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LECTURE 3
NUMERICAL METHODS OF HOMOGENIZATION

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The goal of this lecture is to describe how homogenization theory can be applied to numerical computations of partial differential equations in highly heterogeneous media. In the first chapter we briefly review the classical numerical method for periodic media. It amounts to the separate computation of the cell and homogenized problems. We also give some indications about correctors and boundary layers. In the second chapter we discuss recent numerical methods, inspired from the theory of periodic homogenization, but which can be applied to any kind of disordered heterogeneous media (not necessarily periodic).

Chapter 1

Periodic media

1.1 Classical approach

We consider only periodic media as described in the first lecture. This is of course a serious restriction in many applications (the next chapter is devoted to the non-periodic case). For simplicity we restrict ourselves to a model problem of diffusion. The periodic domain is denoted by Ω (see Figure 1.1), its period by ϵ (assumed to be small in comparison with the size of the domain), and the rescaled unit periodic cell by $Y = (0,1)^N$. The conductivity tensor in Ω is $A\left(\frac{x}{\epsilon}\right)$ where $A(y)$ is Y-periodic and satisfies the coercivity assumption

$$\alpha|\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(y)\xi_i\xi_j \leq \beta|\xi|^2 \quad \forall\, \xi \in \mathbb{R}^N,\ \forall\, y \in Y, \tag{1.1}$$

with $\beta \geq \alpha > 0$. Denoting by $f(x)$ the source term, and enforcing a Dirichlet boundary condition (for simplicity), our model problem reads

$$\left\{ \begin{array}{ll} -\mathrm{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega, \end{array} \right. \tag{1.2}$$

which admits a unique solution $u_\epsilon(x)$.

If one wants to compute numerically the solution u_ϵ, any method (finite differences, finite elements, finite volumes) will require a mesh spacing h that must be smaller than ϵ which the characteristic length of the medium. If ϵ is too small, it yields a very fine mesh and thus a very large number of degrees of freedom. Such discrete problems may be too costly or even impossible to solve because the CPU time, as well as the memory storage, being proportional to some power of the total number of degrees of freedom, are too large.

The classical approach to numerically solve (1.2) is rather to compute the solution of the homogenized problem corresponding to (1.2), namely

$$\left\{ \begin{array}{ll} -\mathrm{div_x}\left(A^*\nabla_x u(x)\right) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{array} \right. \tag{1.3}$$

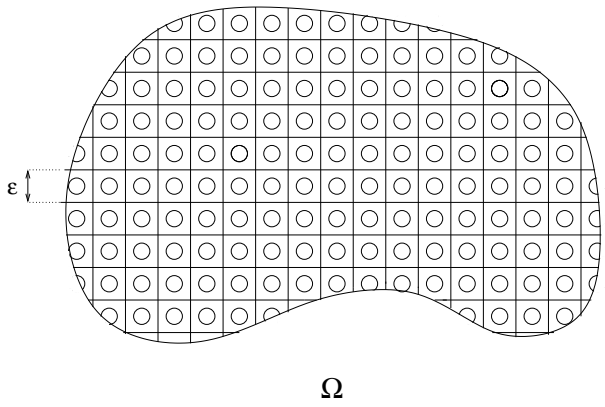

Figure 1.1: A periodic domain.

Since the homogenized tensor A^* is constant, the discretization of (1.3) does not require a small mesh size h. However, we first need to compute the N cell solutions of the cell problems, for $1 \leq i \leq N$,

$$\begin{cases} -\mathrm{div_y} A(y)\,(e_i + \nabla_y w_i(y)) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic}, \end{cases} \tag{1.4}$$

which yield the value of the tensor A^*

$$A^*_{ij} = \int_Y A(y)(e_i + \nabla_y w_i) \cdot e_j \, dy = \int_Y A(y)\,(e_i + \nabla_y w_i) \cdot (e_j + \nabla w_j)\, dy. \tag{1.5}$$

An additional advantage of the cell problems (1.4) is that it allows to improve the approximation of u_ϵ by u by adding the so-called *correctors* to the homogenized solution. Indeed, recall the beginning of the two-scale asymptotic expansion for u_ϵ (and its mathematical justification, see Remark 1.3.7 in the first lecture)

$$u_\epsilon(x) \approx u(x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i \left(\frac{x}{\epsilon}\right). \tag{1.6}$$

In (1.6) the term $\epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i \left(\frac{x}{\epsilon}\right)$ is called the corrector term. When ϵ is small, the corrector term is not very important if one is interested in the values of u_ϵ. However, if the physical quantity of interest is the gradient ∇u_ϵ (some type of flux or of strain), then the corrector is of the same order than the homogenized gradient ∇u, even if ϵ is small, because the approximation in (1.6) is in the sense of the $H^1(\Omega)$-norm and it implies

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

This classical approach of numerical homogenization has been pursued by many authors. Let us mention just a few references: [7], [8], [12], etc.

Remark 1.1.1 *The results of periodic homogenization are also valid for macroscopically modulated oscillating coefficients of the type* $A\left(x, \frac{x}{\epsilon}\right)$*, where* $A(x, y)$ *is a smooth function of* x*, periodic with respect to* y*. Numerically this type of problems is solved exactly as above, except that we compute an effective tensor* $A^*(x)$ *which is piecewise constant in each cell of the coarse mesh of size* h *(used for the computation of the homogenized problem (1.3)).*

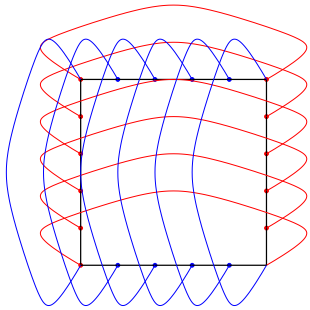

Figure 1.2: Periodic boundary conditions in the unit cell.

The only numerical difficulty in this classical approach is the periodic boundary condition in the cell problems (1.4). Such periodic boundary conditions are frequently not available in usual numerical codes (although they are easy to implement: just merge the degrees of freedom on the boundary with their counterparts on the opposite face of the unit cell Y, see Figure 1.2). Fortunately, under appropriate symmetry conditions, one can replace the periodic boundary condition by a simpler combination of Dirichlet and Neumann conditions.

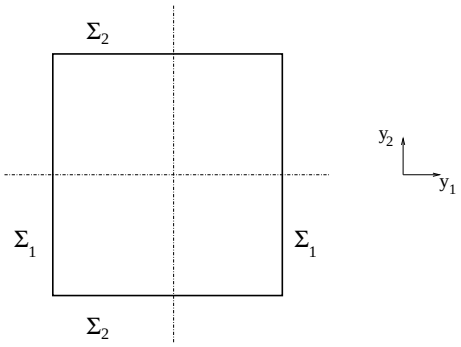

Figure 1.3: Cubic symmetry in the unit cell Y.

Let us assume that the coefficient matrix $A(y)$ has cubic symmetry in Y, i.e. is a diagonal matrix, symmetric with respect to the hyperplanes, parallel to the faces of Y, running through its center (see Figure 1.3). Then, it is easily seen that $-w_i(-y)$ and $w_i(y', y_j)$ for any $j \neq i$ (with $y = (y', -y_j)$) are also solutions of (1.4). This implies that w_i is even with respect to y_j for $j \neq i$, and odd with respect to y_i. Therefore, denoting by

Σ_i the faces of the unit cube Y which are normal to the vector e_i, the cell problem (1.4) is equivalent to

$$\begin{cases} -\mathrm{div}_y A(y)\left(e_i + \nabla_y w_i(y)\right) = 0 & \text{in } Y \\ w_i(y) = 0 & \text{on } \Sigma_i \\ \frac{\partial w_i}{\partial n} = 0 & \text{on } \Sigma_j, j \neq i. \end{cases} \tag{1.7}$$

Of course, one can further reduce the computational domain Y in (1.7) to one of its quadrant because the same type of boundary conditions hold true on the hyperplanes, parallel to the faces of Y, running through its center.

Remark 1.1.2 *There is an alternative method to the computation of the cell and homogenized problems and to the approximation formula (1.6): the so-called Bloch wave method [13], [14], [15]. A variant of this method has also been investigated in [26], [27], [28].*

1.2 Boundary layers

An important issue in the previous classical approach is the possible improvement of the computation by adding *boundary layers*. The starting point is to recognize that the right hand side of (1.6) does not satisfy the Dirichlet boundary condition which is actually imposed to the true solution u_ϵ. Therefore, the approximation (1.6) can be improved, *at least near the boundary* $\partial\Omega$, by adding to its right hand side a so-called *boundary layer*. Introduce a function $u^\epsilon_{1,bl}(x)$, solution of

$$\begin{cases} -\mathrm{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u^\epsilon_{1,bl}\right) = 0 & \text{in } \Omega \\ u^\epsilon_{1,bl} = -\sum_{i=1}^N \frac{\partial u}{\partial x_i}(x) w_i\left(\frac{x}{\epsilon}\right) & \text{on } \partial\Omega. \end{cases} \tag{1.8}$$

Then, we replace (1.6) by

$$u_\epsilon(x) \approx u(x) + \epsilon \sum_{i=1}^N \frac{\partial u}{\partial x_i}(x) w_i\left(\frac{x}{\epsilon}\right) + \epsilon u^\epsilon_{1,bl}(x). \tag{1.9}$$

By construction, the right hand side of (1.9) satisfies the Dirichlet boundary condition as the true solution u_ϵ. One can prove that (1.9) is a better approximation than (1.6), mainly near the boundary. More precisely, without boundary layer the optimal error estimate is

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

while taking into account the boundary layer improves the estimate

$$\left\| u_\epsilon(x) - u(x) - \epsilon \sum_{i=1}^N \frac{\partial u}{\partial x_i}(x) w_i\left(\frac{x}{\epsilon}\right) - \epsilon u^\epsilon_{1,bl}(x) \right\|_{H^1(\Omega)} \leq C\epsilon. \tag{1.10}$$

However, the function $u^\epsilon_{1,bl}(x)$ is not explicit. It is only for rectangular domains with faces aligned with those of the unit cell that one can find an explicit approximation $u^\epsilon_{1,bl}(x)$.

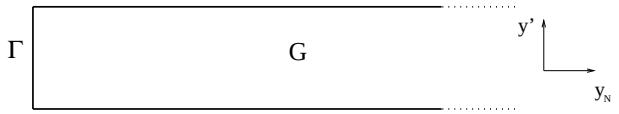

Figure 1.4: Semi infinite band.

For simplicity, assume that $\Omega = (0, L)^N$ where L is a positive length. Denote by Γ that face of Ω where $x_N = 0$ (we use the same name for the corresponding face of the unit cell Y). We define a *semi-infinite band* G by

$$G = (0, 1)^{N-1} \times (0, +\infty),$$

such that $\Gamma = \overline{G} \cap \{y_N = 0\}$ (see Figure 1.4). We use the notation $y = (y', y_N)$ with $y' = (y_1, ..., y_{N-1})$. We define a *semi-infinite band problem*

$$\begin{cases} -\mathrm{div}_y(A(y)\nabla_y w_{i,bl}) = 0 & \text{in } G \\ w_{i,bl} = -w_i & \text{on } \Gamma \\ y' \to w_i(y', y_N) & (0,1)^{N-1}\text{-periodic.} \end{cases} \tag{1.11}$$

One can prove that (1.11) admits a unique solution. Furthermore, this solution converges exponentially fast to a constant when y_N tends to $+\infty$, and its gradient converges exponentially fast to zero. More precisely, there exists a limit c_i and a positive exponent $\gamma > 0$ such that

$$\lim_{y_N \to +\infty} e^{\gamma y_N} \left(|w_{i,bl} - c_i| + |\nabla w_{i,bl}| \right) = 0.$$

The solution $w_{i,bl}$ of (1.11) is called a boundary layer. One can prove that, near Γ, we have

$$u^\epsilon_{1,bl}(x) \approx \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_{i,bl}\left(\frac{x}{\epsilon}\right). \tag{1.12}$$

Of course a similar result holds true for any face of Ω. Finally, plugging the boundary layer approximation (1.12) in (1.9) gives an approximation of u_ϵ which satisfies the same improved error estimate (1.10). Numerically, it is easy to compute approximate solutions of the semi-infinite band problem (1.11): beacuse of the exponential decay of its solution $w_{i,bl}$, one can truncate the semi-infinite band G to just a few cells (typically of the order of 5).

Boundary layers are discussed at length in many papers including [2], [25], [29]. Boundary layers are also very important for the homogenization of oscillating boundaries and for the determination of *effective boundary conditions* (see, e.g. [1], [9], [20], [24]).

Chapter 2

Heterogeneous non-periodic media

2.1 Generalities

The goal is to compute the solution of a partial differential equation in an heterogeneous medium with one, several, or a continuum of lengthscales, characterized by a small parameter ϵ. If the lengthscale ϵ is very small, a direct computation is impossible or too costly. Therefore, we want to use a mesh with a mesh-spacing of size $h >> \epsilon$.

The main idea is to use an homogenization paradigm (i.e. a specific model) to devise an adapted numerical algorithm. For example, in this section and in the next one, we consider again the model problem

$$\begin{cases} -\text{div}\,(A^\epsilon \nabla u_\epsilon) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases} \tag{2.1}$$

where $A^\epsilon(x)$ is not necessarily a periodic function of x. The last section of this chapter will focus on another model problem.

The point is that we do not satisfy ourselves with the mere computation of the solution of the homogenized problem of (2.1). We want, not only the homogenized behavior of the true solution u_ϵ, but also its microscopic fluctuations (the correctors in the terminology of periodic homogenization).

Several multiscale finite element methods for the numerical solution of (2.1) have been proposed. We are going to discuss at length that of Hou et al. [22], [23], but let us also mention a method due to Arbogast [6] for mixed finite element algorithms, a method of Matache, Babuska and Schwab [26] using Bloch waves, the HMM approach of E and Engquist [18] and a wavelet-based method [10], [17]. There are many other methods devoted to numerical homogenization (multigrid, residual free bubble, etc.).

2.2 Multiscale finite element methods

In this section we describe the multiscale finite element method of Hou et al. [22], [23], as well as its extension in [5]. The model problem under consideration is (2.1). We get some inspiration from the periodic case $A^\epsilon = A\left(\frac{x}{\epsilon}\right)$, but the method will be of use for more general cases. However, the convergence proofs are available only in the periodic case, or at least in the *non-resonant case*, i.e. when all heterogeneities length scales are smaller than the mesh size, $h >> \epsilon$.

The main idea is very close to the method of the oscillating test function due to Tartar [30]. Indeed, instead of using the usual P_1 (or affine) finite element basis, we first build an oscillating finite element basis and then compute the solution of (2.1) with this specially adapted basis.

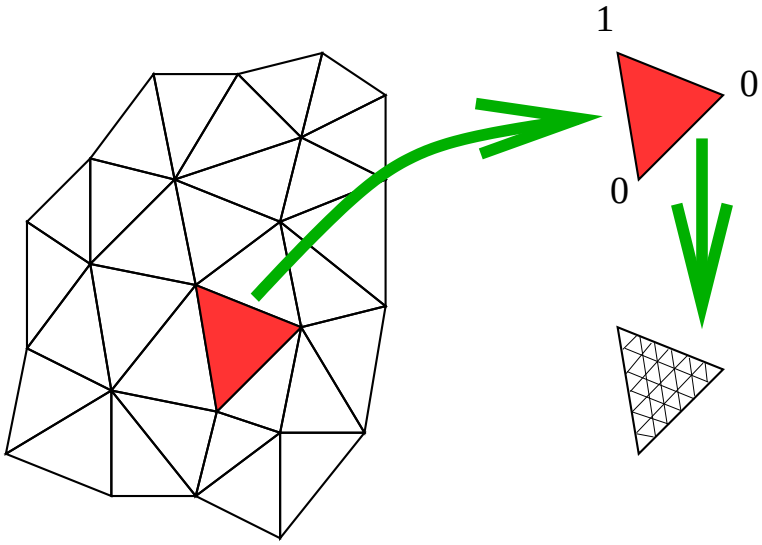

Figure 2.1: Multiscale finite element method.

We start with a coarse mesh of the domain Ω, denoted by $\mathcal{T}_h = (K_l)_{l \in I_h}$. It can be a rectangular or a triangular mesh (see Figure 2.1). We denote by $h > 0$ the mesh spacing in this coarse mesh. We denote by $(x_i)_{1 \leq i \leq N_h}$ the vertices of this coarse mesh. We build a special finite element basis adapted to the problem. Each mesh cell K has its own fine mesh, independent from the other ones (see Figure 2.1). For each mesh cell K and for each of its vertex x_i we compute a base function $\phi^\epsilon_{i,K}$ as the solution of

$$\begin{cases} -\text{div}\left(A^\epsilon \nabla \phi^\epsilon_{i,K}\right) = 0 & \text{in } K \\ \phi^\epsilon_{i,K}(x_j) = \delta_{ij} & \text{at the vertex } x_j \\ \phi^\epsilon_{i,K} & \text{affine on } \partial K \end{cases} \tag{2.2}$$

The boundary value problem (2.2) is similar to the cell problem (1.4). Indeed, introducing

the affine function $e \cdot x + c$ which coincides with the boundary condition of (2.2) (namely $e \cdot x_j + c = \delta_{ij}$), and defining $w^\epsilon_{i,K} = \phi^\epsilon_{i,K} - e \cdot x - c$, (2.2) is equivalent to

$$\begin{cases} -\text{div}\left(A^\epsilon(e + \nabla w^\epsilon_{i,K})\right) = 0 & \text{in } K \\ w^\epsilon_{i,K} = 0 & \text{on } \partial K \end{cases} \tag{2.3}$$

The main difference between (2.3) and the cell problem (1.4) is the boundary condition: Dirichlet for the former, periodic for the latter.

Collecting these functions $\phi^\epsilon_{i,K}$ for all cells K around a single vertex x_i we get a base function ϕ^ϵ_i, with compact support (see Figure 2.2), such that

$$(\phi^\epsilon_i)_{|K} \equiv \phi^\epsilon_{i,K}, \quad \phi^\epsilon_i(x_j) = \delta_{ij} \ \text{ at any vertex } x_j. \tag{2.4}$$

Remark that the computations of the base functions $\phi^\epsilon_{i,K}$ can be made in parallel since they are completely independent.

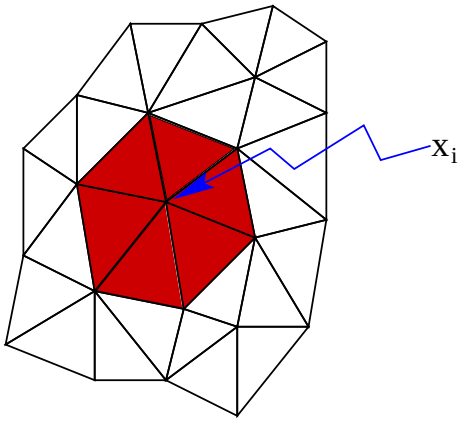

Figure 2.2: Support of the finite element basis function ϕ^ϵ_i.

Finally it remains to compute an approximation u^h_ϵ of the true solution u_ϵ of (2.1) by using the finite element basis $(\phi^\epsilon_i)_{1 \le i \le N_h}$ on the coarse mesh $\mathcal{T}_h$. This last problem is of moderate size, and thus of low cost. However, it incorporates the oscillations of the heterogeneous tensor A^ϵ. This multiscale finite element method is thus a simple conforming method. When implementing this method, there are two delicate issues. First, the rigidity matrix must be computed with a quadrature rule applied on the fine mesh. Second, the numerical solution must be plotted on the fine mesh. This is very important if one want to see the fine oscillations which are incorporated in the finite element basis functions.

In the periodic case, the following convergence result has been proved [22], [23]: there exists a constant $C > 0$ such that

$$\|u_\epsilon - u^h_\epsilon\|_{H^1_0(\Omega)} \le C\left(h + \sqrt{\frac{\epsilon}{h}}\right). \tag{2.5}$$

It is clear that estimate (2.5) is interesting only when $h >> \epsilon$, and that there is a resonance effect when h is of the same order as ϵ. The main idea in the proof of estimate (2.5) is to use asymptotic expansions of the type of (1.6) for u_ϵ and for each basis function ϕ_i^ϵ.

There is a variant of this method [23], called the multi scale finite element method *with oversampling*, which improves the estimate (2.5) by getting rid of the square root. This generalization amounts to compute the base functions $\phi_{i,K}^\epsilon$ on a fine mesh K' which is slightly larger than K, namely $K \subset\subset K'$. The method becomes non-conforming since the different functions $\phi_{i,K}^\epsilon$ do not match at the interface between neighbouring cells, but this variant suppresses all boundary layers effects near the cell boundaries ∂K.

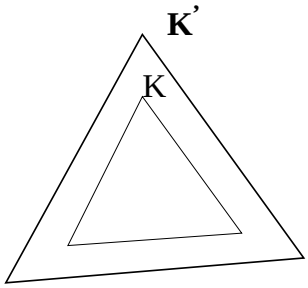

Figure 2.3: Fine mesh for the oversampling method.

Another variant [5] starts by recognizing that the approximation (1.6) is also equivalent (by a first order Taylor expansion) to

$$u_\epsilon(x) \approx u\left(x + \epsilon w\left(\frac{x}{\epsilon}\right)\right) \quad \text{with} \quad w = (w_i)_{1\leq i\leq N}. \tag{2.6}$$

Formula (2.6) suggests a change of variables. Let $(\psi_i)_{1\leq i\leq N_h}$ be a standard finite element basis on the coarse mesh (for example, P_k Lagrange finite elements). This basis is suitable for approximating the homogenized solution u. Then, by composing it with oscillating functions of the type $x + \epsilon w\left(\frac{x}{\epsilon}\right)$, we should obtain a good basis to approximate u_ϵ.

For example, taking a combination of the oscillating functions $\phi_{i,K}^\epsilon$, defined by (2.2), we build a vector ϕ_K^ϵ solution of

$$\begin{cases} -\text{div}\left(A^\epsilon \nabla \phi_K^\epsilon\right) = 0 & \text{in } K \\ \phi_K^\epsilon = x & \text{on } \partial K. \end{cases} \tag{2.7}$$

As already remarked, ϕ_K^ϵ is similar to $x + \epsilon w\left(\frac{x}{\epsilon}\right)$ (in the periodic case). Thus, by composition, we define an oscillating finite element basis

$$\psi_i^\epsilon(x) = \psi_i\left(\phi_K^\epsilon(x)\right) \quad \text{in each cell } K. \tag{2.8}$$

Finally, this basis $(\psi_i^\epsilon)_{1\leq i\leq N_h}$ is used to compute an approximate solution of u_ϵ.

If the coarse basis $(\psi_i)_{1\leq i\leq N_h}$ were P_1 (piecewise affine) finite elements, then this method is exactly that proposed by T. Hou in [22]. However, the advantages of this new method are the following.

1. One can take higher order elements for $(\psi_i)_{1\leq i\leq N_h}$, thus improving the convergence rate. More precisely, in estimate (2.5) the term h can be replaced by h^k if P_k Lagrange finite elements are used.

2. The idea can be generalized to the non-periodic case.

3. One can change the definition of ϕ_K^ϵ, and do, for example, an oversampling method: this will still yield a conforming method.

Remark 2.2.1 *Roughly speaking, the method of Arbogast amounts to replace the Dirichlet boundary condition in (2.2) by a Neumann boundary condition (but it works for mixed finite elements), while the method of Babuska and Schwab uses periodic boundary conditions.*

2.3 Factorization method in neutronics

In this section we describe another method of numerical homogenization which does not rely on the usual model problem (2.1) but rather on the following model of reaction-diffusion equation

$$\left\{\begin{array}{ll} c\left(\frac{x}{\epsilon}\right)\frac{\partial u_\epsilon}{\partial t} - \epsilon^2 \mathrm{div}\left(D\left(\frac{x}{\epsilon}\right)u_\epsilon\right) = \sigma\left(\frac{x}{\epsilon}\right)u_\epsilon & \text{in } \Omega\times\mathbb{R}_*^+ \\ u_\epsilon = 0 & \text{on } \partial\Omega\times\mathbb{R}_*^+ \\ u_\epsilon(0) = u_0 & \text{in } \Omega. \end{array}\right. \tag{2.9}$$

This model, as well as the following numerical method, is frequently used in nuclear reactor physics (or neutronics, see e.g. [3], [4]).

Recall from the second lecture that the asymptotic behavior of (2.9) is given by

$$u_\epsilon(t,x) \approx e^{-\lambda t} w\left(\frac{x}{\epsilon}\right) u\left(\epsilon^2 t, x\right), \tag{2.10}$$

where (λ, w) is the first eigencouple of the following cell spectral problem

$$\left\{\begin{array}{ll} -\lambda c(y)w - \mathrm{div}\left(D(y)w\right) = \sigma(y)w & \text{in } Y \\ y \to w(y) & Y-\text{periodic}, \end{array}\right. \tag{2.11}$$

and u is the solution of the homogenized problem

$$\left\{\begin{array}{ll} \overline{c}\frac{\partial u}{\partial \tau} - \mathrm{div}\left(\overline{D}u\right) = 0 & \text{in } \Omega\times\mathbb{R}_*^+ \\ u = 0 & \text{on } \partial\Omega\times\mathbb{R}_*^+ \\ u(0) = \overline{u}_0 & \text{in } \Omega. \end{array}\right. \tag{2.12}$$

We refer to the second lecture for the precise values of the homogenized coefficients in (2.12). The asympotic result (2.10) allows to compute a correct approximation of the true solution u_ϵ without using a fine mesh. As an example, we reproduce a result of [4] in Figure 2.4 (to which we refer for a precise description of the test case). It is a one-dimensional result (with 20 cells) comparing the true solution u_ϵ and the right hand side of (2.10). The solution is plotted for a very large time (thus, its spatial profile is given by the first eigenfunction).

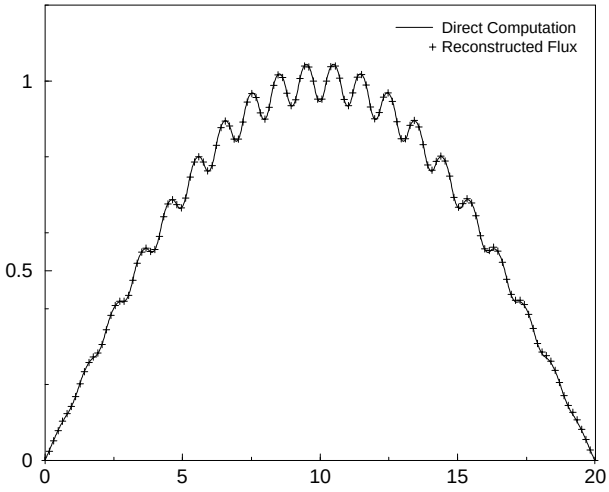

Figure 2.4: Comparison of the left and right hand sides of (2.10).

As another example of the application of (2.10) we display a two-dimensional result of V. Siess (PhD Thesis to appear) in Figure 2.5.

Although the asympotic result (2.10) is restricted to the periodic setting, it can be used to derive a multiscale numerical method in the non-periodic case (see e.g. [11], [16], [31]). When the coefficients in (2.9) are not periodic, one can still compute a cell spectral problem (2.11) for each cell of the domain Ω. Then, in the spirit of (2.10), a change of unknown is performed

$$v_\epsilon\left(\epsilon^2 t, x\right) = \frac{u_\epsilon(t,x)e^{\lambda t}}{w\left(\frac{x}{\epsilon}\right)},$$

and a standard discretization scheme is applied to the new function v_ϵ (the coefficients in the equation for v_ϵ are simply averaged in each cell). Remark that the function v_ϵ is not continuous through the interfaces between cells. Therefore, if a finite element method is used for v_ϵ, it should be a non conforming one.

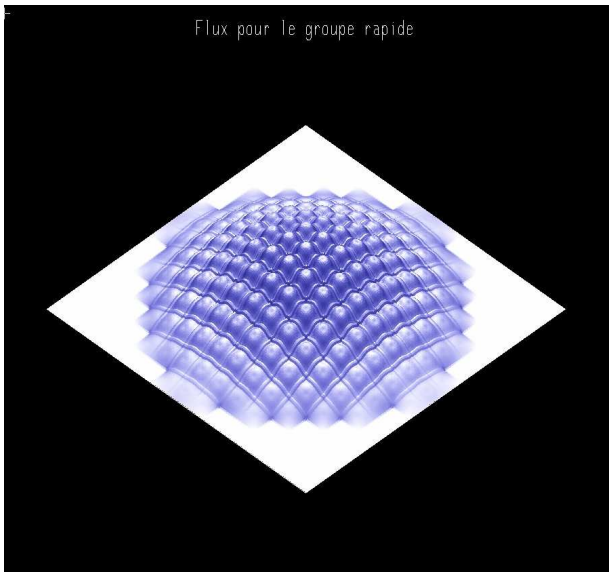

Figure 2.5: Reconstructed solution with (2.10).

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