AN INTRODUCTION TO MULTISCALE FINITE ELEMENT METHODS FOR NUMERICAL HOMOGENIZATION

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MULTIMAT meeting, Paris, 14-16 March 2005

1. Introduction
2. A few words about periodic homogenization
3. A few words about classical finite element methods
4. Multiscale finite element methods
5. Another homogenization paradigm

-I- INTRODUCTION

Goal of numerical homogenization: compute the behavior of an heterogeneous medium (with lengthscale ϵ) using a mesh of size $h >> \epsilon$.

☞ A homogenized model is not enough: we want some details about microscopic fluctuations.

☞ There may be many scales ϵ: beware of resonances $h \approx \epsilon$.

☞ A model problem or a paradigm of homogenization must be chosen in order to guide the conception of a multiscale numerical method.

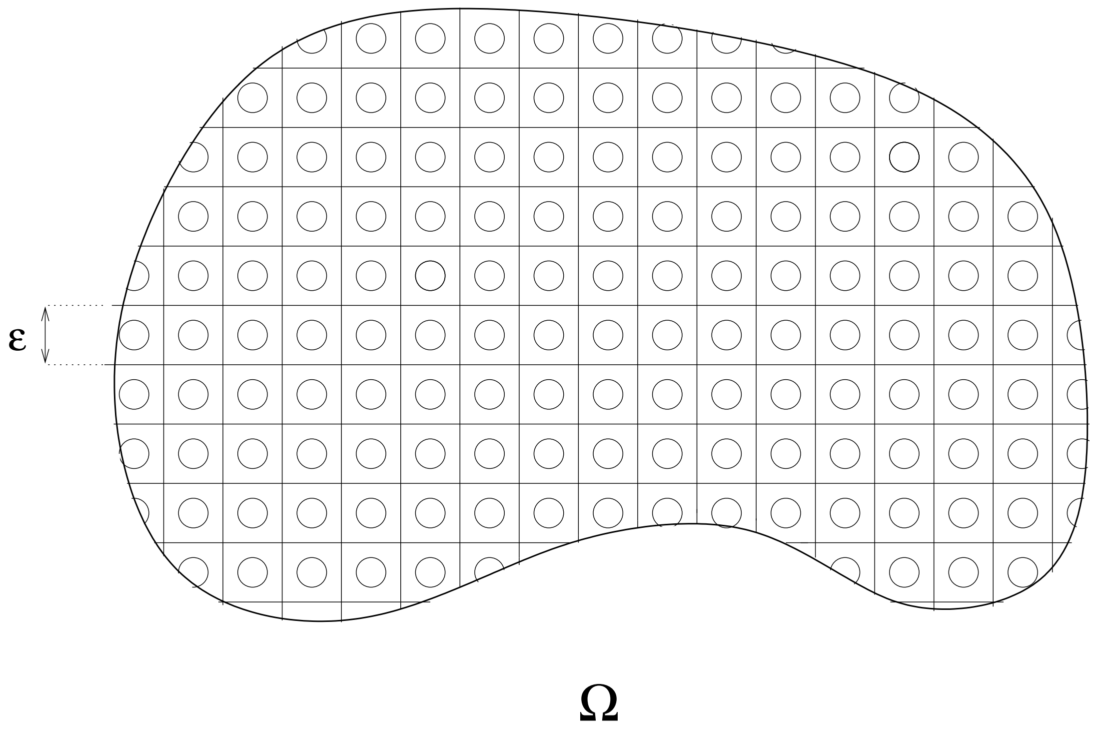
☞ Many works on this topic: Arbogast, Hou, Efendiev, Babuska, Matache, Schwab, E, Engquist, Capdeboscq, Vogelius...

☞ Although the real problems are not periodic, we shall use periodic homogenization as a guideline.

-II- BASIC FACTS IN PERIODIC HOMOGENIZATION

Model problem: diffusion in a periodic medium characterized by the tensor

$$A(y) \quad \text{with} \quad y = \frac{x}{\epsilon} \in Y = (0,1)^N$$



DEFINITION OF HOMOGENIZATION

- ☞ Rigorous version of averaging
- ☞ Process of asymptotic analysis
- ☞ Extract effective or homogenized parameters for heterogeneous media
- ☞ Derive simpler macroscopic models from complicated microscopic models
- ☞ Different methods :
  - two-scale asymptotic expansions for periodic media
  - H- or G-convergence for general media
  - stochastic, or variational methods

TWO-SCALE ASYMPTOTIC EXPANSIONS

Stationary diffusion equation

$$\begin{cases} -\mathrm{div}\,\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases}$$

with a coefficient tensor $A(y)$ which is Y-periodic, uniformly coercive and bounded

$$\alpha|\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(y)\xi_i\xi_j \leq \beta|\xi|^2, \quad \forall\, \xi \in \mathbb{R}^N, \forall\, y \in Y \quad (\beta \geq \alpha > 0).$$

HOMOGENIZATION AND ASYMPTOTIC ANALYSIS

- Direct solution too costly if ϵ is small
- Averaging: replace $A(y)$ by effective homogeneous coefficients
- Asymptotic analysis: limit as $\epsilon \to 0$
  yields a rigorous definition of the homogenized parameters
- Error estimates: compare exact and homogenized solutions
- Similar to Representative Volume Element method
- Huge literature

Representative Volume Element method

Mesoscale $\epsilon << h << 1$. A Representative Volume Element is a cube of size h. We average all quantities in this cube:

☞ u is the average of the field u_ϵ

☞ ξ is the average of the gradient ∇u_ϵ

☞ σ is the average of the flux $A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon$

☞ e is the average of the energy density $A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon \cdot \nabla u_\epsilon$

Definition of the homogenized tensor A^*:

$$\sigma = A^*\xi, \quad e = A^*\xi \cdot \xi, \quad \xi = \nabla u.$$

Questions: is it possible to find such a tensor A^* ? Does it depend on ϵ, h, f, u, the boundary conditions ? How to compute it ?

Asymptotic analysis

Rather than considering a single heterogeneous medium with a fixed lengthscale ϵ_0, the problem is embedded in a sequence of similar problems parametrized by a lengthscale ϵ.

Homogenization amounts to perform an asymptotic analysis when $\epsilon \to 0$

$$\lim_{\epsilon \to 0} u_\epsilon = u.$$

The limit u is the solution of an homogenized problem, the conductivity tensor of which is called the effective or homogenized conductivity.

This yields a coherent definition of homogenized properties which can be rigorously justified by quantifying the resulting error estimate.

TWO-SCALE ASYMPTOTIC EXPANSIONS

Ansatz for the solution

$$u_\epsilon(x) = \sum_{i=0}^{+\infty} \epsilon^i u_i\left(x, \frac{x}{\epsilon}\right),$$

with $u_i(x, y)$ function of both variables x and y, periodic in y

Derivation rule

$$\nabla\left(u_i\left(x, \frac{x}{\epsilon}\right)\right) = \left(\epsilon^{-1}\nabla_y u_i + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right)$$

$$\nabla u_\epsilon(x) = \epsilon^{-1}\nabla_y u_0\left(x, \frac{x}{\epsilon}\right) + \sum_{i=0}^{+\infty} \epsilon^i\left(\nabla_y u_{i+1} + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right)$$

CASCADE OF EQUATIONS

$$-\epsilon^{-2}\left[\operatorname{div}_y A\nabla_y u_0\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{-1}\left[\operatorname{div}_y A(\nabla_x u_0+\nabla_y u_1)+\operatorname{div}_x A\nabla_y u_0\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{0}\left[\operatorname{div}_x A(\nabla_x u_0+\nabla_y u_1)+\operatorname{div}_y A(\nabla_x u_1+\nabla_y u_2)\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\sum_{i=1}^{+\infty}\epsilon^{i}\left[\operatorname{div}_x A(\nabla_x u_i+\nabla_y u_{i+1})+\operatorname{div}_y A(\nabla_x u_{i+1}+\nabla_y u_{i+2})\right]\left(x,\frac{x}{\epsilon}\right)$$

$$= f(x).$$

$\boxed{\epsilon^i \text{ equation}}$

$$-\mathrm{div}_y\ \left(A(y)\nabla_y u_{i+2}(x,y)\right) = f\left(u_i, u_{i+1}\right)(x,y) \quad \text{in} \quad Y$$

- This is a partial differential equation in y.
- We supplement it with periodic boundary conditions.
- The macroscopic variable x is just a parameter.

Technical lemma on cell problems

Definition.

$$L^2_\#(Y) = \left\{ \phi(y) \ Y\text{-periodic, such that } \int_Y \phi(y)^2 dy < +\infty \right\}$$

$$H^1_\#(Y) = \left\{ \phi \in L^2_\#(Y) \text{ such that } \nabla\phi \in L^2_\#(Y)^N \right\}$$

Lemma. Let $f(y) \in L^2_\#(Y)$ be a periodic function. There exists a solution in $H^1_\#(Y)$ (unique up to an additive constant) of

$$\begin{cases} -\mathrm{div}\ (A(y)\nabla w(y)) = f & \text{in } Y \\ y \to w(y) & Y\text{-periodic,} \end{cases}$$

if and only if $\int_Y f(y)dy = 0$ (this is called the Fredholm alternative).

$\boxed{\epsilon^{-2} \text{ equation}}$

$$-\mathrm{div}_y\ (A(y)\nabla_y u_0(x,y)) = 0 \quad \text{in} \quad Y$$

where x is just a parameter.

Its unique solution does not depend on y

$$u_0(x,y) \equiv u(x)$$

ϵ^{-1} equation

$$-\mathrm{div}_y\, A(y)\nabla_y u_1(x,y) = \mathrm{div}_y\, A(y)\nabla_x u(x) \quad \text{in} \quad Y$$

which is an equation for u_1. Introducing the cell problem

$$\begin{cases} -\mathrm{div}_y\, A(y)\left(e_i + \nabla_y w_i(y)\right) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic}, \end{cases}$$

by linearity we compute

$$u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(y).$$

ϵ^0 equation

$$-\mathrm{div}_y\, A(y)\nabla_y u_2(x,y) = \mathrm{div}_y\, A(y)\nabla_x u_1 + \mathrm{div}_x\, A(y)\left(\nabla_y u_1 + \nabla_x u\right) + f(x)$$

which is an equation for u_2. Its compatibility condition (Fredholm alternative) is

$$\int_Y \left(\mathrm{div}_y\, A(y)\nabla_x u_1 + \mathrm{div}_x\, A(y)\left(\nabla_y u_1 + \nabla_x u\right) + f(x)\right) dy = 0.$$

Replacing u_1 by its value yields the homogenized equation

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

with the constant homogenized tensor

$$A^*_{ij} = \int_Y \left[\left(A(y)\nabla_y w_i\right)\cdot e_j + A_{ij}(y)\right] dy = \int_Y A(y)\left(e_i + \nabla_y w_i\right)\cdot\left(e_j + \nabla w_j\right) dy.$$

COMMENTS

- Explicit formula for the effective parameters (no longer true for non-periodic problems).
- A^* does not depend on ϵ, f, u or the boundary conditions (still true in the non-periodic case).
- A^* is positive definite (not necessarily isotropic even if $A(y)$ was so).
- One can check that

$$\lim_{\epsilon \to 0} u_\epsilon = u, \quad \lim_{\epsilon \to 0} \nabla u_\epsilon = \nabla u, \quad \lim_{\epsilon \to 0} A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon = A^* \nabla u,$$

$$\lim_{\epsilon \to 0} A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \cdot \nabla u_\epsilon = A^* \nabla u \cdot \nabla u.$$

- Same results for evolution problems.
- Very general method, but heuristic and not rigorous.

CONVERGENCE

Theorem.

$$u_\epsilon(x) = u(x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i\left(\frac{x}{\epsilon}\right) + r_\epsilon(x) \quad \text{with} \quad \|r_\epsilon\|_{H^1(\Omega)} \leq C\sqrt{\epsilon}$$

In particular, it implies

$$\left\| \nabla u_\epsilon(x) - \nabla u(x) - \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x)(\nabla_y w_i)\left(\frac{x}{\epsilon}\right) \right\|_{L^2(\Omega)^N} \leq C\sqrt{\epsilon}$$

☞ Correctors are important for the gradient.

☞ We could have expected $\|r_\epsilon\|_{H^1(\Omega)} \leq C\epsilon$ and $\|r_\epsilon\|_{L^2(\Omega)} \leq C\epsilon^2$, but this is not true in general.

☞ "Bad estimates" are due to boundary layers effects.

☞ Generalization to the non-periodic case.

HARMONIC VARIABLES (S. Kozlov)

$$u_\epsilon(x) \approx u(x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i \left(\frac{x}{\epsilon}\right)$$

This ansatz looks like a Taylor expansion.

Corollary. Assume $u \in W^{2,\infty}(\Omega)$. Define $w = (w_1, ..., w_N)$. Then

$$u_\epsilon(x) = u\left(x + \epsilon w\left(\frac{x}{\epsilon}\right)\right) + s_\epsilon(x) \quad \text{with} \quad \|s_\epsilon\|_{H^1(\Omega)} \le C\sqrt{\epsilon}.$$

(There is a generalization to the non-periodic case.)

Remark. In 2-d, $x \to \left(x + \epsilon w\left(\frac{x}{\epsilon}\right)\right)$ is a change of variables (cf. Nesi).

-II- CLASSICAL FINITE ELEMENT METHODS

Stationary diffusion equation

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

Sobolev space

$$H_0^1(\Omega) = \left\{ \phi \text{ such that } \int_\Omega \left(\phi^2 + |\nabla\phi|^2\right) dx < +\infty \text{ and } \phi = 0 \text{ on } \partial\Omega \right\}$$

Variational formulation: find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega A(x)\nabla u \cdot \nabla\phi \, dx = \int_\Omega f\phi \, dx \quad \forall\, \phi \in H_0^1(\Omega)$$

Galerkin method for a finite dimensional subspace $V_h \subset H_0^1(\Omega)$: find an approximate solution $u_h \in V_h$ such that

$$\int_\Omega A(x)\nabla u_h \cdot \nabla \phi_h \, dx = \int_\Omega f \phi_h \, dx \quad \forall \phi_h \in V_h$$

Let $(\phi_j)_{1\leq j\leq n_{dl}}$ be a basis of V_h and write $u_h = \sum_{j=1}^{n_{dl}} U_j \phi_j$ to get

$$\sum_{j=1}^{n_{dl}} U_j \int_\Omega A(x)\nabla \phi_j \cdot \nabla \phi_i \, dx = \int_\Omega f \phi_i \, dx$$

Introducing

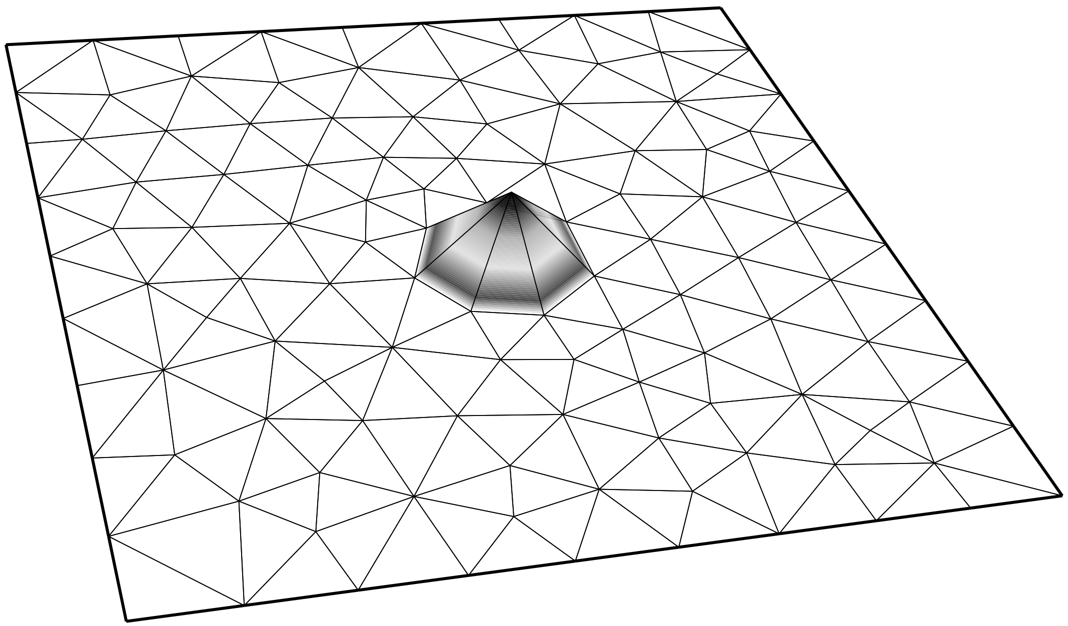
$$\mathcal{K}_h = \left(\int_\Omega A(x)\nabla\phi_j \cdot \nabla\phi_i \, dx \right)_{1\leq i,j\leq n_{dl}}, \quad \text{and} \quad b = \left(\int_\Omega f\phi_i \, dx \right)_{1\leq i\leq n_{dl}}$$

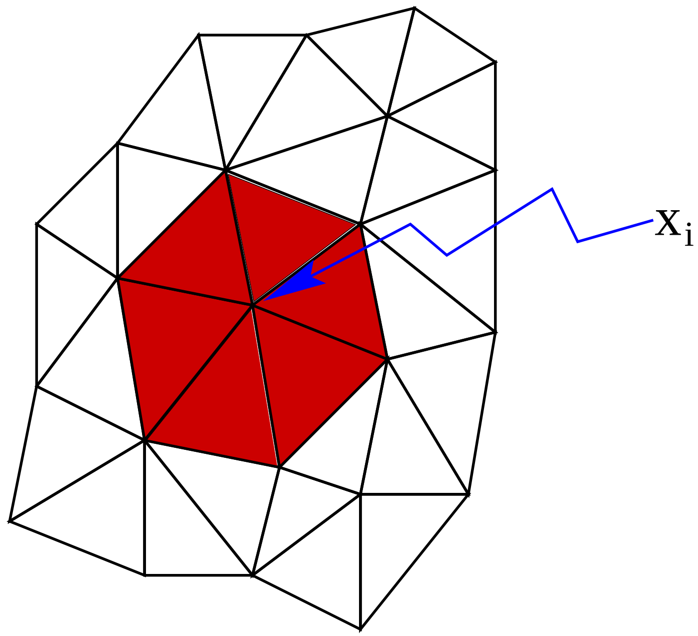
we have to solve a linear system in $\mathbb{R}^{n_{dl}}$

$$\mathcal{K}_h U = b$$

Typically V_h is associated to a mesh.

Example: $P1$ Lagrange finite elements.





Basis function: ϕ_i affine on each (triangular) cell, equal to 1 on the node x_i and 0 on all others nodes.

$$u_h(x) = \sum_{i=1}^{n_{dl}} U_i \phi_i(x) \quad \Rightarrow \quad U_i = u_h(x_i)$$

Convergence

Theorem. For a sequence of "uniformly regular" meshes in 2-d or 3-d, there exists a constant C, independent of h and u such that

$$\|u - u_h\|_{H^1(\Omega)} \leq Ch\|u\|_{H^2(\Omega)}$$

(roughly, $\|u\|_{H^2(\Omega)} \approx \|\nabla\nabla u\|_{L^2(\Omega)}$)

Remark. In the case of oscillating coefficients $A\left(\frac{x}{\epsilon}\right)$, we have

$$u_\epsilon(x) \approx u(x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i\left(\frac{x}{\epsilon}\right) \quad \Rightarrow \quad \|u_\epsilon\|_{H^2(\Omega)} \approx \epsilon^{-1}$$

so the $P1$ Finite Element method can converge only if $h << \epsilon$.

Ingredients of the convergence proof

Céa's lemma. Let u be the exact solution and u_h the approximate one in V_h. Then

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

Interpolation lemma ($P1$ FEM in 2-d or 3-d). For any function $v \in H^2(\Omega)$ define its interpolate in V_h

$$r_h v(x) = \sum_{i=1}^{n_{dl}} v(x_i) \phi_i(x)$$

There exists a constant C, independent of h and v such that

$$\|v - r_h v\|_{H^1(\Omega)} \leq Ch \|v\|_{H^2(\Omega)}.$$

Remark. For a multiscale finite element methods we must improve the interpolation lemma by changing the basis functions.

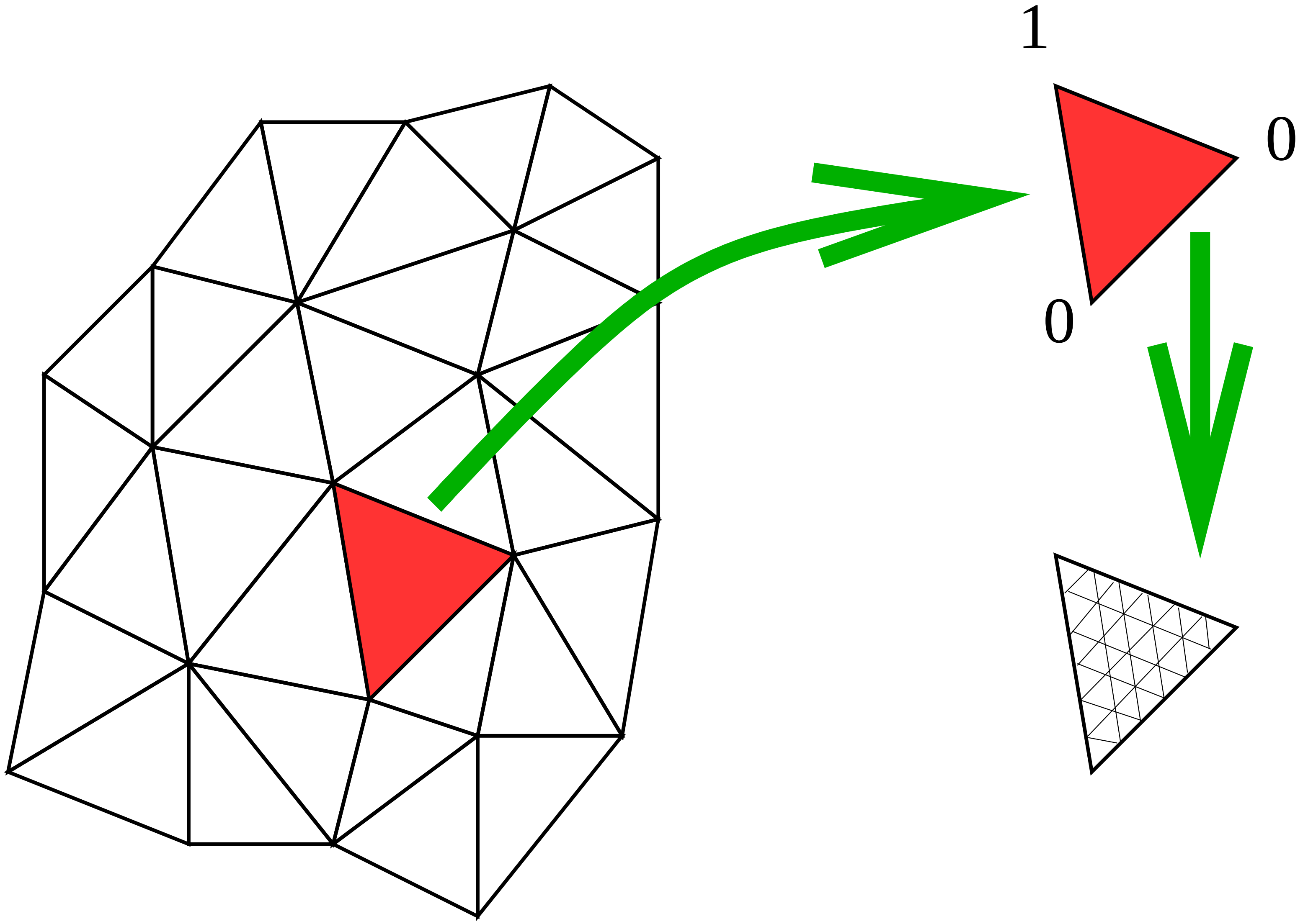
-IV- MULTISCALE FINITE ELEMENT METHODS

Model problem

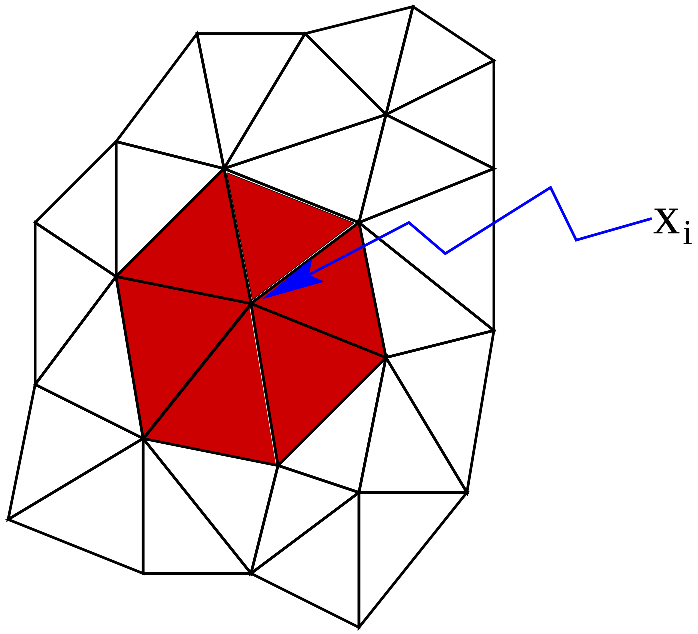
$$\begin{cases} -\text{div } (A^\epsilon(x)\nabla u_\epsilon) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases}$$

- Macro/micro approach: use a coarse mesh for defining the nodal values of u_ϵ and a fine mesh for computing the basis functions ϕ_i^ϵ.
- We pre-compute locally oscillating basis functions ϕ_i^ϵ that depend on A^ϵ.
- The problem dimension is that of the coarse mesh.
- Multiscale FEM are defined for non-periodic problems but their quantitative convergence analysis is made in the periodic case.
- There are other problems and other methods...
- Main references for this example: Hou, Efendiev, Wu, Babuska, Matache, Schwab, Brizzi...

COARSE AND FINE MESHES



Multiscale Finite Element Method of T. Hou



For each coarse triangle K, there is a fine mesh on which we compute ϕ_i^ϵ solution of

$$\left\{ \begin{array}{ll} -\text{div}\ (A^\epsilon \nabla \phi_i^\epsilon) = 0 & \text{in } K \\ \phi_i^\epsilon(x_j) = \delta_{ij} & \text{at the nodes of } K \\ \phi_i^\epsilon(x) & \text{affine on } \partial K \end{array} \right.$$

Multiscale Finite Element Method of T. Hou (continued)

- By definition, the function ϕ_i^ϵ is continuous across cell boundaries ∂K.
- This yields a conformal F.E.M.
- The F.E. basis functions ϕ_i^ϵ encodes the oscillations of A^ϵ.
- Idea similar to the famous oscillating test function method of Tartar in homogenization theory.
- The computation of all ϕ_i^ϵ can be done in parallel (once and for all).
- The previous definition is similar to the cell problem: if $e \cdot x$ is the affine boundary condition, then $w_i^\epsilon = \phi_i^\epsilon - e \cdot x$ satisfies

$$\begin{cases} -\text{div}\ (A^\epsilon(e + \nabla w_i^\epsilon)) = 0 & \text{in } K \\ w_i^\epsilon = 0 & \text{on } \partial K \end{cases}$$

Convergence of the method (in the periodic case)

Theorem. Let u_ϵ be the exact solution and u_ϵ^h the computed solution by the multiscale FEM. Then

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C \left(\epsilon + h + \sqrt{\frac{\epsilon}{h}} \right).$$

- ☞ The classical finite element method does not converge if $h >> \epsilon$.
- ☞ Resonance effect when $h \approx \epsilon$ for the multiscale FEM.
- ☞ Although we analyze the convergence of the FEM in the periodic case, it is well defined for non-periodic problems.

Sketch of the proof

Denoting by V_h^ϵ the finite dimensional space spanned by the (ϕ_i^ϵ), Céa's lemma implies

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C \inf_{v_\epsilon^h \in V_h^\epsilon} \|u_\epsilon - v_\epsilon^h\|_{H^1(\Omega)}.$$

We choose $v_\epsilon^h = \Pi_h^\epsilon u$ where u is the homogenized solution and Π_h^ϵ is the interpolation operator defined by

$$(\Pi_h^\epsilon v)(x) = \sum_i v(x_i)\phi_i^\epsilon(x)$$

On the other hand, using the homogenization ansatz

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C\left(\|u_\epsilon - u - \epsilon u_1^\epsilon\|_{H^1(\Omega)} + \|u + \epsilon u_1^\epsilon - \Pi_h^\epsilon u\|_{H^1(\Omega)}\right)$$

$$\leq C\left(\sqrt{\epsilon} + \|u + \epsilon u_1^\epsilon - \Pi_h^\epsilon u\|_{H^1(\Omega)}\right)$$

Then using the homogenization ansatz for the basis function ϕ_i^ϵ on each coarse cell K

$$\left\| \phi_i^\epsilon - \phi_i - \epsilon \sum_{k=1}^{d} w_k \left(\frac{x}{\epsilon}\right) \frac{\partial \phi_i}{\partial x_k} \right\|_{H^1(K)} \leq C \sqrt{\frac{\epsilon}{h}} \sqrt{|K|}$$

where C is independent of h (the size of K).

This implies

$$\|u+\epsilon u_1^\epsilon - \Pi_h^\epsilon u\|_{H^1(\Omega)} \leq C \left(\sqrt{\frac{\epsilon}{h}} + \|u - \Pi_h u\|_{H^1(\Omega)} + \epsilon \|w\left(\frac{x}{\epsilon}\right) \nabla(u - \Pi_h u)\|_{H^1(\Omega)} \right)$$

where Π_h is the usual interpolation operator on the coarse mesh. Recall that

$$\|u - \Pi_h u\|_{H^1(\Omega)} \leq Ch\|u\|_{H^2(\Omega)}$$

which yields the result.

Another multiscale method (Allaire-Brizzi)

Based on the harmonic variables of Kozlov

$$u_\epsilon(x) \approx u\left(x + \epsilon w\left(\frac{x}{\epsilon}\right)\right)$$

with $w = (w_1, ..., w_N)$ solutions of the cell problems.

New idea: to compute an approximation of u_ϵ we use a standard finite element method for u composed with the map $x \rightarrow \left(x + \epsilon w\left(\frac{x}{\epsilon}\right)\right)$.

INGREDIENTS

- As many other methods we use a coarse mesh for u and a fine mesh for w.
- On the coarse mesh: standard P_k F.E.M. with basis functions (ϕ_i) (of any order $k \geq 1$).
- On the fine mesh: for each coarse triangle K we compute a locally oscillating function χ^ϵ solution of

$$\begin{cases} -\mathrm{div}\ \left(A\left(\frac{x}{\epsilon}\right)\nabla\chi^\epsilon\right) = 0 & \text{in } K \\ \chi^\epsilon(x) = x & \text{on } \partial K \end{cases}$$

- Typically $\chi^\epsilon(x) \approx x + \epsilon w\left(\frac{x}{\epsilon}\right)$.

Definition of the multiscale FEM: basis functions $\phi_i^\epsilon(x) = \phi_i \circ \chi^\epsilon(x)$.

CONVERGENCE (in the periodic case)

Theorem. If u_ϵ^h is the approximated solution in the subspace spanned by $(\phi_i^\epsilon = \phi_i \circ \chi^\epsilon)$, then

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C \left(h^k + \sqrt{\frac{\epsilon}{h}} \right).$$

If the oscillating functions χ^ϵ are computed with a $P_{k'}$ FEM on the fine mesh of size h', then

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C \left(h^k + \sqrt{\frac{\epsilon}{h}} + \left(\frac{h'}{\epsilon}\right)^{k'} \right).$$

Idea of the proof

By Céa's lemma

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \le C \inf_{v_\epsilon^h \in V_h^\epsilon} \|u_\epsilon - v_\epsilon^h\|_{H^1(\Omega)}.$$

We choose $v_\epsilon^h = (\Pi_h u) \circ \chi^\epsilon$ where Π_h is the usual interpolation operator on the coarse mesh. Then

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \le C \left(\|u_\epsilon - u \circ \chi^\epsilon\|_{H^1(\Omega)} + \|(u - \Pi_h u) \circ \chi^\epsilon\|_{H^1(\Omega)} \right).$$

(But this estimate has to be done on each coarse cell K.)

A standard computation yields the result.

REMARKS

- Each oscillating function χ^ϵ is computed independently of the others (natural parallelism).
- The complexity of the macroscopic computation is linked to the coarse mesh.
- No periodicity is required.
- When $k = 1$, we recover exactly the previous method of Hou et al.
- We perform numerical experiments for $k = 2$.
- One can choose a larger support for χ^ϵ (over-sampling in order to avoid boundary layer effects) and still have a conforming F.E.M.
- Our method works in any dimension and for any type of mesh.

SOME IMPROVEMENTS

☞ The error estimate in $\sqrt{\epsilon/h}$ indicates a resonance effect.

☞ It is due to boundary layers.

☞ It cannot be removed completely but some ideas are helpful.

First idea: Replace the affine boundary conditions on ∂K for ϕ_i^ϵ by oscillating boundary conditions: for example, in 2-d

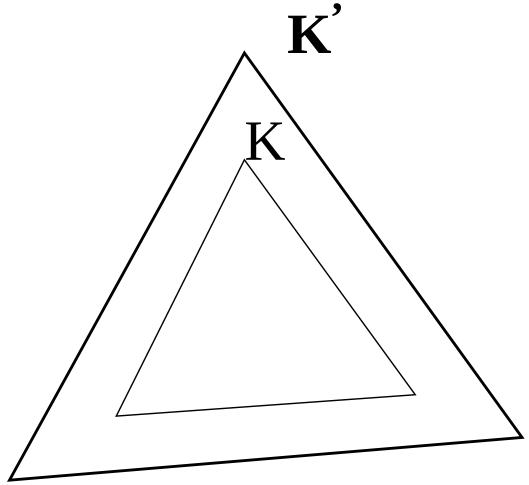
$$\left\{ \begin{array}{rcll} -\mathrm{div}\,(A^\epsilon(x)\nabla\phi_i^\epsilon) & = & 0 & \text{in } K, \\ \phi_i^\epsilon & = & b_i^\epsilon(x) & \text{on } \partial K, \end{array} \right.$$

where on each side of ∂K, parametrized by a curvilinear coordinate $s \in [0,1]$,

$$-\frac{d}{ds}\left(A^\epsilon \frac{d\, b_i^{\epsilon,K}}{ds} \right) = 0$$

with the boundary conditions $b_i^\epsilon(x(0)) = x_i(0)$ and $b_i^\epsilon(x(1)) = x_i(1)$.

Second idea: Oversampling method (T. Hou)



Oversampling method: compute ϕ_i^ϵ on a larger fine mesh K' such that $K \subset\subset K'$ (overlap).

Non-conforming F.E. method with a better convergence rate

$$\|u_\epsilon - u_\epsilon^h\|_{H^1(\Omega)} \leq C\left(h + \epsilon + \frac{\epsilon}{h}\right)$$

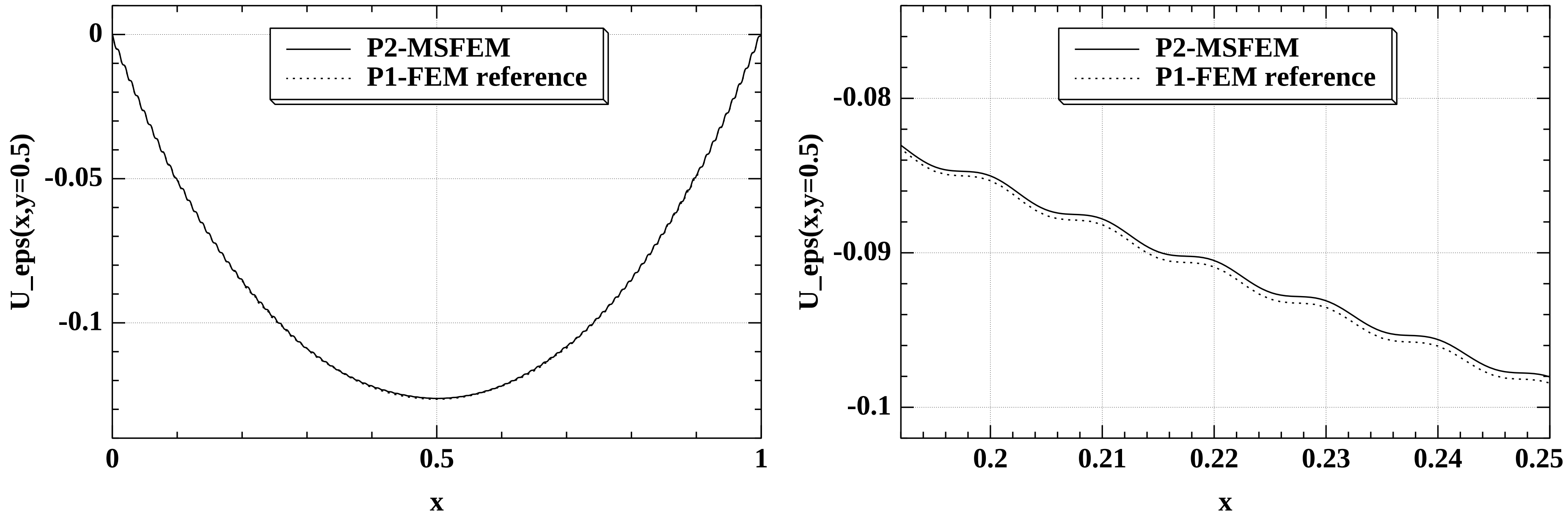
NUMERICAL EXPERIMENTS

Test proposed by T. Hou in the 2-D periodic case

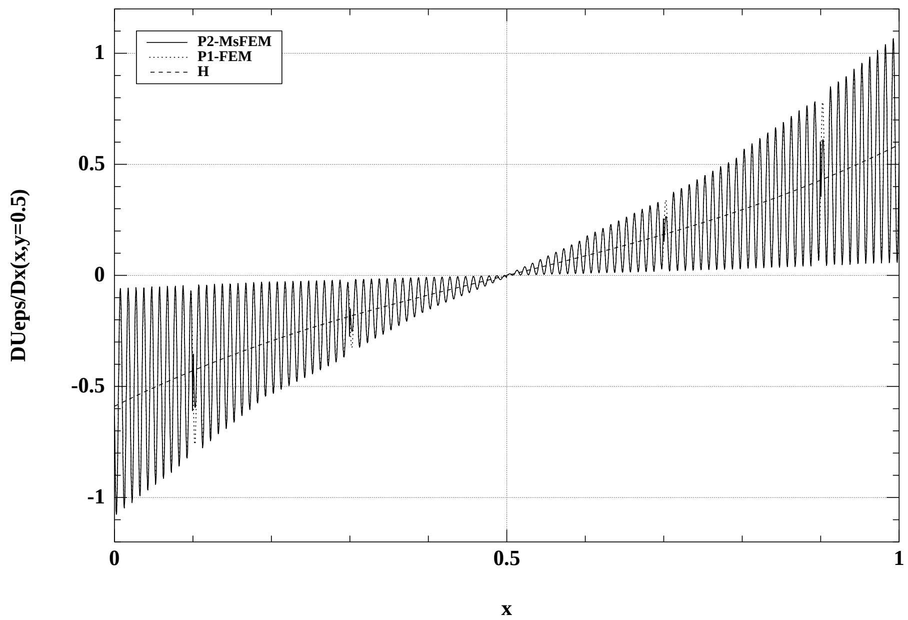
$$A(y) = \frac{1}{(2 + 1.8\sin(2\pi y_1))(2 + 1.8\sin(2\pi y_2))}.$$

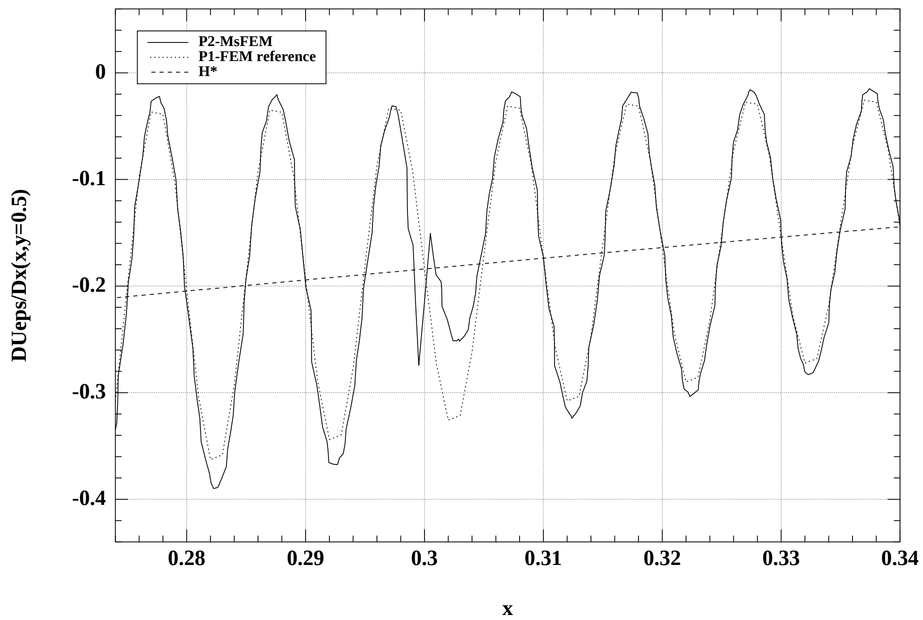
Method of Allaire-Brizzi with $P2$ F.E.

- ☞ $A^* = 1/(2\sqrt{4 - (1.8)^2})$
- ☞ constant source term $f = -1$
- ☞ $\Omega = (0,1)^2$ with Dirichlet boundary conditions
- ☞ $\epsilon = 0.01$
- ☞ coarse triangular mesh with $h = 1/5$
- ☞ fine triangular mesh with $h' = 4.10^{-4}$



Cross section (left) and close-up (right) at $y = 0.5$ of the reference and multiscale solutions: $\epsilon = 10^{-2}, h = 1/5,\ h' = 4.10^{-4}$





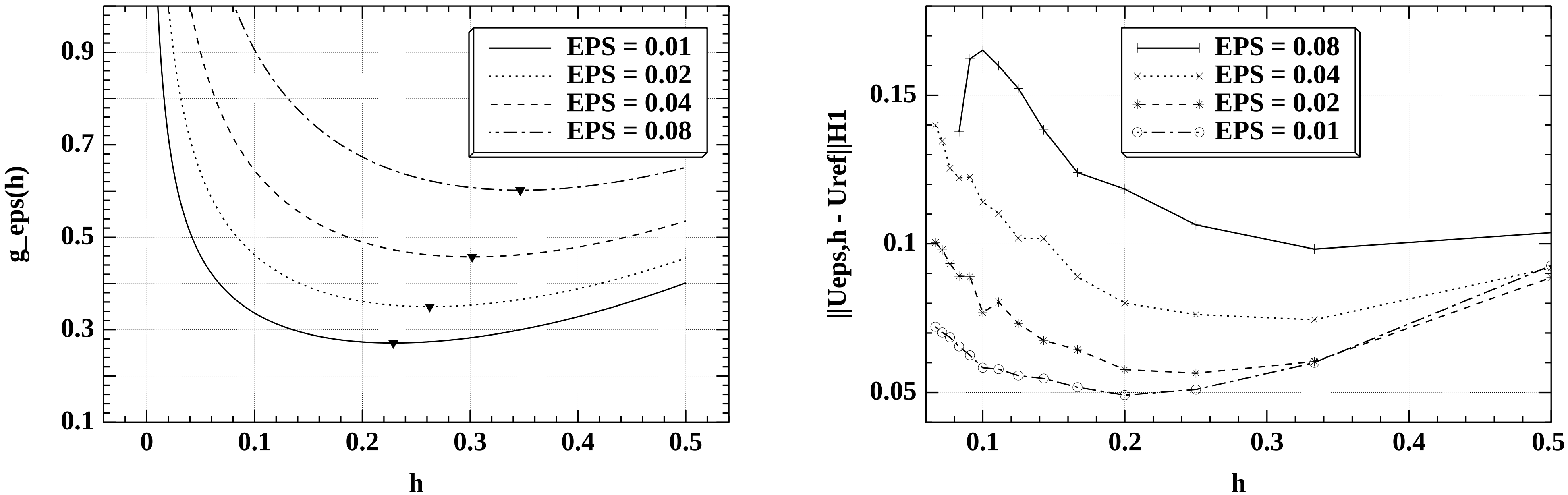
Cross-section (left) and close-up (right) of the partial derivative $\partial u^\epsilon/\partial x$ at $y = 0.5$ of the reference and multiscale solutions: $\epsilon = 10^{-2}, h = 1/5$, $h' = 4.10^{-4}$. Here, H stands for the homogenized solution.

Predicted error estimate when $k = 2$, $k' = 1$

$$g^\epsilon(h) \; = \; h^2 + \sqrt{\frac{\epsilon}{h}} + \frac{h'}{\epsilon}.$$

If we assume that h' is very small compare to ϵ, the optimal mesh size is

$$h \; \simeq \; \epsilon^{1/5}.$$



Error estimate (in the H^1 norm) predicted by the previous formula (left) and computed (right) as a function of h for different values of ϵ with $h' = 4.\ 10^{-4}$.

h	$\| u_h^\epsilon - u^\epsilon \|_{L^2(\Omega)}$	$\| u_h^\epsilon - u^\epsilon \|_{H_0^1(\Omega)}$	$\| u_h^\epsilon - u^\epsilon \|_{L^\infty(\Omega)}$
0.0666	0.372 E-02	0.721 E-01	0.673 E-02
0.0769	0.327 E-02	0.685 E-01	0.792 E-01
0.0833	0.287 E-02	0.654 E-01	0.522 E-02
0.1000	0.105 E-03	0.583 E-01	0.196 E-02
0.1250	0.146 E-02	0.557 E-01	0.273 E-02
0.1666	0.116 E-02	0.517 E-01	0.313 E-02
0.2000	0.412 E-03	0.491 E-01	0.243 E-02
0.2500	0.702 E-03	0.509 E-01	0.405 E-02
0.3333	0.195 E-02	0.600 E-01	0.604 E-02
0.5000	0.536 E-02	0.926 E-01	0.107 E-01

Error estimates (in various norms) as a function of h for $\epsilon = 10^{-2}$ and $h' = 4.\ 10^{-4}$.

h	N	CPU1 (s)	CPU2 (s)	CPU1/N (s)
0.0666	450	81918	1.05	182
0.0769	338	65508	0.46	193
0.1000	200	47520	0.11	237
0.1250	128	25640	0.04	200
0.2000	50	9897	0.01	197
0.2500	32	6367	0.01	198
0.3333	18	3619	0.01	201
0.5000	8	1849	0.01	231

CPU times (in seconds). N is the total number of elements in the coarse mesh. CPU1 is the total sequential time for computing the oscillating functions $w^{\epsilon,h}$ (thus CPU1/N is the corresponding parallel time). CPU2 is the inherently sequential time for the coarse mesh computation (assembling and solving).

	$P1$ multiscale FEM		$P2$ multiscale FEM	
h	$\lVert u_h^\epsilon - u^\epsilon \rVert_{L^2(\Omega)}$	$\lVert u_h^\epsilon - u^\epsilon \rVert_{H^1(\Omega)}$	$\lVert u_h^\epsilon - u^\epsilon \rVert_{L^2(\Omega)}$	$\lVert u_h^\epsilon - u^\epsilon \rVert_{H^1(\Omega)}$
0.0666	0.442E-02	0.828E-01	0.346E-02	0.714E-01
0.1000	0.289E-02	0.840E-01	0.955E-03	0.581E-01
0.1250	0.415E-02	0.921E-01	0.131E-02	0.547E-01
0.2000	0.676E-02	0.117E+00	0.412E-03	0.491E-01
0.2500	0.929E-02	0.134E+00	0.702E-03	0.509E-01
0.3333	0.133E-01	0.154E+00	0.195E-02	0.600E-01
0.5000	0.155E-01	0.168E+00	0.536E-02	0.926E-01

Comparison $P1$ (left) and $P2$ (right): error estimates (in various norms) as a function of h for $\epsilon = 10^{-2}$ and $h' = h/500$.

2-d non-periodic problem

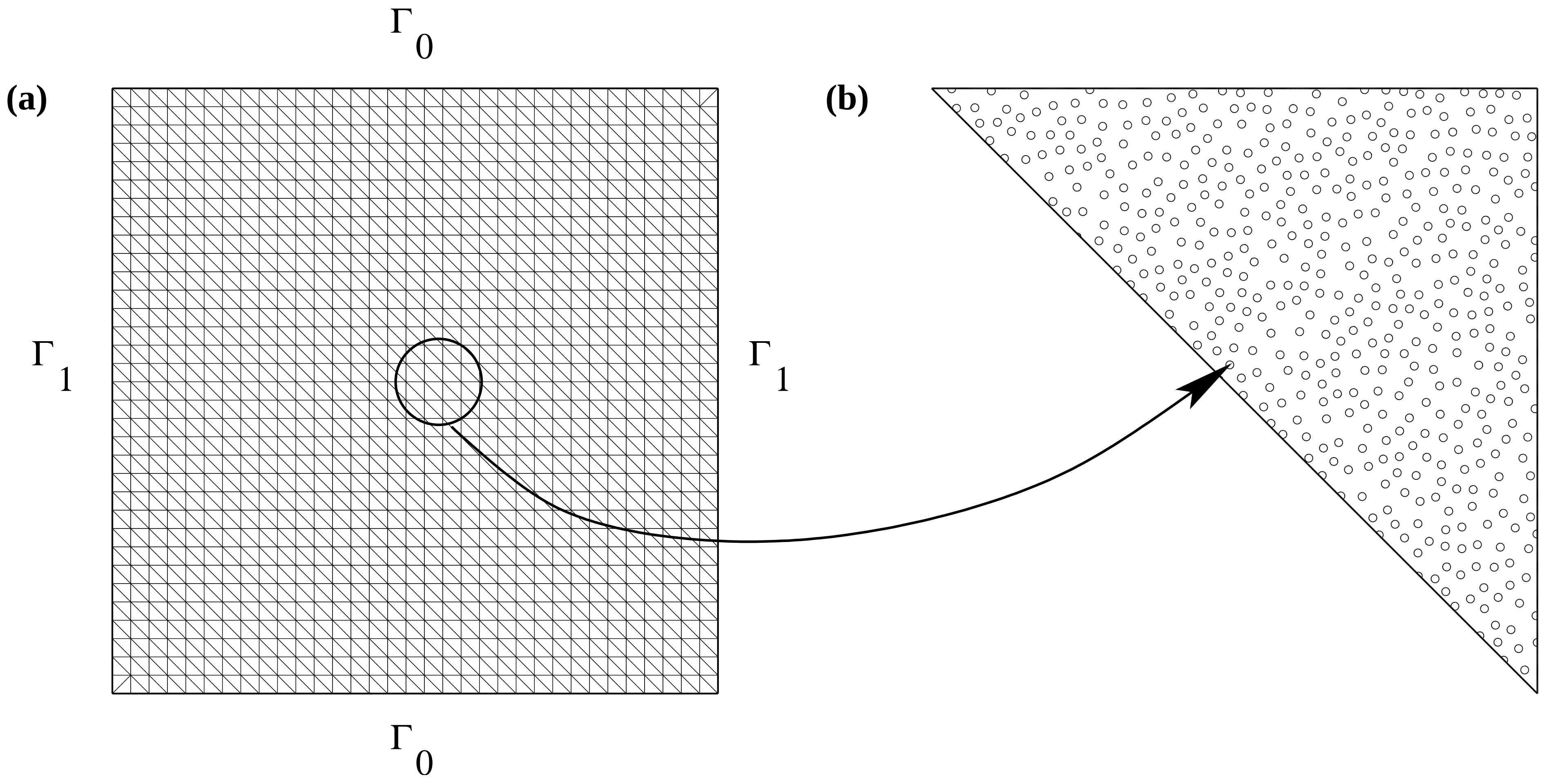
Discontinuous coefficients:

$$A^\epsilon(x) = \begin{cases} 1 & \text{in the matrix} \\ 100 & \text{in the inclusions} \end{cases}$$

10^6 monodisperse spherical inclusions in a matrix.

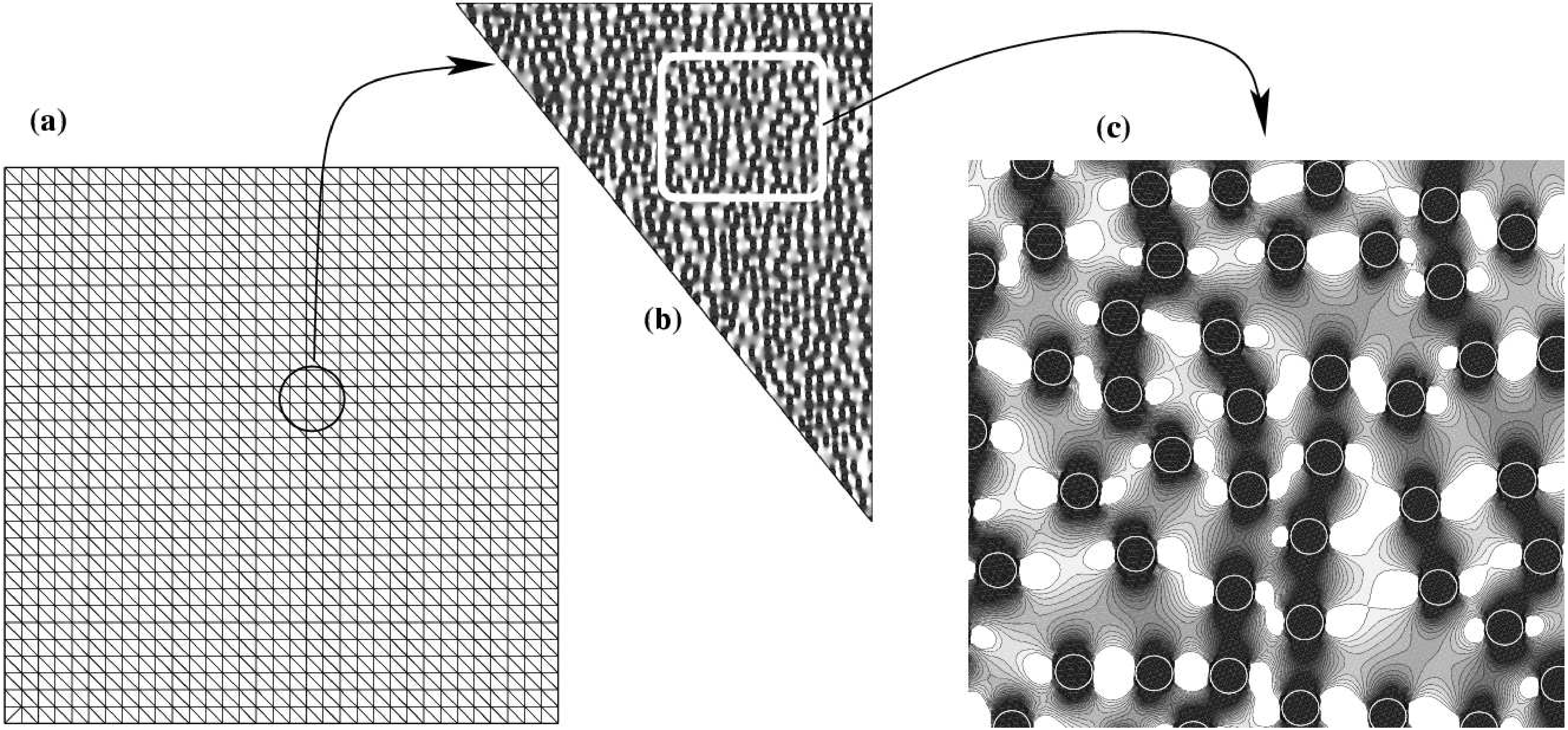
Domain $\Omega = (0,1)^2$, without source term.

Boundary conditions: Neumann on the vertical sides, Dirichlet 0 (bottom) and 1 (top).

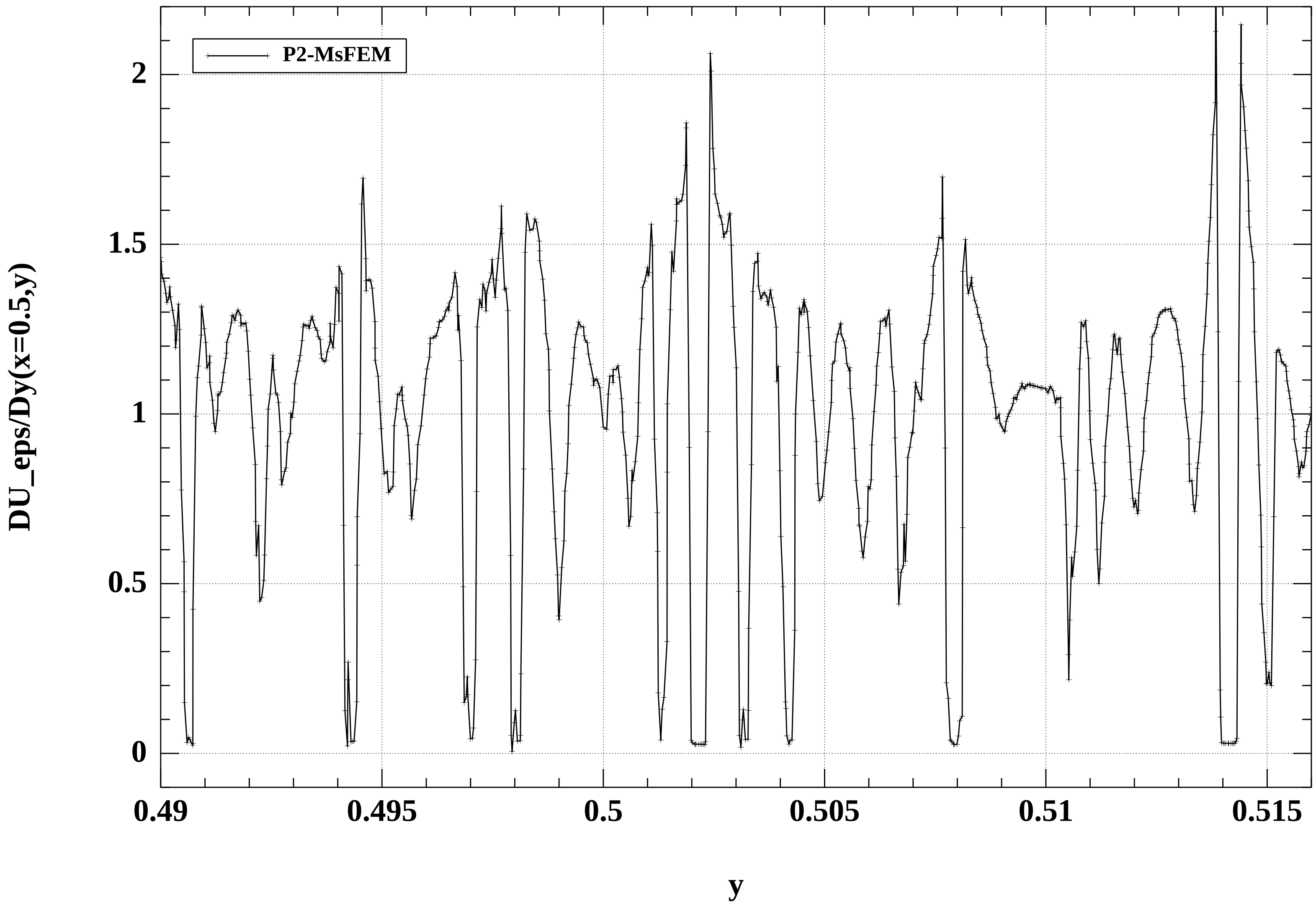


Coarse mesh.

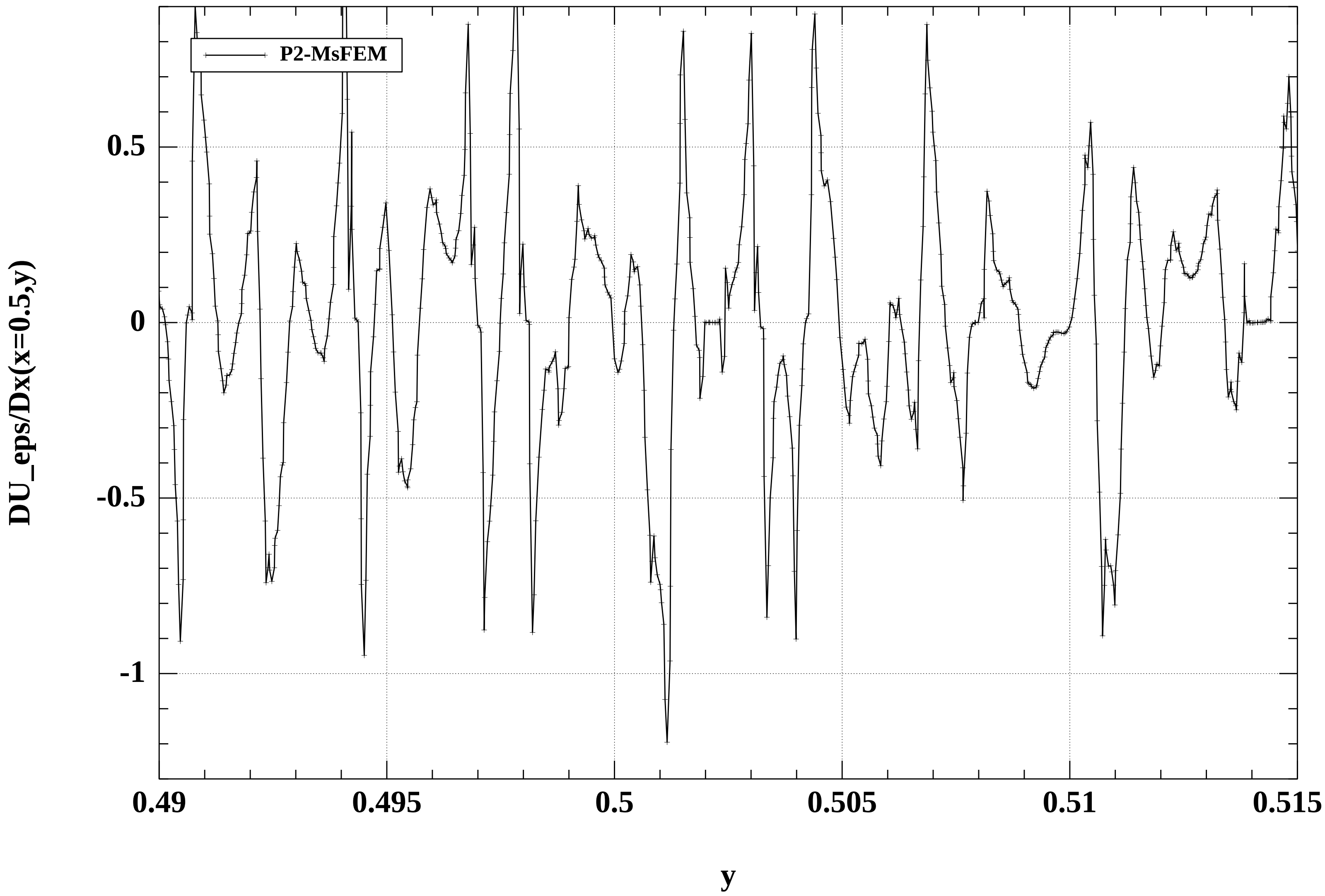
Close-up on the inclusions.



Flux density $|A^\epsilon \nabla u^\epsilon|$ in a coarse mesh cell and close-up.



Close-up of the vertical cross-sections of the partial derivative $\partial u^\epsilon / \partial y(x = 0.5, y)$.



Close-up of the vertical cross-sections of the partial derivative $\partial u^\epsilon/\partial x(x = 0.5, y)$.

-V- ANOTHER HOMOGENIZATION PARADIGM

- ☞ Different model problem and diferent scaling.
- ☞ A diferent homogenization paradigm yields a different multiscale method.
- ☞ Previously the solution was behaving like

$$u_\epsilon(x) \approx u(x) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right),$$

Now we want to have large oscillations in the leading term

$$u_\epsilon(x) \approx u_0\left(x, \frac{x}{\epsilon}\right) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right),$$

- ☞ Such a model can be found in neutronic diffusion, radiative transport, semiconductors...

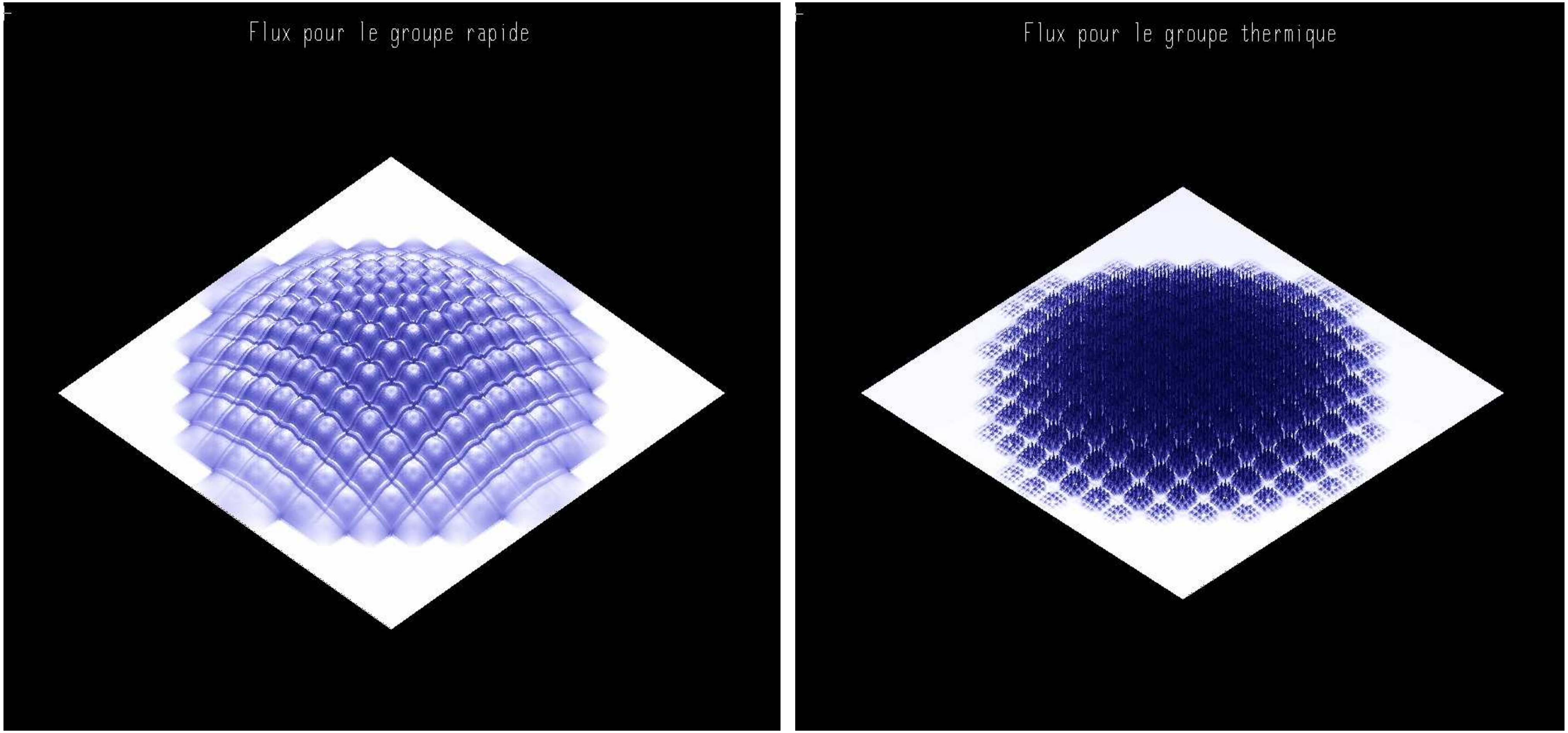
Example: neutronic diffusion model

$$\left\{ \begin{array}{ll} c\left(\frac{x}{\epsilon}\right)\frac{\partial u_\epsilon}{\partial t} - \epsilon^2 \mathrm{div}\ \left(A\left(\frac{x}{\epsilon}\right)u_\epsilon\right) = \sigma\left(\frac{x}{\epsilon}\right)u_\epsilon & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \\ u_\epsilon(0) = u_0 & \end{array} \right.$$

$$\boxed{u_\epsilon(t,x) \approx e^{-\lambda t} w\left(\frac{x}{\epsilon}\right) u\left(\epsilon^2 t, x\right)}$$

$$\left\{ \begin{array}{ll} -\lambda c(y) w - \mathrm{div}\ (A(y)w) = \sigma(y) w & \text{in } Y \\ y \to w(y) & Y - \text{periodic} \end{array} \right.$$

$$\left\{ \begin{array}{ll} c^* \frac{\partial u}{\partial \tau} - \mathrm{div}\ \left(\tilde{A}^* u\right) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \\ u(0) = \overline{u}_0 & \end{array} \right.$$



Two groups neutronic diffusion computation (Allaire and Siess)

HYDRODYNAMIC LIMIT OF KINETIC EQUATION

Transport or kinetic equation: particle density $\phi(x,v)$ in $\Omega \times V$

$$\left\{ \begin{array}{l} \dfrac{\partial \phi_\epsilon}{\partial t} + \epsilon v \cdot \nabla \phi_\epsilon = \displaystyle\int_V \sigma\left(\frac{x}{\epsilon}, v', v\right) \phi_\epsilon(x,v') dv' - \Sigma\left(\frac{x}{\epsilon}, v\right) \phi_\epsilon(x,v) \\ \phi_\epsilon = 0 \qquad \text{on } \Gamma_- = \{(x,v) \in \partial\Omega \times V \,|\, v \cdot n(x) < 0\}, \end{array} \right.$$

☞ Singular perturbations: mean free path of the order of ϵ, characteristic time of observation of the order of $1/\epsilon^2$.

☞ Hydrodynamic or fluid limit: change of type of the equations.

☞ Origin of the scaling: change of variables $y = x/\epsilon \quad \Rightarrow$ cells of size 1, domain of size $1/\epsilon$, no more ϵ in the equations.

CONVERGENCE RESULT

$$\boxed{\phi_\epsilon(t,x,v) \approx e^{-\lambda t}\psi\left(\frac{x}{\epsilon},v\right) u\left(\epsilon^2 t,x\right)}$$

Spectral cell problem:

$$\begin{cases} -\lambda\psi + v\cdot\nabla_y\psi = \int_V \sigma\left(y,v',v\right)\psi(y,v')dv' - \Sigma\left(y,v\right)\psi(y,v) & \text{in } Y \\ y \to \psi(y,v) & Y-\text{periodic} \end{cases}$$

First eigenvalue λ and first eigenfunction $\psi(y,v) > 0$ (local equilibrium between transport and scattering).

Change of unknown: $u_\epsilon(\epsilon^2 t,x,v) = \dfrac{\phi_\epsilon(t,x,v)}{\psi\left(\frac{x}{\epsilon},v\right)}e^{\lambda t}$

Homogenized problem for u_ϵ:

$$\begin{cases} c^* \dfrac{\partial u}{\partial \tau} - \mathrm{div}\, \left(A^* \nabla u\right) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \\ u(0) = \overline{u}_0 & \end{cases}$$

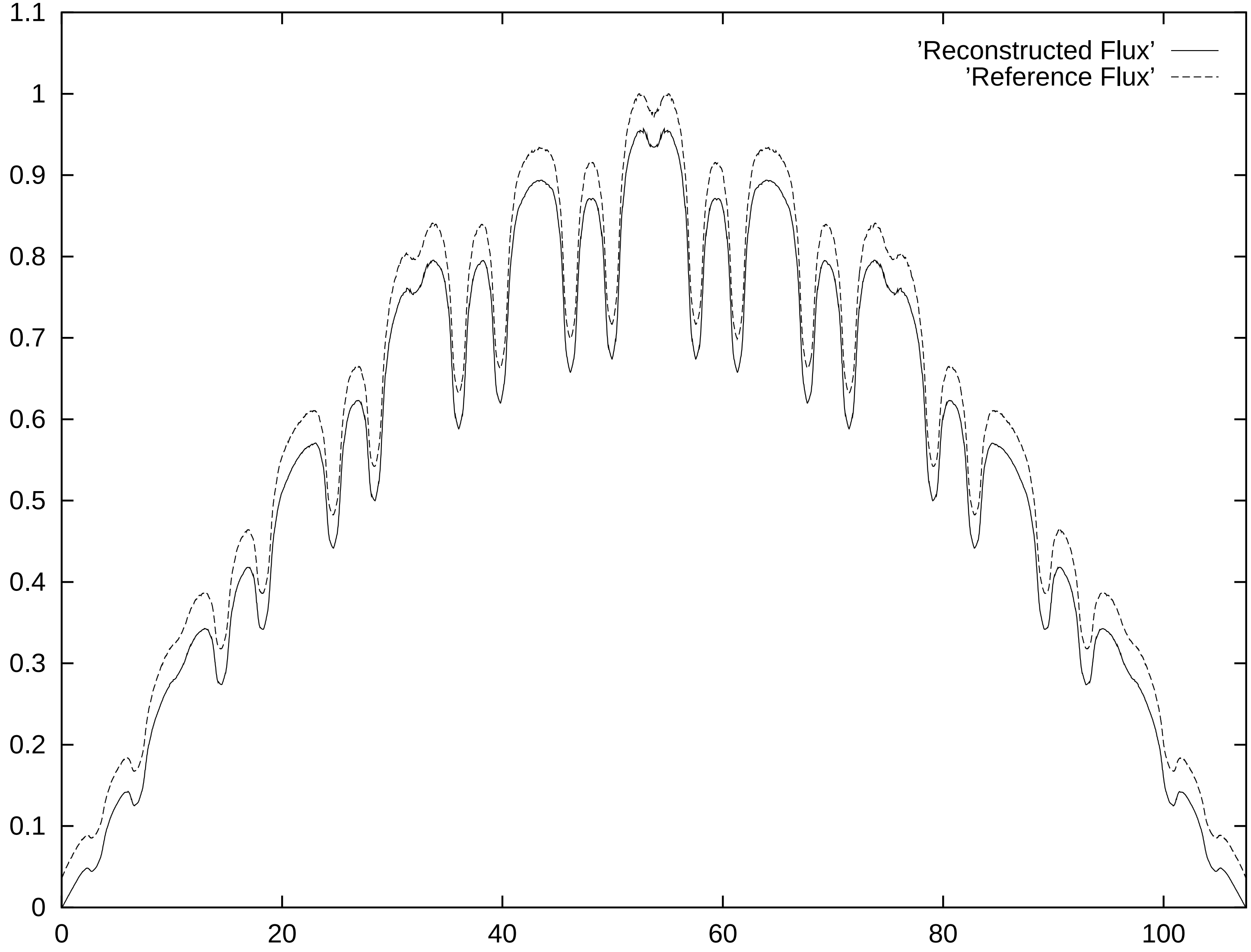
☞ Conclusion: microscopic transport equation, homogenized diffusion equation.

☞ At the basis of many numerical methods.

☞ Complicated but explicit formula for c^* and A^*.

☞ Boundary layers are very important.

☞ Many contributions: Keller, Larsen, Bensoussan-Lions-Papanicolaou, Sentis, Allaire-Bal...


'Reconstructed Flux'
'Reference Flux'
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
0
20
40
60
80
100

A short list of references

Homogenization theory:

Bensoussan, A.; Lions, J.-L.; Papanicolaou, G.; *Asymptotic analysis for periodic structures*; North-Holland: Amsterdam, 1978.

Jikov, V. V.; Kozlov, S. M.; Oleinik, O. A.; *Homogenization of Differential Operators and Integral Functionals*; Springer Verlag: New York, Berlin, 1994.

Multiscale finite element methods:

T. Hou, X.-H. Wu, *A multiscale finite element method for elliptic problems in composite materials and porous media,* J.Comput.Phys. 134, pp.169-189 (1997).

W. E, B. Engquist, *The heterogeneous multiscale methods,* Commun. Math. Sci. 1, 87–132 (2003).

A.-M. Matache, I. Babuska, C. Schwab, *Generalized p-FEM in homogenization,* Numer. Math. 86, 319–375 (2000).

T. Arbogast, *Numerical subgrid upscaling of two-phase flow in porous media,* in Numerical treatment of multiphase flows in porous media, Lecture Notes in Physics, vol. 552, Chen, Ewing and Shi eds., pp.35-49 (2000).

Homogenization of transport equations:

G. Allaire, G. Bal, *Homogenization of the criticality spectral equation in neutron transport,* M2AN 33, pp.721-746 (1999).