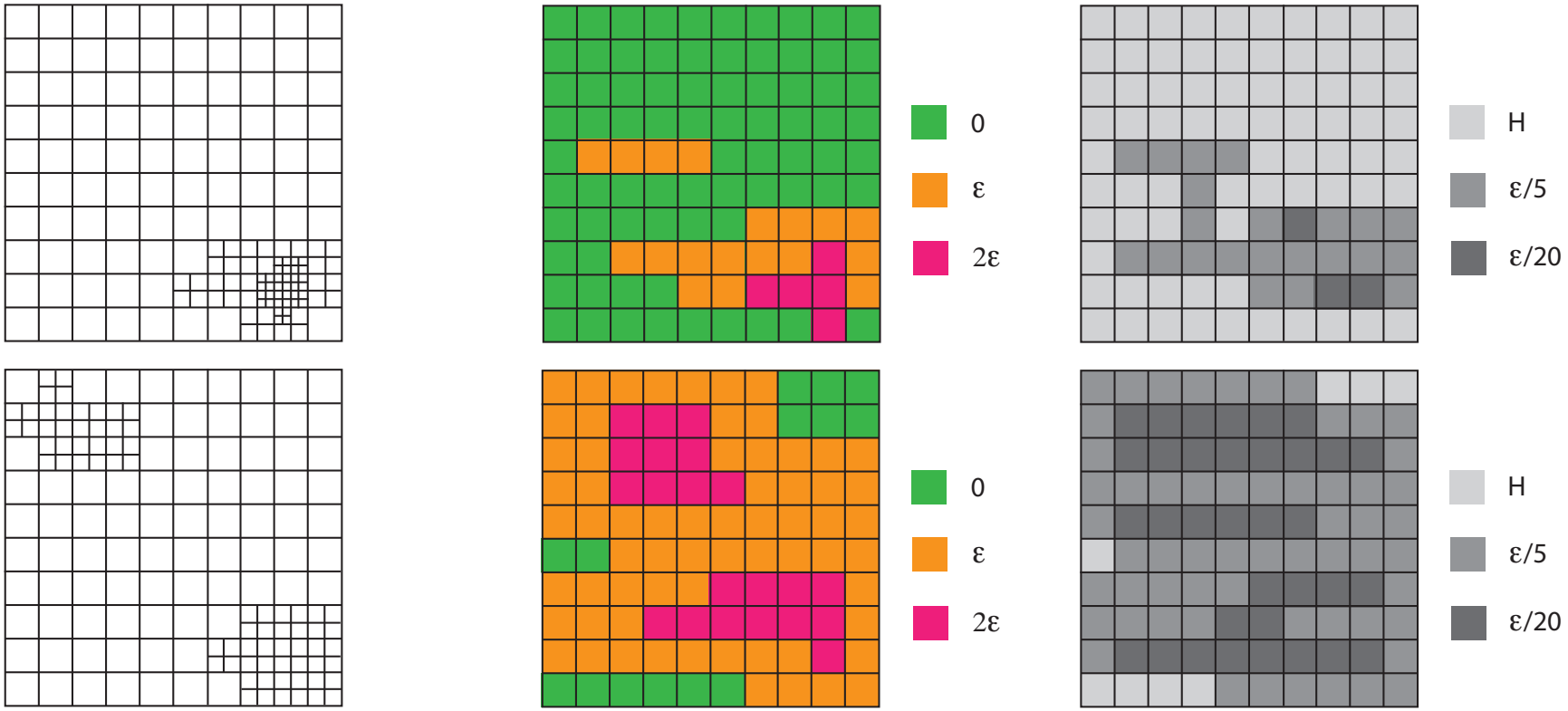
Primal pb (exact)

Primal pb (MsFEM)

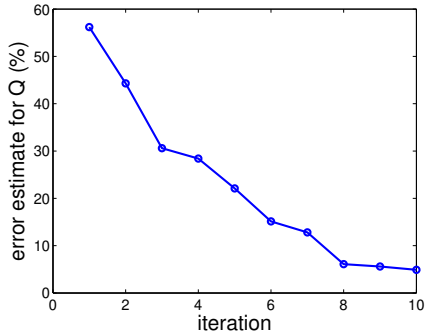
Adjoint problem (exact)

Crude computation: no oversampling, 10×10 macro elements, $h = H/10$

Darcy flow: adaptive strategy (error threshold: 1%)



Final MsFEM discretization for Q (top) and for the global error (bottom)

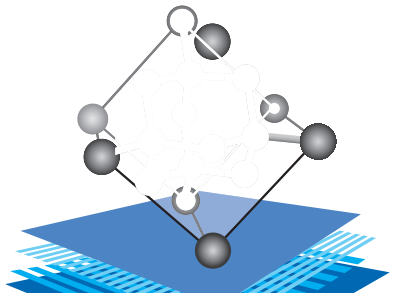


Conclusions

- We have introduced an a posteriori error estimation method:
  - compatible with the offline/online spirit of the MsFEM approach
  - ok for global error and error on quantities of interest
- Estimated Error $\approx$ True Error (within 10%)

Other works:

- Review article (L. Chamoin, F.L.): arXiv preprint 2110.02160
- A priori and a posteriori estimates for a different variant of MsFEM: F.L., P.-L. Rothé, C. Le Bris, U. Hetmaniuk, SIAM MMS 2022.



https://team.inria.fr/matherials/

Support from ONR and EOARD
is gratefully acknowledged.