Multi-Scale Finite Element Methods for Reaction-Diffusion Equations

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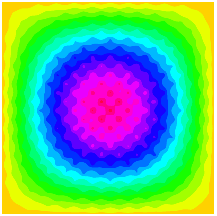
MATHerials

Multiscale models

We seek a numerical approximation of the **first eigencouple** $(u^\varepsilon, \lambda^\varepsilon)$ of the reaction-diffusion problem:

$$\frac{1}{\varepsilon^2}\sigma^\varepsilon u^\varepsilon - \operatorname{div}(A^\varepsilon \nabla u^\varepsilon) = \frac{\lambda^\varepsilon}{\varepsilon^2} u^\varepsilon \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial\Omega$$

Solution u^ε:



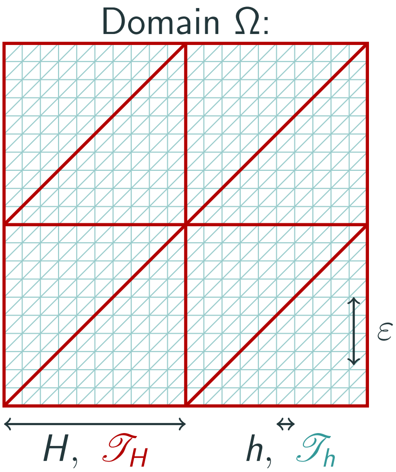
A^ε and σ^ε vary on a small scale ε

Finite element method (e.g. $\mathbb{P}_1$)

- Solution on a coarse mesh is wrong even on the macroscopic scale
- We would need a very fine mesh to get an accurate solution: prohibitively computationally expensive

We could use the homogenization theory in a periodic framework, but we do not want to restrict ourselves to this framework, or to the $\varepsilon \ll 1$ framework.

Multiscale Finite Element Method – MsFEM (Hou and Wu 1997)



- We discretize our domain Ω using a coarse mesh T_H. Each element of that coarse mesh is itself discretized on a fine mesh ($H > \varepsilon$ and $h \ll \varepsilon$).
- Instead of using $\mathbb{P}_1$ basis functions, we associate to each node i of the coarse mesh T_H, a well adapted basis function ϕ_i^ε.
- The basis functions ϕ_i^ε are computed off-line by solving local problems posed on each element of the coarse mesh (using the fine mesh discretization).

MsFEM

Multiscale Finite Element Method – MsFEM (Hou and Wu 1997)

1. Offline stage: compute local basis functions (expensive)

2. Online stage: one coarse global problem (inexpensive)

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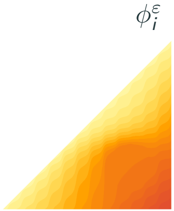
Multiscale basis functions:

$$\forall K \in \mathscr{T}_H, \quad \begin{cases} \mathscr{F}^\varepsilon(\phi_i^\varepsilon) = 0 & \text{in } K \\ +\text{Boundary conditions} & \text{on } \partial K \end{cases}$$

where $\mathscr{F}^\varepsilon$ is the operator of local problems we have to define.

2. Online stage: one coarse global problem (inexpensive)



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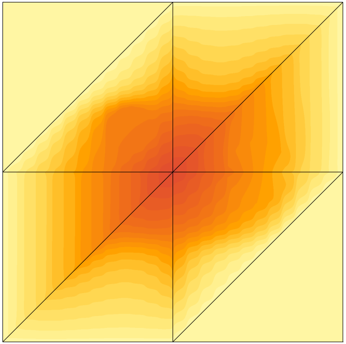
Variational Formulation: Find $u_H^\varepsilon \in V_H^\varepsilon = \text{span}\left\{\phi_j^\varepsilon\right\}$, $\lambda_H^\varepsilon \in \mathbb{R}$ s.t. $\forall \phi_i^\varepsilon$:

$$\frac{1}{\varepsilon^2}\int_\Omega \sigma^\varepsilon u_H^\varepsilon \phi_i^\varepsilon + \int_\Omega A^\varepsilon \nabla u_H^\varepsilon \cdot \nabla \phi_i^\varepsilon = \frac{\lambda_H^\varepsilon}{\varepsilon^2}\int_\Omega u_H^\varepsilon \phi_i^\varepsilon$$

ϕ_i^ε



Homogenization in a periodic framework

Theorem 1 (G. Allaire, Y. Capdeboscq, 2000)

Let $(\psi(y), \lambda^\infty)$ *be the first eigencouple of the cell problem:*

$$\sigma(y)\psi(y) - \operatorname{div}(A(y)\nabla\psi(y)) = \lambda^\infty\psi(y) \text{ in } Y, \quad y \mapsto \psi(y) \ Y\text{-periodic}$$

Then,

$$\boxed{u^\varepsilon(x) = v(x)\psi\left(\frac{x}{\varepsilon}\right) + o(1)}$$

and

$$\lambda^\varepsilon = \lambda^\infty + O(\varepsilon^2)$$

(v, ν) is the first eigencouple of the homogenized problem:

$$-\operatorname{div}(A^*\nabla v) = \nu v \quad \text{in } \Omega, \quad v = 0 \quad \text{on } \partial\Omega \tag{1}$$

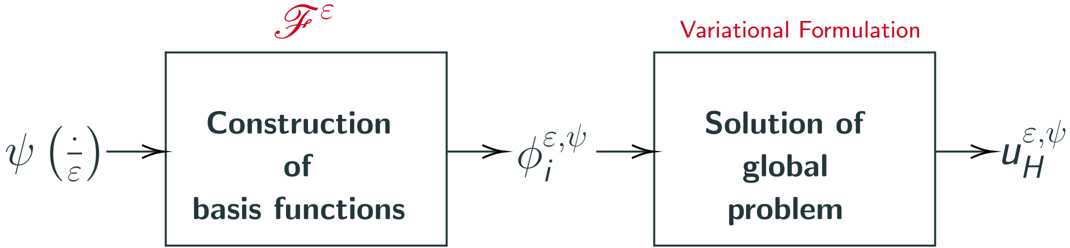
where A^* is the constant homogenized matrix, depending only on the coefficients A and σ.

Preliminary MsFEM approach

$$u^\varepsilon(x) = v(x)\psi\left(\frac{x}{\varepsilon}\right) + o(1)$$

The basis functions have to encode the microscopic behaviour of the solution.

- As a preliminary step, we first assume we know the eigenfunction ψ (we compute it off-line on a fine mesh).
- This function ψ is then used to construct the basis functions $\phi_i^{\varepsilon,\psi}$.



Preliminary MsFEM approach: Construction of basis functions

- We seek the first eigencouple $(u^\varepsilon, \lambda^\varepsilon)$ of the problem:

$$\frac{1}{\varepsilon^2}\sigma\left(\frac{x}{\varepsilon}\right) u^\varepsilon - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla u^\varepsilon\right) = \frac{\lambda^\varepsilon}{\varepsilon^2} u^\varepsilon \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial\Omega$$

  where A and σ are periodic functions.
- With the change of variables $v^\varepsilon = \dfrac{u^\varepsilon}{\psi(\frac{\cdot}{\varepsilon})}$, we get a generalized purely diffusive eigenvalue problem:

$$-\operatorname{div}\left(\psi^2\left(\frac{x}{\varepsilon}\right) A\left(\frac{x}{\varepsilon}\right)\nabla v^\varepsilon\right) = \frac{\nu^\varepsilon}{\varepsilon^2}\psi^2\left(\frac{x}{\varepsilon}\right) v^\varepsilon \text{ in } \Omega, \quad v_\varepsilon = 0 \text{ sur } \partial\Omega$$

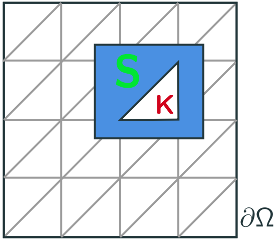
- We can solve this problem with the MsFEM-lin basis functions χ_i^ε:

$$\forall K \in \mathscr{T}_H, \quad \begin{cases} -\operatorname{div}\left(\psi^2\left(\frac{\cdot}{\varepsilon}\right) A\left(\frac{\cdot}{\varepsilon}\right)\nabla \chi_i^\varepsilon\right) = 0 & \text{in } K \\ \chi_i^\varepsilon = \chi_i^{\mathbb{P}_1} & \text{on } \partial K \end{cases}$$

- We use for the initial problem the basis functions $\boxed{\phi_i^{\varepsilon,\psi} = \chi_i^\varepsilon \psi(\frac{\cdot}{\varepsilon})}$.

  Spoiler: it works very nicely !

Actual numerical approach (1/3): A first (bad) idea



We now need to find a proxy for $\psi(\cdot/\varepsilon)$:

For each element **K** of the coarse mesh T_H, we construct a square-shaped oversampling patch **S**.

A possible idea: We consider the first eigencouple $(\widetilde{\psi}_S^\varepsilon, \widetilde{\lambda}_S^\varepsilon)$ of the problem on **S**:

$$\frac{1}{\varepsilon^2}\sigma^\varepsilon \widetilde{\psi}_S^\varepsilon - \mathrm{div}\left(A^\varepsilon \nabla \widetilde{\psi}_S^\varepsilon\right) = \frac{\lambda_S^\varepsilon}{\varepsilon^2}\widetilde{\psi}_S^\varepsilon \text{ in } \mathbf{S}, \quad x \mapsto \widetilde{\psi}_S^\varepsilon \ \mathbf{S}\text{-periodic}$$

- If **S** contains an integer number of periodic cells, then $\widetilde{\psi}_K^\varepsilon := \widetilde{\psi}_S^\varepsilon|_K = \psi(\frac{\cdot}{\varepsilon})$.
- If not, then $\widetilde{\psi}_K^\varepsilon$ can be very different of $\psi(\frac{\cdot}{\varepsilon})$!

Actual numerical approach (2/3): A filter idea

Suppose we want to approximate the average of g a 1-periodic function on $\mathbb{R}$
but we only have access to the function $g^\varepsilon := g(\frac{\cdot}{\varepsilon})$ over the domain $\Omega = (0,1)$.

- If $\dfrac{1}{\varepsilon}$ is an integer, then:

$$\frac{1}{|\Omega|}\int_\Omega g^\varepsilon = \frac{1}{\mathbb{Y}}\int_{\mathbb{Y}} g$$

- In general we have:

$$\left|\frac{1}{|\Omega|}\int_\Omega g^\varepsilon - \frac{1}{\mathbb{Y}}\int_{\mathbb{Y}} g\right| = O(\varepsilon)$$

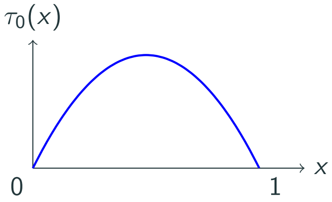
$\Rightarrow$ The idea now is to add a filter function to "mitigate" the fact that we are off by a certain fraction of a period at the boundary of the domain.

Actual numerical approach (2/3): A filter idea

Suppose we want to approximate the average of g a 1-periodic function on $\mathbb{R}$ **but** we only have access to the function $g^\varepsilon := g(\frac{\cdot}{\varepsilon})$ over the domain $\Omega = (0, 1)$.

- Let τ_0 a function so that

$$\begin{cases} \tau_0 > 0 \text{ in } (0,1) \\ \int_0^1 \tau_0(x)\, dx = 1 \\ \tau_0(0) = \tau_0(1) = 0 \end{cases}$$



- Then we have:

$$\left|\frac{1}{|\Omega|}\int_\Omega \tau_0 g^\varepsilon - \frac{1}{\mathbb{Y}}\int_{\mathbb{Y}} g\right| = O(\varepsilon^2)$$

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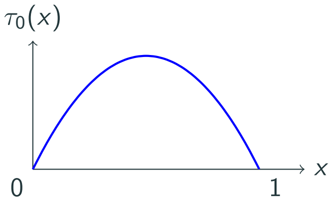


- Then we have:

$$\left|\frac{1}{|\Omega|}\int_\Omega \tau_0 g^\varepsilon - \frac{1}{\mathbb{Y}}\int_\mathbb{Y} g\right| = O(\varepsilon^2)$$

- And if $\tau_0^{(p)}(0) = \tau_0^{(p)}(1) = 0$ for $0 \le p \le P$, then the error is of order $O(\varepsilon^{P+2})$.

Actual numerical approach: MsFEM with oversampling

- The initial idea: We consider the first eigencouple $(\widetilde{\psi}_S^\varepsilon, \widetilde{\lambda}_S^\varepsilon) \in \left(H^1_{per}(\mathbf{S}), \mathbb{R}\right)$ s.t.

$$\forall v \in H^1_{per}(\mathbf{S}), \quad \int_{\mathbf{S}} \sigma^\varepsilon \widetilde{\psi}_S^\varepsilon v + \varepsilon^2 \int_{\mathbf{S}} A^\varepsilon \nabla \widetilde{\psi}_S^\varepsilon \cdot \nabla v = \lambda_S^\varepsilon \int_{\mathbf{S}} \widetilde{\psi}_S^\varepsilon v$$

- We define a filter τ on $\mathbf{S}$, such that τ and $\nabla\tau$ are zero on $\partial\mathbf{S}$.
- The new idea: We consider the first eigencouple $\widetilde{\psi}_S^\varepsilon \in H^1(\Omega), \lambda^\varepsilon \in \mathbb{R}$ (the smallest eigenvalue) and $\mu^\varepsilon \in \mathbb{R}^d$ (Lagrange multiplier) such that $\forall v \in H^1(\Omega), \mu \in \mathbb{R}^d$:

$$\begin{cases} \varepsilon^2 \int_{\mathbf{S}} \tau A^\varepsilon \nabla \widetilde{\psi}_S^\varepsilon \cdot \nabla v + \int_{\mathbf{S}} \tau \sigma^\varepsilon \widetilde{\psi}_S^\varepsilon v = \lambda^\varepsilon \int_{\mathbf{S}} \tau \widetilde{\psi}_S^\varepsilon v + \int_{\mathbf{S}} \tau \nabla v \cdot \mu^\varepsilon, \\ \int_{\mathbf{S}} \tau \nabla \widetilde{\psi}_S^\varepsilon \cdot \mu = 0 \end{cases}$$

Recall that in 1D, $\int_{\mathbf{S}} \nabla \widetilde{\psi}_S^\varepsilon = 0$ is equivalent to periodic BC. We note $\widetilde{\psi}^\varepsilon := \widetilde{\psi}_S^\varepsilon|_K$ on K.

Recall the Preliminary MsFEM method

$$\frac{1}{\varepsilon^2}\sigma\left(\frac{x}{\varepsilon}\right)u^\varepsilon - \operatorname{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla u^\varepsilon\right) = \frac{\lambda^\varepsilon}{\varepsilon^2}u^\varepsilon \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial\Omega$$

Assuming we know ψ,

- We introduce the MsFEM-lin basis functions χ_i^ε:

$$\forall K \in \mathscr{T}_H, \quad \begin{cases} -\operatorname{div}\left(\psi^2\left(\frac{\cdot}{\varepsilon}\right)A\left(\frac{\cdot}{\varepsilon}\right)\nabla\chi_i^\varepsilon\right) = 0 & \text{in } K \\ \chi_i^\varepsilon = \chi_i^{\mathbb{P}_1} & \text{on } \partial K \end{cases}$$

- We then use the basis functions $\boxed{\phi_i^{\varepsilon,\psi} = \chi_i^\varepsilon\psi(\frac{\cdot}{\varepsilon})}$.

$\Rightarrow$ And we now have at our disposal an accurate approximation of $\psi\left(\frac{\cdot}{\varepsilon}\right)$!

Actual MsFEM method

We proceed as in the preliminary approach, replacing everywhere $\psi(\frac{\cdot}{\varepsilon})$ by $\widetilde{\psi}^\varepsilon$.

- Rather than considering the MsFEM-lin basis functions χ_i^ε:

$$\forall K \in \mathcal{T}_H, \quad \begin{cases} -\operatorname{div}\left(\psi^2\left(\frac{\cdot}{\varepsilon}\right) A\left(\frac{\cdot}{\varepsilon}\right)\nabla\chi_i^\varepsilon\right) = 0 & \text{in } K \\ \chi_i^\varepsilon = \chi_i^{\mathbb{P}_1} & \text{on } \partial K \end{cases}$$

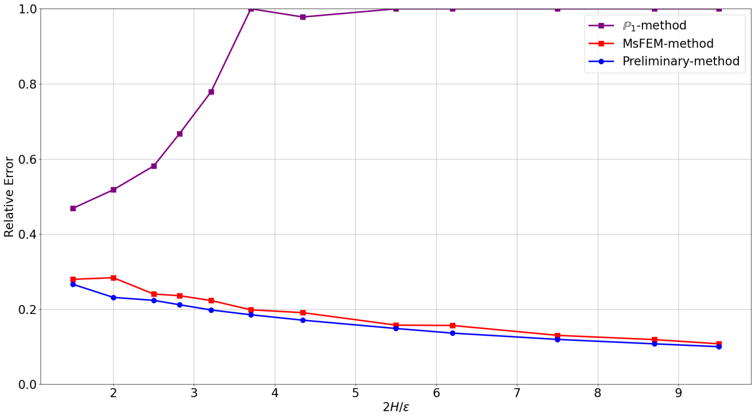
  we consider the functions $\overline{\chi}_i^\varepsilon$:

$$\forall K \in \mathcal{T}_H, \quad \begin{cases} -\operatorname{div}\left((\widetilde{\psi}^\varepsilon)^2 A\left(\frac{\cdot}{\varepsilon}\right)\nabla\overline{\chi}_i^\varepsilon\right) = 0 & \text{in } K \\ \overline{\chi}_i^\varepsilon = \chi_i^{\mathbb{P}_1} & \text{on } \partial K \end{cases}$$

- For the preliminary method we use the basis functions $\boxed{\phi_i^{\varepsilon,\psi} = \chi_i^\varepsilon \psi(\frac{\cdot}{\varepsilon})}$.
- For the actual method we use the basis functions $\boxed{\phi_i^{\varepsilon,\widetilde{\psi}} = \overline{\chi}_i^\varepsilon \widetilde{\psi}^\varepsilon}$.

H^1 relative error (periodic coefficients)

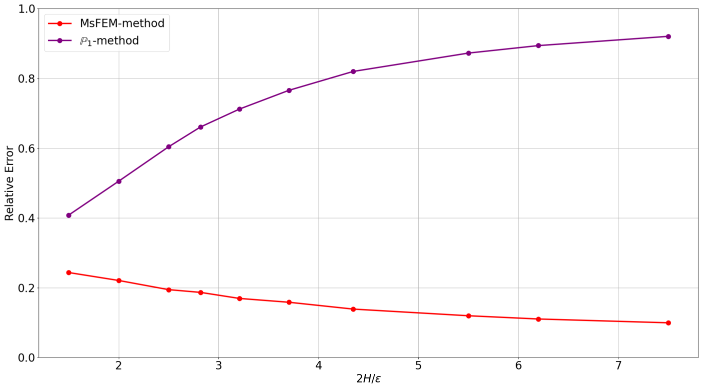
$$A(x,y) = 6 + 5\cos(2\pi(x+2y))\sin(2\pi(x-y)) \qquad \sigma(x,y) = 20\,(2+\cos(2\pi(x-2y))\sin(2\pi(x-y)))$$



H^1 error around 15-20%

H^1 relative error (Quasi-periodic coefficients)

$$A^\varepsilon(x,y) = \left(5 + 1.25\left(\cos\left(\frac{2\pi x}{\varepsilon}\right) + \cos\left(\frac{2\sqrt{2}\pi x}{\varepsilon}\right)\right)\left(\sin\left(\frac{2\pi y}{\varepsilon}\right) + \sin\left(\frac{2\sqrt{2}\pi y}{\varepsilon}\right)\right)\right)$$
$$\sigma^\varepsilon(x,y) = 40\left(2 + 0.25\left(\cos\left(\frac{2\pi x}{\varepsilon}\right) + \cos\left(\frac{2\sqrt{2}\pi x}{\varepsilon}\right)\right)\left(\sin\left(\frac{2\pi y}{\varepsilon}\right) + \sin\left(\frac{2\sqrt{2}\pi y}{\varepsilon}\right)\right)\right)$$



H^1 error around 15-20% again

Multi-query contexts

MsFEM (as any multiscale numerical approach) is beneficial in multi-query problems. Here, the multi-query context comes:

- In the time-dependent setting, from the fact that we consider several time steps.
- For the eigenproblem, from the fact that we can consider several eigencouples (and not only the first one).
- For the eigenproblem, with a spatial recombination of the diffusion and reaction coefficients.

Multi-query context: consideration of several eigencouples

We can seek a numerical approximation of other eigencouples $(u^{\varepsilon,m}, \lambda^{\varepsilon,m})$ of the reaction-diffusion problem:

$$\frac{1}{\varepsilon^2}\sigma^\varepsilon u^{\varepsilon,m} - \operatorname{div}(A^\varepsilon \nabla u^{\varepsilon,m}) = \frac{\lambda^{\varepsilon,m}}{\varepsilon^2} u^{\varepsilon,m} \text{ in } \Omega, \quad u^{\varepsilon,m} = 0 \text{ on } \partial\Omega$$

where $u^{\varepsilon,m}$ is the eigenvector associated to the m-th eigenvalue $\lambda^{\varepsilon,m}$.

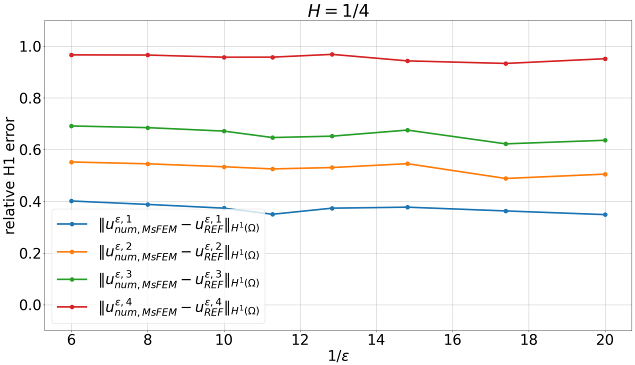
We have actually the following homogenization result (in the periodic setting):

$$\boxed{u^{\varepsilon,m}(x) = v^m(x)\psi\left(\frac{x}{\varepsilon}\right) + o(1)}$$

where (v^m, ν^m) is the m-th eigencouple of the homogenized problem:

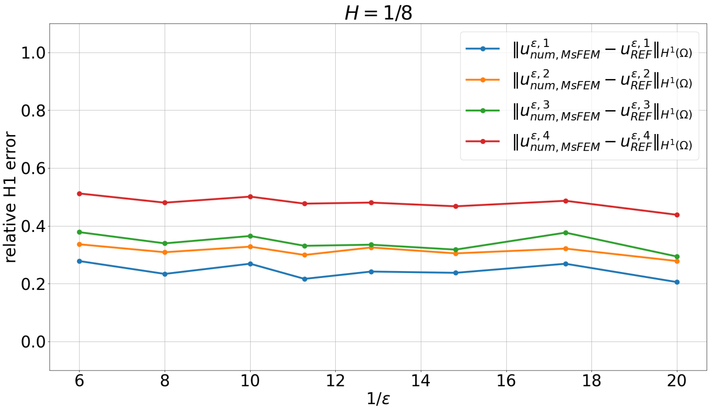
$$-\operatorname{div}(A^* \nabla v) = \nu v \quad \text{in } \Omega, \quad v = 0 \quad \text{on } \partial\Omega \tag{2}$$

Multi-query context: consideration of several eigencouples

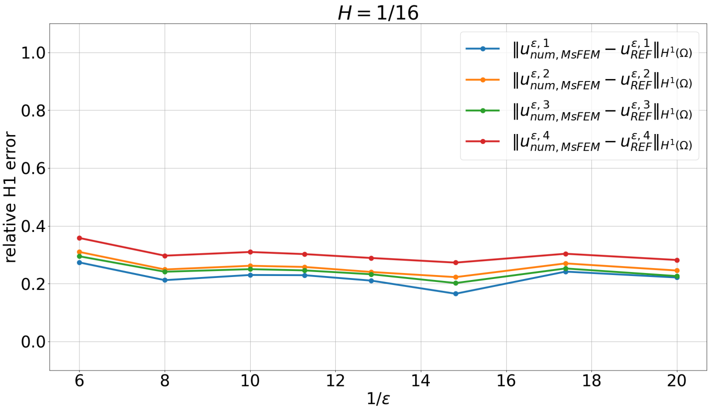


- The first eigenvalue is simple.
- Eigenvectors $u^{\varepsilon,1}$ and $u^{\varepsilon,2}$ are associated to the same double eigenvalue.
- The eigenvector $u^{\varepsilon,3}$ is associated to a simple eigenvalue.

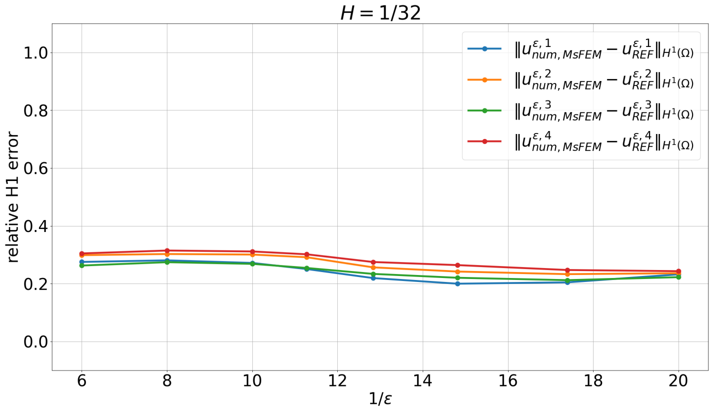
Multi-query context: consideration of several eigencouples



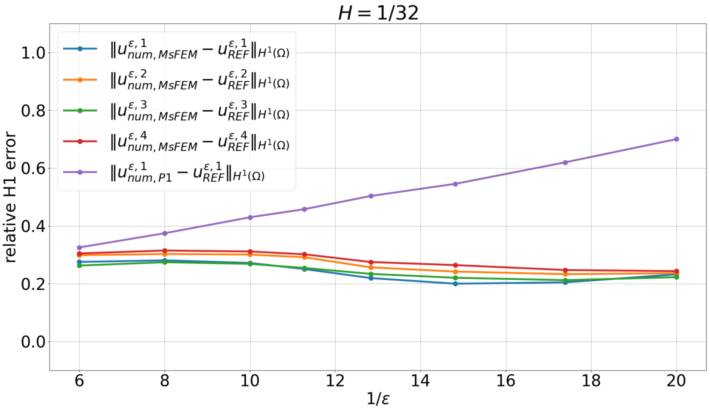
Multi-query context: consideration of several eigencouples



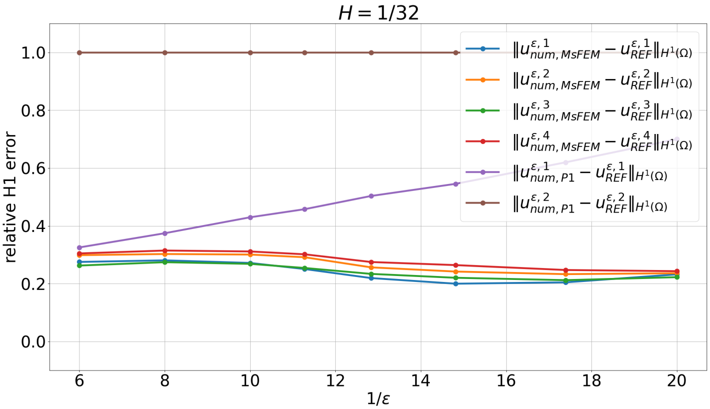
Multi-query context: consideration of several eigencouples



Multi-query context: consideration of several eigencouples



Multi-query context: consideration of several eigencouples



Conclusion

- We have introduced a preliminary MsFEM approach, restricted to the periodic setting. It yields accurate results and is amenable to an error analysis.
- We have next introduced an approximation of ψ using filtering ideas, the resulting practical MsFEM approach yields accurate results (only a small loss wrt preliminary approach).

This MsFEM approach can also be applied to solve the problems (not presented here):

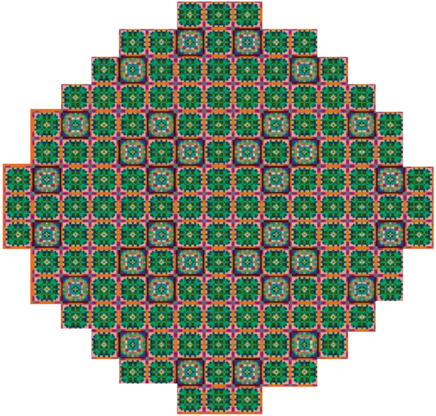
- The time-dependent problem, either with a time-stepping method, or by decomposing the solution on the eigenvectors of the operator.
- The vectorial reaction diffusion problem (relevant from the application viewpoint; mathematically challenging because not self-adjoint).

The support from ONR and EOARD is gratefully acknowledged.

References

- Grégoire Allaire and Yves Capdeboscq, *Homogenization of a spectral problem in neutronic multigroup diffusion*, Computer Methods in Applied Mechanics and Engineering **187** (2000), no. 1, 91–117.
- Grégoire Allaire and François Malige, *Analyse asymptotique spectrale d'un problème de diffusion neutronique*, Comptes Rendus de l'Académie des Sciences - Series I - Mathematics **324** (1997), no. 8, 939–944.
- Xavier Blanc and Claude Le Bris, *Homogenization Theory for Multiscale Problems: An introduction*, MS&A, vol. 21, Springer Nature Switzerland, Cham, 2023.
- Thomas Y. Hou and Xiao-Hui Wu, *A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media*, Journal of Computational Physics **134** (1997), no. 1, 169–189.

Multi-query context: spatial recombination of the coefficients



Assemblies are reordered to obtain the most homogeneous neutron flux in the reactor core.

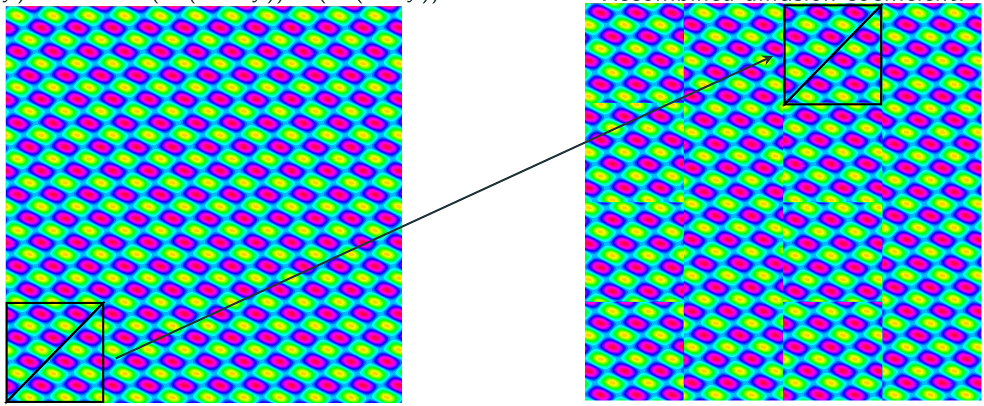
For each spatial combination, the first eigencouple $(u^\varepsilon, \lambda^\varepsilon)$ has to be computed.

The number of combinations is huge, so MsFEM is going to be really beneficial in this context.

Multi-query context: spatial recombination of the coefficients

$A(x,y) = 6 + 5\cos(2\pi(x+2y))\sin(2\pi(x-y))$:

Recombined diffusion coefficient:



The basis functions are reordered, in the same way as the coefficients, so that we do not have to do any offline computation again.

Appendix

A^* is the homogenized matrix defined by:

$$A^*_{ij} = \int_Y \psi^2(y)A(y)\left(\nabla w_j + e_j\right) \cdot e_i dy$$

where w_i are the correctors, solutions of:

$$-\operatorname{div}_y \left(\psi^2 A\left(\nabla_y w_i + e_i\right)\right) = 0 \quad \text{in } Y, \quad y \mapsto w_i(y) \ \ Y\text{-periodic}$$