Multi-Scale Finite Element Methods for Reaction-Diffusion Equations

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Multiscale models

Our study focuses on the **multi-scale reaction diffusion equation** with highly oscillatory coefficients. One possible application is to model the neutron flux in a nuclear reactor core whose microstructure is heterogeneous.

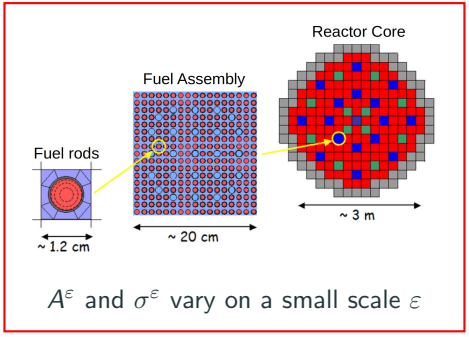
Two settings are interesting for the reaction diffusion equation: the **time-dependent setting** and the associated **eigenvalue problem**. We focus here on the latter.

$\Rightarrow$ Our goal is to develop a Multi-scale Finite Element Method, to solve this eigenvalue problem numerically.

Multiscale models

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

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



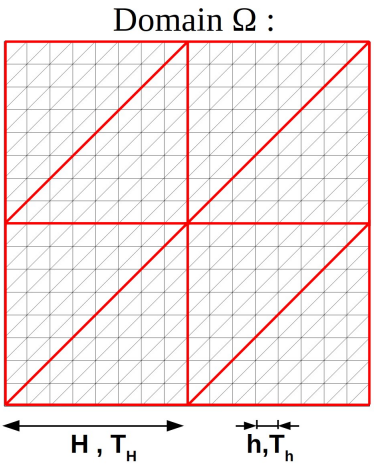
A^ε and σ^ε vary on a small scale ε

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.

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)

MsFEM

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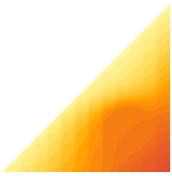
Multiscale basis functions:

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

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

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

ϕ_i^ε



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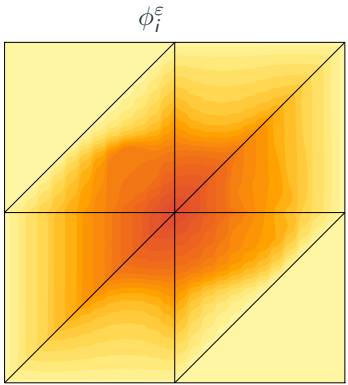
Variational Formulation: Find $u_H^\varepsilon \in V_H^\varepsilon = \text{span}\left\{\phi_j^\varepsilon\right\}$, $\lambda_H^\varepsilon \in \mathbb{R}$ s.t. $\forall\, \phi_i^\varepsilon$:

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



Homogenization

The delicate task lies in finding the adequate operator $\mathscr{F}^\varepsilon$ to use in the local problems. We make partial use of homogenization theory in a periodic framework to guide our intuition.

In this periodic framework, we therefore seek the first eigencouple $(u^\varepsilon, \lambda^\varepsilon)$ of:

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

where A and σ are periodic functions.

Homogenization

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,

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

and

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

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

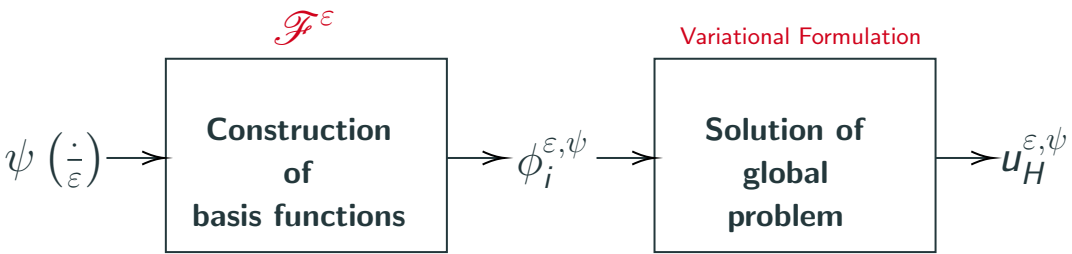
$$-\operatorname{div}(A^*\nabla v) = \nu v \quad \text{in } \Omega, \quad v = 0 \quad \text{on } \partial\Omega \tag{1}$$

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

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

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 method: 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:

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

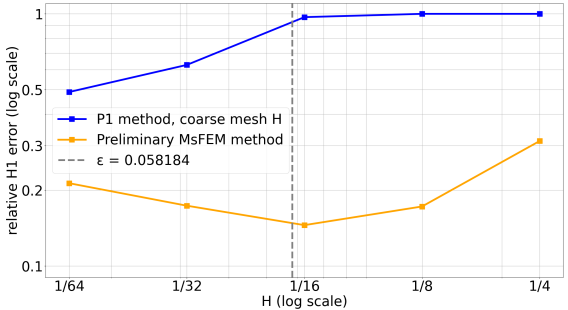
We can solve this problem with the MsFEM-lin basis functions χ_i^ε:

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

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

Preliminary MsFEM method: Numerical results

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



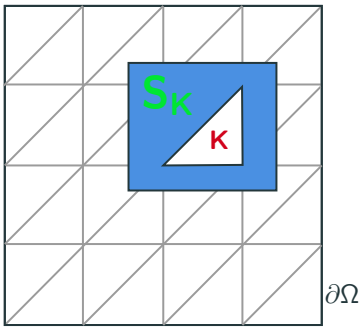
We compute on a fine mesh T_h a reference solution u^{ε}_{ref} with the $\mathbb{P}^1$ Finite Element Method. We define the relative H^1 error as:

$$\frac{\left\| u^{\varepsilon}_{num} - u^{\varepsilon}_{ref} \right\|_{H^1(\Omega)}}{\left\| u^{\varepsilon}_{ref} \right\|_{H^1(\Omega)}}$$

- The $\mathbb{P}^1$-method error confirms the multiscale character of the problem.
- The preliminary MsFEM method gives a much better approximation of the solution.

$\Rightarrow$ We will now try to obtain results as accurate as those of this preliminary method without the a priori knowledge of the function ψ.

Actual numerical approach: MsFEM with oversampling



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 $\mathbf{S_K}$.

We compute on the fine mesh T_h the first eigencouple $\left(\tilde{\psi}^{\varepsilon}_{S_K}, \tilde{\lambda}^{\varepsilon}_{S_K}\right)$ of the problem on $\mathbf{S_K}$:

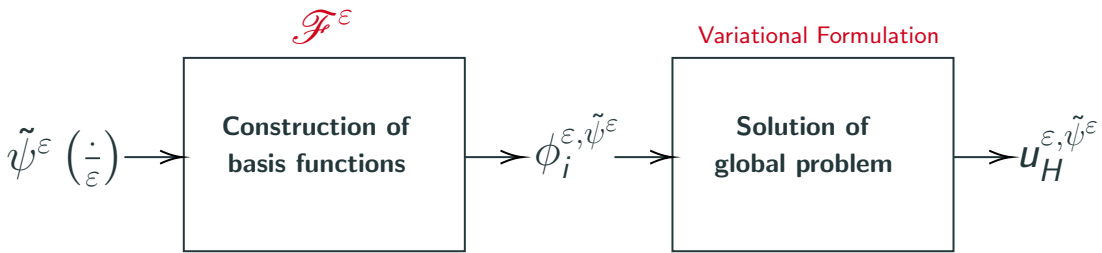
$$\frac{1}{\varepsilon^2}\sigma^{\varepsilon}\tilde{\psi}^{\varepsilon}_{S_K} - \operatorname{div}\left(A^{\varepsilon}\nabla\tilde{\psi}^{\varepsilon}_{S_K}\right) = \frac{\lambda^{\varepsilon}_{S_K}}{\varepsilon^2}\tilde{\psi}^{\varepsilon}_{S_K} \text{ in } \mathbf{S_K}, \quad x \mapsto \tilde{\psi}^{\varepsilon}_{S_K} \ \mathbf{S_K}\textbf{-periodic}$$

We then define $\forall\, \mathbf{K} \in T_H$: $\tilde{\psi}^{\varepsilon}_{K} = \tilde{\psi}^{\varepsilon}_{S_K}|_K$

Actual numerical approach: MsFEM with oversampling

We are aiming at (and we indeed numerically observe that): $\tilde{\psi}_K^\varepsilon(x) \approx \psi(\frac{x}{\varepsilon})$ on K.

We then use the same construction of basis functions as in the preliminary method, but with $\tilde{\psi}^\varepsilon = \{\tilde{\psi}_K^\varepsilon\}_{K \in \mathcal{T}_H}$ instead of $\psi(\frac{\cdot}{\varepsilon})$:



$\Rightarrow$ This MsFEM-with-oversampling method does not rely on the periodicity of the problem.

MsFEM with oversampling: construction

Denote $\tilde{\psi}^\varepsilon$ the function such that: $\tilde{\psi}^\varepsilon|_K = \tilde{\psi}^\varepsilon_K$.

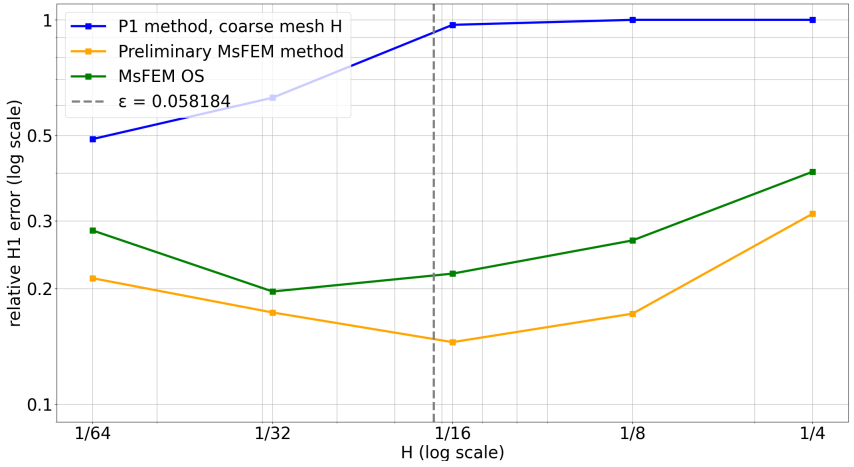
- From the function $\tilde{\psi}^\varepsilon$, construct the MsFEM-lin basis functions $\chi_i^{\varepsilon,\tilde{\psi}^\varepsilon}$:

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

- Therefore, for the initial problem, we use the basis functions $\boxed{\phi_i^{\varepsilon,\tilde{\psi}^\varepsilon} = \chi_i^{\varepsilon,\tilde{\psi}^\varepsilon}\,\tilde{\psi}^\varepsilon}$.

Actual numerical approach: MsFEM with oversampling

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



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:

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

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

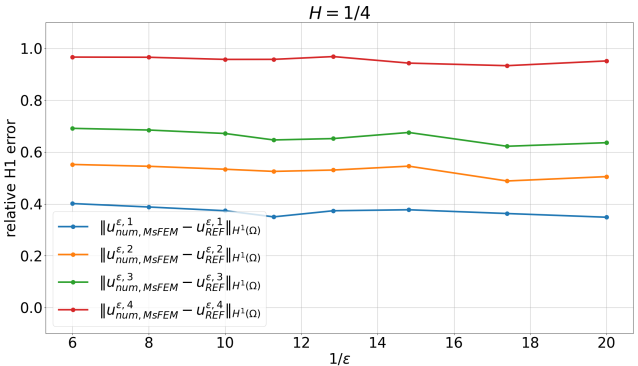
We have actually the following homogenization result (in the periodic setting):

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

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

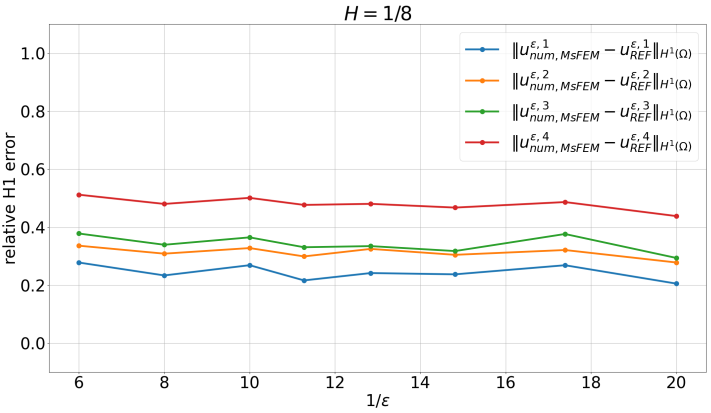
$$-\operatorname{div}\left(A^*\nabla v\right) = \nu v \quad \text{in } \Omega, \quad v = 0 \quad \text{on } \partial\Omega \tag{2}$$

Multi-query context: consideration of several eigencouples

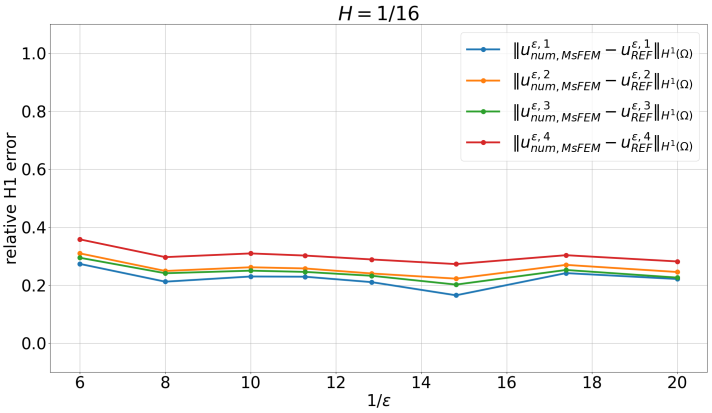


- The first eigenvalue is simple.
- Eigenvectors $u^{\varepsilon,1}$ and $u^{\varepsilon,2}$ are associated to the same double eigenvalue.
- The eigenvector $u^{\varepsilon,3}$ is associated to a simple eigenvalue.

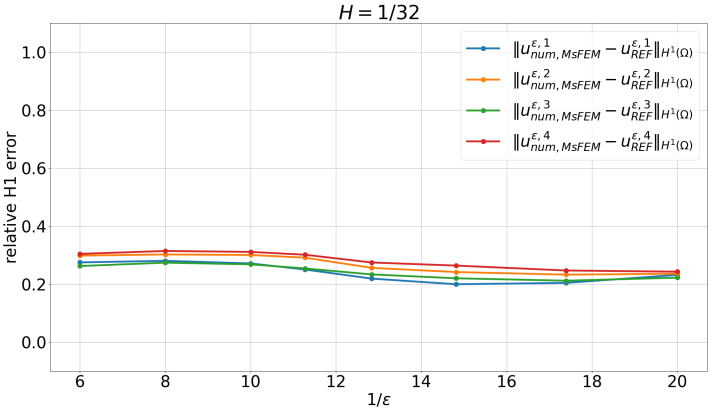
Multi-query context: consideration of several eigencouples



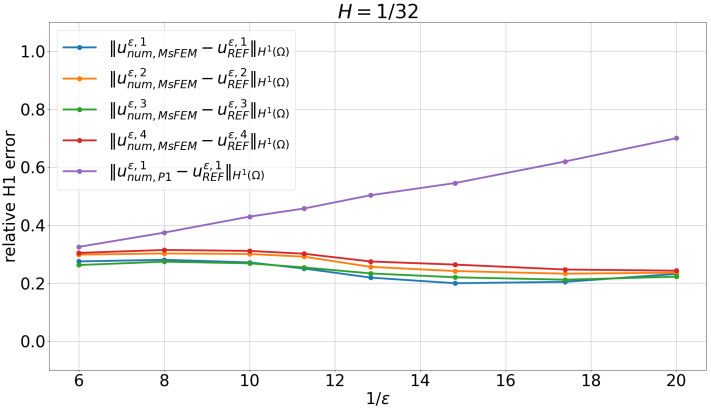
Multi-query context: consideration of several eigencouples



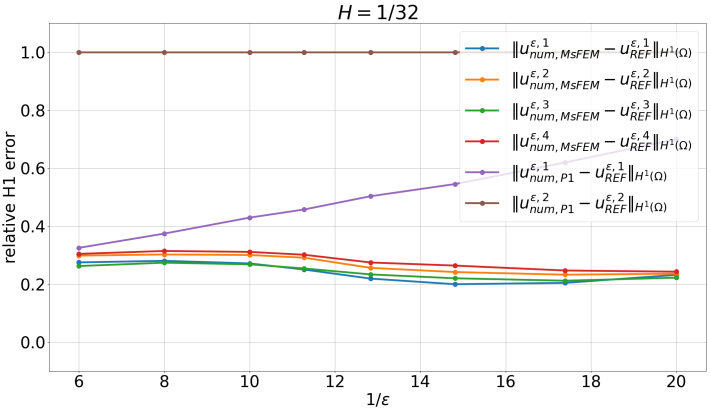
Multi-query context: consideration of several eigencouples



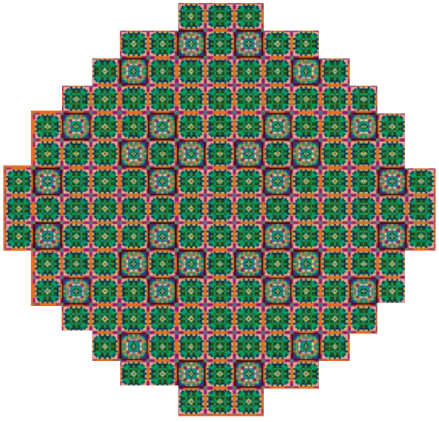
Multi-query context: consideration of several eigencouples



Multi-query context: consideration of several eigencouples



Multi-query context: spatial recombination of the coefficients



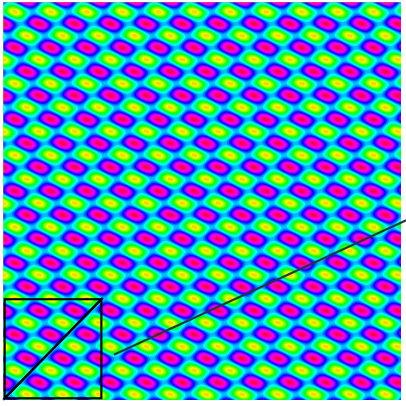
Assemblies are reordered to obtain the most homogeneous neutron flux in the reactor core.

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

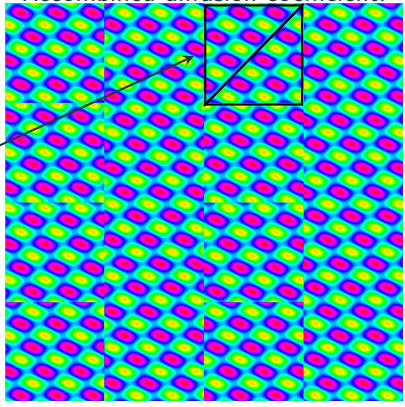
The number of combinations is huge, so MsFEM is going to be really beneficial in this context.

Multi-query context: spatial recombination of the coefficients

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

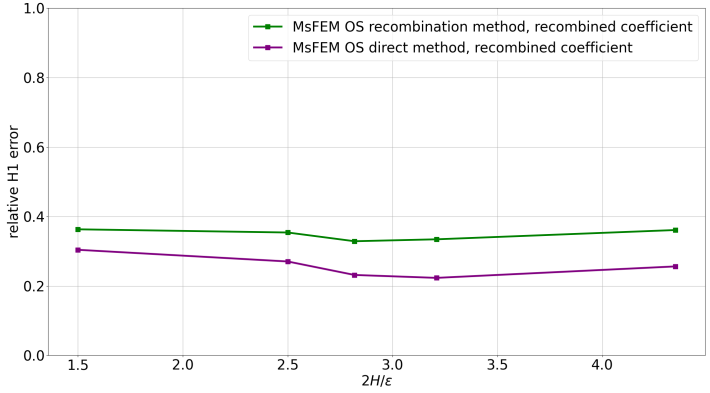


Recombined diffusion coefficient:



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

Multi-query context: spatial recombination of the coefficients



if we do not go through the offline stage again, the error increases from 30% to 35%,

while the computation time is very significantly reduced.

Future Work

- Resolution of the time-dependent problem with the MsFEM-with-oversampling method, either with a time-stepping method, or by decomposing the solution on the eigenvectors of the operator.

- Adaptation of the MsFEM-with-oversampling method to other reaction diffusion equations, such as vectorial variants.

The support from ONR and EOARD is gratefully acknowledged.

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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:

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