ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

MATHICSE
Mathematics Institute of Computational Science and Engineering
School of Basic Sciences - Section of Mathematics

MATHICSE Technical Report
Nr. 10.2013
March 2013 (updated November 2013)

Numerical homogenization methods

Assyr Abdulle

http://mathicse.epfl.ch

Phone: +41 21 69 37648

Address:
EPFL - SB - MATHICSE (Bâtiment MA)
Station 8 - CH-1015 - Lausanne - Switzerland

Fax: +41 21 69 32545

Title: Numerical homogenization methods

Name: Assyr Abdulle

Affil./Addr.: Chair of Computational Mathematics and Numerical Analysis

ANMC - MATHICSE - Mathematics Section

École Polytechnique Fédérale de Lausanne (EPFL)

Station 8, 1015 Lausanne, Switzerland

E-mail: assyr.abdulle@epfl.ch ⋆

Numerical homogenization methods

Synonyms

multiscale methods for homogenization problems, upscaling methods, representative volume element methods

Definition

Numerical homogenization methods are techniques for finding numerical solutions of partial differential equations (PDEs) with rapidly oscillating coefficients (multiple scales). In mathematical analysis, homogenization can be defined as a theory for replacing a PDE with rapidly oscillating coefficients by a PDE with averaged coefficients (an effective PDE), that describes the macroscopic behavior of the original equation. Numerical techniques that are able to approximate the solution of an effective PDE (often unknown in closed form) and local fluctuation of the oscillatory solution without resolving the full oscillatory equation by direct discretization are coined "numerical homogenization methods". These methods are also called multiscale methods as they typically combine numerical solvers on different scales.

⋆ Version of 1. November 2013

Overview

Homogenization

Consider a general family of PDEs $L_\varepsilon(u_\varepsilon) = f$ with oscillating coefficients depending on a small parameter $\varepsilon > 0$ with solution $u_\varepsilon : \Omega \longrightarrow \mathbb{R}$, where Ω is an open subset of $\mathbb{R}^d,\ 1 \leq d \leq 3$. The parameter ε emphasizes the multiscale nature of the above family of PDEs, and represents a typical microscopic length scale of a heterogeneity in the system (multiple microscopic length scales could be considered as well). One can think of the solution as containing low $\mathcal{O}(1)$ frequency components and high $\mathcal{O}(1/\varepsilon)$ frequency components. Solving numerically a given PDE of the above family using classical numerical approximations such as the finite element method (FEM), the finite difference method (FDM) or the finite volume method (FVM), would usually amount in a number of degrees of freedom (DOF) (or unknowns of the discrete system) proportional to $\mathcal{O}(\varepsilon^{-d})$, which can be prohibitive for small ε. If the family of solutions converges (in some appropriate sense) to a limit denoted u_0 when the size of the heterogeneity $\varepsilon \to 0$ and if that limit is the solution of an averaged (homogenized) equation $L_0(u_0) = f$, we then have an effective (upscaled, averaged) model that can be treated with a classical method at a cost independent of ε. The rigorous study of these questions is the core of the mathematical homogenization theory [10; 26; 28].

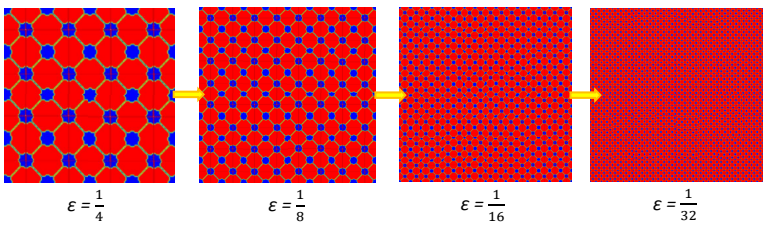

Fig. 1. Heterogeneous domain with periodic heterogeneities of size $\varepsilon \to 0$.

Numerical approaches

In most practical situations, the averaged equation described in the previous section is not known in explicit form. Furthermore, even if known, the data of the averaged equation are usually not known explicitly but rely for each $x \in \Omega$ on yet another PDE. Numerical approaches for homogenization problems were pioneered by Babuška [8] and have since then enjoyed considerable developments. In what follows we explain the main ideas of a few numerical homogenization strategies that have been developed in the applied mathematics community. There is also an abundant related literature on multiscale computational methods in the field of material sciences, that share similar ideas as the ones described below (unit cell methods, continuous/discontinuous computational homogenization methods). The emphasis there is rather on applications (bulk modeling, crack modeling, failure) and we refer to recent reviews for references [27; 21].

Among the computational methods that we will describe, we will focus on techniques based on finite element methods (FEMs), but the main ideas are also applicable to other type of discretizations. We choose for $L_\varepsilon(u_\varepsilon) = f$ an elliptic multiscale problem that reads in weak form: Find $u_\varepsilon \in V(\Omega)$ such that

$$B(u_\varepsilon, v) = \int_\Omega a^\varepsilon \nabla u_\varepsilon \cdot \nabla v dx = (f, v) \quad \forall v \in V(\Omega), \tag{1}$$

where $(f, v) = \int_\Omega f v dx$ and $V(\Omega)$ is a Sobolev space that we choose to be $H_0^1(\Omega)$ (the space of square-integrable functions that vanishes on $\partial\Omega$ with square-integrable derivatives). Here a^ε is an oscillating tensor with fast $\mathcal{O}(1/\varepsilon)$ and slow frequencies. The homogenized problem corresponding to the above equation reads: Find $u_0 \in V(\Omega)$ such that

$$B_0(u_0, v) = \int_\Omega a^0 \nabla u_0 \cdot \nabla v dx = (f, v) \quad \forall v \in V(\Omega). \tag{2}$$

The solution u_ε can be expected to behave as $u_0 + \varepsilon u_1$, with $\|u_1\|_{L^2(\Omega)} = \mathcal{O}(1)$ but $\|\nabla u_1\|_{L^2(\Omega)} = \mathcal{O}(1/\varepsilon)$. A standard finite element (FE) approximation of (1) consists in

a solution u_h of (1) in a finite dimensional space spanned by piecewise polynomials on a partition $\mathcal{T}_h$ of Ω with mesh size h (see below). However, a good approximation of u_ε by u_h (the FE solution) is usually obtained only if $h \ll \varepsilon$ in which case the complexity (DOF) scales as $\mathcal{O}(\varepsilon^{-d})$. Two main classes of numerical homogenization methods have been developed to address this issue:

1. methods based on a reduced model generated from the original fine scale problem,
2. methods that sample the original fine scale problem on patches to recover effective data of a macroscopic model and use correctors to reconstruct the fine scale solution.

Notations

In what follows we will consider for simplicity Ω to be both polygonal and convex and we restrict ourselves to simplicial FEs. We consider a family of macroscopic (conformal, shape regular) triangulations $\mathcal{T}_H$ of $\Omega = \cup_{K\in\mathcal{T}_H} K$, with elements K of diameter H_K and $H = \max_{K\in\mathcal{T}_H}$ the size of the triangulation (mesh size). For a macroscopic triangulation, $H > \varepsilon$ is allowed. On a (polygonal) subset D of Ω we also consider a microscopic triangulation $D = \cup_{T\in\mathcal{T}_h} T$, with elements T of diameter h_T and a meshsize h that satisfies $h < \varepsilon$. We then consider the following FE spaces

$$V_H(\Omega) = \{v_H \in V(\Omega);\ v_H|_K \in \mathcal{P}^1(K),\ \forall K \in \mathcal{T}_h\}, \tag{3}$$

$$V_h(D) = \{v_h \in V(D);\ v_h|_T \in \mathcal{P}^1(T),\ \forall T \in \mathcal{T}_h\}, \tag{4}$$

where $\mathcal{P}^1(K)$ is the space of piecewise linear polynomials on K (resp. T). For a cubic domain $D = Y$ we also consider

$$W_h(D) = \{v_h \in W^1_{per}(D);\ v_h|_T \in \mathcal{P}^1(T),\ \forall T \in \mathcal{T}_h\}, \tag{5}$$

where $W^1_{per}(D)$ is a Sobolev space of periodic functions (the closure of smooth periodic functions on D for the H^1 norm, where functions differing by a constant are identified). We consider here piecewise linear polynomials and conformal meshes for simplicity but

emphasize that the methods described below have been generalized to higher order piecewise polynomial spaces and other types of FEs.

Supplementing oscillatory functions to a coarse FE space

The idea to enrich a coarse FE space with oscillatory functions goes back to Babuška and Osborn [9], where the methodology is described for one-dimensional problems. This idea has inspired generalizations to higher dimensions in various directions. We describe such a generalization in the context of numerical homogenization.

Multiscale Finite Element Method (MsFEM)

The main idea is to supplement oscillating functions to a coarse FE space. We consider the FE space (3). For each vertex $x_\nu,\ \nu = 1, 2, \ldots, N$ of the mesh $\mathcal{T}_H$ that does not intersect the boundary $\partial\Omega$, we denote by $\varphi_{\nu,H}$ the nodal basis function such that $\varphi_{\nu,H}(x_\mu) = \delta_{\nu\mu}$, where $\delta_{\nu\mu}$ is the Kronecker delta. We thus have $V_H(\Omega) = \text{span}\{\varphi_{\nu,H},\ \nu = 1, 2, \ldots, N\}$. For each macro element K we also consider its $d+1$ vertices that we denote $x_{K,j},\ j = 1, \ldots, d+1$, and the $d+1$ basis functions $\varphi_{\nu,H}$ that do not vanish in K will be denoted by $\varphi_{K,j,H}$. We next define the oscillatory functions that will enrich the coarse finite FE space $V_H(\Omega)$. For that we consider the FE space (4) with $D = K$ and $q = 1$ and for each $j = 1, \ldots, d+1$, the following microscopic problem: Find $\phi_{K,j,h}$ such that $\phi_{K,j,h} - \varphi_{K,j,H} \in V_h(K)$ and

$$\int_K a^\varepsilon \nabla\phi_{K,j,h} \cdot \nabla z_h dx = 0 \quad \forall z_h \in V_h(K). \tag{6}$$

The multiscale finite element space is defined as $V_{MsFEM} := \text{span}\{\phi_{K,j,h};\ j = 1, \ldots, d+1,\ K \in \mathcal{T}_H\}$, and the multiscale method is defined by the following problem [24]: Find $u_{Hh} \in V_{MsFEM}$ such that

$$B(u_{Hh}, v_{Hh}) = (f, v_{Hh}) \quad \forall v_{Hh} \in V_{MsFEM}, \tag{7}$$

where $B(\cdot,\cdot)$ is defined in (1). We observe that $V_{MsFEM} \subset V(\Omega)$ and the method is conforming. The accuracy of the method has been studied in [24; 7] for (locally) periodic coefficients, i.e., tensors $a^\varepsilon(x) \in \mathbb{R}^{d\times d}$ of the form $a^\varepsilon(x) = a(x, x/\varepsilon) = a(x, y)$ that are Y-periodic in y (here Y is a unit cube). Assuming appropriate regularity on the solutions of (1),(2) and on the tensor a^ε one can show

$$\|u^\varepsilon - u_{Hh}\|_{H^1(\Omega)} \leq C_1 \left(H + \left(\frac{h}{\varepsilon}\right)\right) + C_2 \left(\frac{\varepsilon}{H}\right)^{1/2},$$

that is, linear convergence in the macroscopic and microscopic mesh sizes up to a so-called resonance error $(\varepsilon/H)^{1/2}$. This term originates from the mismatch of the artificial boundary conditions imposed on the local problems (6) and the possible mismatch between the macroscopic mesh size H and the ideal sample size (e.g., an integer number of the period in the periodic case). One idea to decrease the resonance error is oversampling that consists in solving (6) in a larger domain $K_O \supset K$ but using only the micro functions restricted to K to construct the basis of V_{MsFEM}. In doing so, it is shown in [19] that the influence of the boundary layer in the larger domain K_O on the basis functions of V_{MsFEM} is reduced and the resonance error can be decreased to $\varepsilon/H + \sqrt{\varepsilon}$. We note that in this reformulation, two basis functions constructed in two adjacent macro elements K, K' might not match on the boundary $K \cap K'$, i.e., $V_{MsFEM} \not\subset V(\Omega)$; hence, the method is nonconforming.

Computational work

Assuming that the cost of the linear algebra *scales linearly* with the unknowns of the linear system, we have a total cost proportional to the number of macro elements times the DOF for the multiscale basis. In view of the above error estimates setting the micro mesh $\frac{h}{\varepsilon} \simeq H = \frac{1}{N_{mac}}$ (for optimal convergence rates) we find cost$= \mathcal{O}((N_{mac})^d) \cdot$

$\mathcal{O}\big((\frac{H}{h})^d\big) = \mathcal{O}((N_{mac})^d \cdot \varepsilon^{-d})$. It should be noted that the computation of the basis functions can be performed in parallel, and that for problems with different source terms or for some time-dependent problems, the basis functions can be computed once. Furthermore, for problems with scale separation, the macroscopic elements K could be replaced by a smaller region of the size of the local period resulting in a reduced cost. We refer to [18] for a comprehensive review of the MsFEM.

MsFEM using harmonic coordinates

In [7] MsFEM type methods using (localized) harmonic coordinates have been proposed. On each element K one considers $\boldsymbol{\phi}_{K,h} = \{\phi_{K,1,h}, \ldots, \phi_{K,d,h}\}$, where $\phi_{K,j,h},\ j = 1, \ldots, d$, are the d solutions of the microscopic problem (6), and a function $\boldsymbol{\phi}_h : \Omega \to \mathbb{R}^d$ such that $\boldsymbol{\phi}_{h|K} = \boldsymbol{\phi}_{K,h}\ \forall K \in \mathcal{T}_H$. We can then define a multiscale finite element basis as $\tilde{V}_{MsFEM} := \text{span}\{\varphi_{\nu,H} \circ \boldsymbol{\phi}_h;\ \nu = 1, 2, \ldots, N\}$, where $\varphi_{\nu,H}$ are the standard piecewise polynomials on the macroscopic mesh $\mathcal{T}_H$. This change of coordinates simplifies the construction and analysis of higher order MsFEM. We also refer to [31] for related work on the approximation of oscillatory problems with rough and high contrast coefficients.

Supplementing upscaled data for coarse FE computation and reconstruction

The general numerical strategy is to get an effective model by performing local computations. These local computations can in turn also be used to reconstruct the fine scale solution. As the effective data usually depend on $x \in \Omega$, one has in general an infinite number of such local problems to solve (except for the case of a periodic fine scale tensor). For numerical computation one needs thus to select sampling points $x_i \in \Omega,\ i = 1, \ldots, p$, where such local computations have to be performed. A classical

approach consists in selecting sampling points $x_i \in \Omega,\ i = 1, \ldots, p$, and pre-computing an approximation of the effective tensor $a^0(x_i)$ at these points. This approach does however not offer much control on the overall numerical discretization (that depends on the accuracy of the precomputed data), neither does it offer an efficient strategy for non-periodic, nonlinear or time dependent problems. A local switch to a fine scale approximation is also difficult with this strategy. An efficient approach is to supplement the effective data (relying on a micro FEM) simultaneously to the coarse FE discretization (relying on a macro FEM). A representative method for this approach is described below.

Heterogeneous Multiscale Method

We start by motivating the computational strategy. Consider u_ε the solution of the fine scale problem (1) and assume that it can be well approximated by $u_0 + \varepsilon u_1$, that we write $u_0 + \tilde{u}_1$, where we suppose $\|\tilde{u}_1\|_{L^\infty(\Omega)} = \mathcal{O}(\varepsilon), \|\nabla \tilde{u}_1\|_{L^\infty(\Omega)} = \mathcal{O}(1)$. As before we consider a coarse triangulation of the computational domain $\Omega = \cup_{K \in \mathcal{T}_H} K$, and in addition, within each K we consider a sampling domain $K_\delta \subset K$ that consists of a cube of size δ centered in a node $x_K \in K$, with δ of size comparable to ε (provided $\delta \geq \varepsilon$). Locally, we would like our numerical approximation u_h of u_ε to satisfy $u_h = u_H + \tilde{u}_h$, where u_H belongs to a macro FE space $V_H(\Omega)$ and $\tilde{u}_h$ to a micro FE space $\tilde{V}_h(K_\delta)$. If $\tilde{u}_h$ is an approximation of $\tilde{u}_1$ we should have $\frac{1}{|K_\delta|} \int_{K_\delta} \tilde{u}_h dx = \mathcal{O}(\varepsilon)$, where $|K_\delta|$ denotes the measure (volume) of K_δ, and we will assume for the time being that functions in $\tilde{V}_h(K_\delta)$ have zero mean. We next consider (1), where we approximate the right-hand side f by a macroscopic function f_H that is piecewise constant on $\mathcal{T}_H$. If now u_h is an approximation of the fine scale problem (1) we have $u_h - u_H = \tilde{u}_h \in \tilde{V}_h(K_\delta)$ and

$$\int_{K_\delta} a^\varepsilon(x) \nabla u_h \cdot \nabla \tilde{z}_h dx = \int_{K_\delta} f_H \tilde{z}_h dx = 0 \quad \forall \tilde{z}_h \in \tilde{V}_h(K_\delta), \tag{8}$$

where we have used that $\tilde{z}_h$ has zero mean over K_δ and f_H is constant in K. Substituting now $\tilde{u}_h + u_H$ for u_h in the above equations yields $\tilde{u}_h = \sum_{j=1}^d \tilde{\chi}_{K,j,h} \partial u_H/\partial x_j$, where $\chi_{K,j,h}, j = 1, \dots d$ are the solutions of the problem

$$\int_{K_\delta} a^\varepsilon(x) \nabla \chi_{K,j,h} \cdot \nabla \tilde{z}_h dx = \int_{K_\delta} a^\varepsilon(x) \boldsymbol{e}_j \nabla \tilde{z}_h dx \quad \forall \tilde{z}_h \in \tilde{V}_h(K_\delta), \tag{9}$$

where $\boldsymbol{e}_j, j = 1, \dots d$ are the vectors of the canonical basis of $\mathbb{R}^d$. Inserting now $\tilde{z}_h = u_h - u_H$ in (8), recalling that u_H is linear on K, reveals that

$$\begin{aligned} \frac{1}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x) \nabla u_h \cdot \nabla u_h dx &= \frac{1}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x) \nabla u_h \cdot \nabla u_H dx \\ &= \frac{1}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x)(I + \tilde{\Psi}_{K,h}) dx \nabla u_H \cdot \nabla u_H \\ &= \frac{1}{|K|} \int_K a_K^0 \nabla u_H \cdot \nabla u_H dx, \end{aligned} \tag{10}$$

where $a_K^0 = \frac{1}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x)(I + \tilde{\Psi}_{K,h}) dx$, and $\tilde{\Psi}_{K,h}$ is a $d \times d$ matrix given by $\tilde{\Psi}_{K,h} = (\nabla \chi_{K,1,h}, \dots, \nabla \chi_{K,d,h})$. The above relation suggests to consider a macroscopic effective energy

$$\begin{aligned} J(v_H) &= \frac{1}{2} \sum_{K \in \mathcal{T}_H} \int_K a_K^0 \nabla v_H \cdot \nabla v_H dx - \int_\Omega f v_H dx \\ &= \frac{1}{2} \sum_{K \in \mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x) \nabla v_h \cdot \nabla v_h dx - \int_\Omega f v_H dx, \end{aligned}$$

for a function $v_H \in V_H(\Omega)$ and motivates the definition of the variational form of the finite element heterogeneous multiscale method (FE-HMM) [16; 1; 17]: Find $u_H \in V_H(\Omega)$ such that

$$B_H(u_H, v_H) = \sum_{K \in \mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x) \nabla u_h \cdot \nabla v_h dx = \int_\Omega f v_H dx \quad \forall v_H \in V_H(\Omega), \tag{11}$$

where u_h (respectively v_h) is such that $u_h - u_H \in \tilde{V}_h(K_\delta)$ (respectively $v_h - v_H \in \tilde{V}_h(K_\delta)$) and a solution of (8). We make the following observations:

- $B_H(u_H, v_H) = \sum_{K \in \mathcal{T}_H} |K| a_K^0 \nabla u_H \cdot \nabla v_H$, which resembles a FEM with *numerical quadrature* for an upscaled problem,

- the micro problem (8) is well posed for various micro FEM spaces $\tilde{V}_h(K_\delta)$ provided that the tensor a^ε is uniformly elliptic and bounded. In particular $\tilde{V}_h(K_\delta) = W_h(K_\delta)$ or $V_h(K_\delta)$ are possible choices (for this latter space one does not need to enforce the zero mean property),
- higher order methods rely on higher order quadrature formula, e.g., $B_H(u_H, v_H) = \sum_{K\in\mathcal{T}_H}\sum_{j=1}^{J}\omega_{K,j}a^0_{K,j}\nabla u_H(x_{K,j})\cdot\nabla v_H(x_{K,j})$, for appropriate nodes $x_{K,j}$ and weights $\omega_{K,j}$,
- variational crimes are inherent to the method and the Galerkin orthogonality for $u_0 - u_H$ with respect to $B_0(\cdot,\cdot)$ does not hold.

Assuming appropriate regularity on the solution of (2) and on the tensor a^ε one can show for locally periodic coefficients [1; 17; 2] with $\tilde{V}_h(K_\delta) = V_h(K_\delta)$ that

$$\|u_0 - u_H\|_{H^1(\Omega)} \leq C_1\left(H + \left(\frac{h}{\varepsilon}\right)^2\right) + C_2\frac{\varepsilon}{\delta},$$

where C_1, C_2 are independent of H, h, ε. We observe that the micro error is quadratic in the H^1 norm (this result holds also for non symmetric tensors a^ε [14; 5]). The macroscopic error relies on error estimates for FEM with numerical quadrature. The term $\frac{\varepsilon}{\delta}$ is a resonance error that originates from the mismatch of the artificial boundary conditions imposed on K_δ. If $\delta/\varepsilon \in \mathbb{N}$ and $V_h(K_\delta) = W_h(K_\delta$ then $C_2 = 0$. This error bound can also be improved using a modified cell problem as studied recently in [22].

Fine scale approximation

A fine scale approximation can be recovered by a the following simple post-processing procedure following the methodology developed in [30]. Suppose that we want to know a fine scale approximation in $D \subset \Omega$. Consider $D \subset D_\eta \subset \Omega$, where $\text{dist}(\partial D, \partial D_\eta) = \eta$. We next consider the following problem in D_η: find $u_{Hh} - u_H \in \tilde{V}_h(D_\eta)$ such that

$$\int_{D_\eta} a^\varepsilon(x)\nabla u_{Hh}\cdot\nabla\tilde{z}_h dx = 0 \quad \forall\tilde{z}_h \in \tilde{V}_h(D_\eta),$$

where u_H is the solution of 11. For the error, we have [17]

$$\int_D |\nabla(u^\varepsilon - u_{Hh})|^2 dx \leq \frac{C}{\eta} \left(\|u_0 - u_H\|_{L^\infty(D_\eta)} + \|u_\varepsilon - u_H\|_{L^\infty(D_\eta)} \right).$$

For locally periodic homogenization problem it is also possible to define a simpler reconstruction. Indeed, extend the function u_h available in each K_δ periodically in K (we denote this extension by $\tilde{u}_{h,K}$) and consider the reconstruction

$$u_{Hh}(x) = u_H(x) + \tilde{u}_{h,K}(X), \ x \in K, \forall K \in \mathcal{T}_H.$$

If we assume that $\tilde{V}_h(K_\delta) = W_h(K_\delta)$ and $\delta/\varepsilon \in \mathbb{N}$ then [1; 17]

$$\left(\sum_{K \in \mathcal{T}_H} \|\nabla u^\varepsilon - \nabla u_{Hh}\|^2_{L^2(K)} \right)^{1/2} \leq C \left(H + \frac{h}{\varepsilon} + \sqrt{\varepsilon} \right),$$

where C is independent of H, h, ε.

Computational work

Assuming that the cost of the linear algebra *scales linearly* with the unknowns of the linear system we have a total cost proportional to the number of macro elements times the DOF for the micro functions in each sampling domain. In view of the above error estimates, setting the micro mesh $\frac{h}{\varepsilon} \simeq \sqrt{H}$ which implies $h = \frac{\varepsilon}{N_{mac}^{1/2}}$ with $H = \frac{1}{N_{mac}}$ we obtain cost= $\mathcal{O}((N_{mac})^d) \cdot \mathcal{O}\big((\frac{\delta}{h})^d\big) = \mathcal{O}((N_{mac})^{3d/2})$, for the approximation of u_0 and setting $\frac{h}{\varepsilon} \simeq H$ we obtain cost= $\mathcal{O}((N_{mac})^d) \cdot \mathcal{O}\big((\frac{\delta}{h})^d\big) = \mathcal{O}((N_{mac})^{2d})$, for the approximation of the fine scale solution u_ε (locally periodic case). As can be seen from the above estimates, the complexity in this approach is independent of ε. This is a consequence of choosing a computational strategy based on localizing the fine scale computations. We refer to [3; 15; 4] for recent reviews.

Other approaches

There have been a number of other approaches that have been developed for (or that can be applied to) homogenization problems. We describe the main ideas of a few representative algorithms.

Variational Multiscale and Residual Free Bubble Methods

First developed to address the issue of stabilizing FEM, the Variational Multiscale Method (VMM) introduced in [25] and the Residual Free Bubble Method (RFB) [13] have evolved into general frameworks for the construction of effective numerical methods for the approximation of the solution of a PDE with multiple scales. In the VMM one starts to decompose the numerical approximation u_h of the PDE into $u_h = u_H + \tilde{u}$, where u_H represents coarse scales and $\tilde{u}$ represents fine scales. Likewise, a finite dimensional space $V_h \in V(\Omega)$ large enough to resolve the fine scale details is decomposed into coarse V_H and fine scale part $\tilde{V}$. One then seeks a solution $u_h = u_H + \tilde{u} \in V_H \oplus \tilde{V}$ such that

$$\begin{aligned} B(u_H + \tilde{u}, v_H) &= (f, v_H) \quad \forall v_H \in V_H, \\ B(u_H + \tilde{u}, \tilde{v}) &= (f, \tilde{v}) \quad \forall \tilde{v} \in \tilde{V}. \end{aligned} \tag{12}$$

Writing the second equation as $B(\tilde{u}, \tilde{v}) = (f, \tilde{v}) - B(u_H, \tilde{v}) = (f - \mathcal{L}(u_H), \tilde{v})$ on can write formally $\tilde{u} = M(f - \mathcal{L}(u_H))$ (M is a bounded linear operator on $\tilde{V}$ obtained by restricting $f - \mathcal{L}(u_H)$ to $\tilde{V}$) to obtain a variational problem in V_H

$$B(u_H, v_H) + B\left(M(f - \mathcal{L}(u_H)), v_H\right) = (f, v_H) \quad \forall v_H \in V_H.$$

For an actual numerical solution, the operator M has to be approximated and localized. In the RFB, one starts with the coarse FE space V_H and seek to enlarge it by adding localized FE enrichments that belong to the so-called bubble space, i.e., one chooses

$\tilde{V} = V_B = \{v \in V;\ v_{|\partial K} = 0\}$. Considering (12) with $\tilde{V}$ replaced by V_B, we see that the fine scale equation is now localized. Although the VMM and the RFB have originally not been introduced for homogenization problems, it has been shown that they share similarities with the MsFEM [32].

Sparse Tensor Product FEM

This computational approach is based on the two-scale convergence theory and its generalization [29; 6]. The two-scale convergence is a rigorous justification of the ansatz made in the introduction, namely that the solution u_ε behaves as $u_0 + \varepsilon u_1$ for periodic homogenization problems with locally periodic tensors a^ε. Consider the function u_1 as a mapping $\Omega \to W^1_{per}(Y)$ that is square integrable and denote the set of such functions as $L^2(\Omega; W^1_{per}(Y))$. Using test functions of the form $v + \varepsilon v_1$ in the variational form (1) and "passing to the limit" one arrives at the following two-scale problem: Find $u_0 \in V(\Omega), u_1 \in L^2(\Omega; W^1_{per}(Y))$ such that

$$\int_\Omega \int_Y a(x,y)\,(\nabla_x u_0 + \nabla_y u_1) \cdot (\nabla_x v + \nabla_y v_1)\,dydx = (f, v), \tag{13}$$

for all test functions $v \in V(\Omega)$ and $v_1 \in L^2(\Omega; W^1_{per}(Y))$. To turn this homogenization technique into a numerical approach the ideas are now to

- define a tensor product FE space as a subspace of $V(\Omega) \times L^2(\Omega; W^1_{per}(Y)$ to discretize the "augmented variational problem";
- construct a sparse tensor product FE space based on hierarchical sequences of FE spaces in the component domains.

It is shown in [23] that the complexity of solving the augmented system numerically (with an appropriate sparse tensor product FEM) is comparable to the complexity of a standard FEM for a single scale problem in Ω.

Projection-based Numerical Homogenization

Starting with a fine scale discretization of the equation (1), the idea is to project this discretized problem into a lower dimensional space and successively eliminate the fine scale component [12; 20]. Consider

$$L_j u_j = f_j,$$

a fine scale discretization of a multiscale problem $L_\varepsilon(u_\varepsilon) = f$ in a finite dimensional subspace $V_j = V_j(\Omega)$ of $V(\Omega)$. Here V_j is supposed to be large enough to resolve the fine scale details of the original problem. One considers next a decomposition

$$V_j = V_{j-1} \oplus W_{j-1},$$

where V_{j-1}, W_{j-1} represent the coarse and fine scale components of functions in V_j. Next, one defines the projection $v_j^p = P(v_j)$ for functions in V_j using the projection operator $P : V_j \to V_{j-1}$ and defines $v_j^q = Q(v_j) := v_j - P(v_j)$, for the operator $Q : V_j \to W_{j-1}$. A natural way to construct these projections is by using a wavelet basis. It is then seen that u_j^p, the coarse scale part of u_j, satisfies the equation

$$\bar{L}_j u_j^p = \bar{f}_j$$

where $\bar{L}_j = PL_jP - PL_jQ(QL_jQ)^{-1}QL_jP$, and $\bar{f} = Pf_j - PL_jQ(QL_jQ)^{-1}Qf_j$. The coarse grid operator $\bar{L}_j$ can be seen to be the Schur complement of the operator $G_jL_jG_j^*$, where $G_j = (P_j \; Q_j)$ and G_j^* is its adjoint. This procedure can then be iterated to eliminate successively the fine-scale components. An issue with this approach is that the $\bar{L}_j$ might not be sparse in general even if one starts with a sparse operator L_{j+1}. However, for classes of problems for which the element of $\bar{L}_j$ have a fast decay away from the main diagonal, $\bar{L}_j$ can be well approximated by a sparse matrix [11].

Numerical illustration

As mentioned earlier, most of the numerical methods described in this article can be generalized to time dependent problems. To illustrate numerical homogenization techniques, we consider a parabolic homogenization problem studied in [5]

$$L_\varepsilon u_\varepsilon = \partial_t u_\varepsilon - \nabla \cdot (a^\varepsilon \nabla u_\varepsilon) = f \quad \text{in } \Omega \times (0,T),$$

with initial and boundary conditions as described below. The numerical homogenization algorithm is chosen to be the FE-HMM. For the multiscale tensor a^ε, we choose a log-normal stochastic field with mean zero and variance $\sigma = 0.01$. Here ε plays the role of the correlation lengths of the log-normal field given by $\varepsilon_{x_1} = 0.01$ and $\varepsilon_{x_2} = 0.02$. Other data are given by $f(x,t) = 1$ and $u_\varepsilon(x,0) = 7(0.5 - x_1)(0.5 + x_1)(1 + x_2)$ in Ω. The computational domain Ω consists of a half disk partitioned with a coarse mesh using 576 (macro) triangles, and a rectangle meshed using 784 (macro) quadrilaterals, which leads to about $M_{macro} \approx 1100$ DOF, when using piecewise linear and piecewise bilinear polynomials, respectively. We consider mixed boundary conditions, with Dirichlet conditions on the three edges of the rectangular, and Neumann conditions on the boundary of the half disk. We perform two numerical experiments: First we use the FE-HMM on a coarse mesh, second we use a standard FEM using a mesh resolving the correlation lengths leading to around 10^6 DOF. As the tensor a^ε is not periodic, we choose sampling domains K_δ with a size a few times larger than the correlation lengths in each spatial dimension. In Figure 2 we illustrate the capability of the FE-HMM method to capture the correct macroscopic behavior on a coarse macroscopic mesh.

References

1. A. Abdulle. On a priori error analysis of fully discrete heterogeneous multiscale FEM. *SIAM, Multiscale Model. Simul.*, 4(2):447–459, 2005.

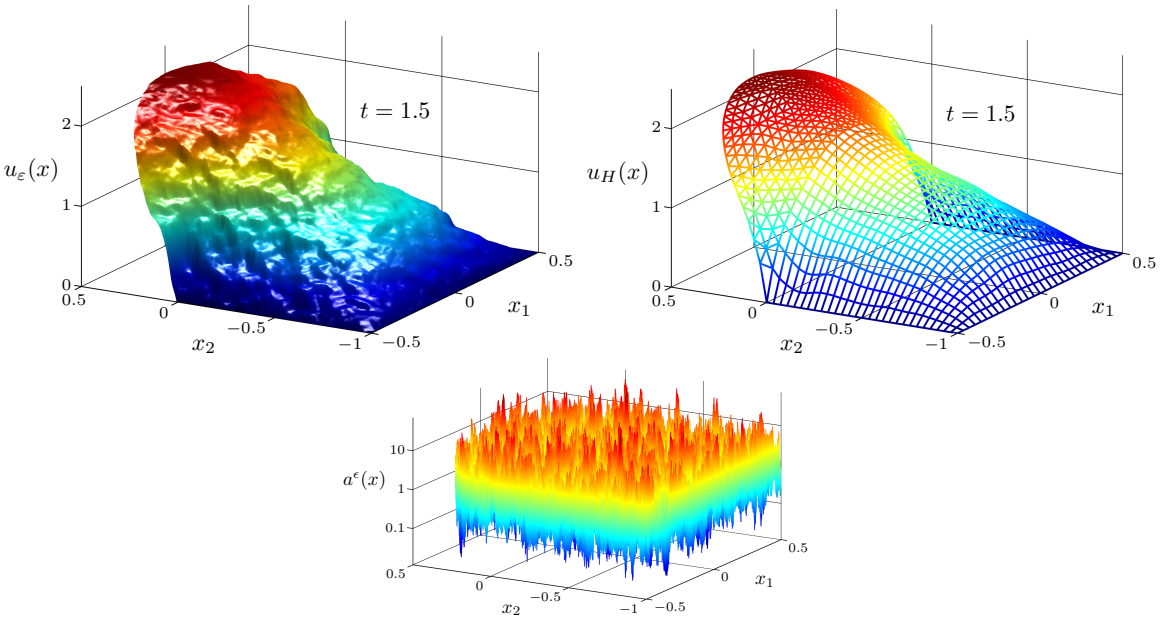

Fig. 2. Fine scale computation (left figure), a realization of the stochastic tensor (middle figure) and FE-HMM (right figure).

2. A. Abdulle. Analysis of a heterogeneous multiscale FEM for problems in elasticity. *Math. Models Methods Appl. Sci.*, 16(4):615–635, 2006.
3. A. Abdulle. A priori and a posteriori error analysis for numerical homogenization: a unified framework. *Ser. Contemp. Appl. Math. CAM*, 16:280–305, 2011.
4. A. Abdulle, W. E, B. Engquist, and E. Vanden-Eijnden. The heterogeneous multiscale method. *Acta Numer.*, 21:1–87, 2012.
5. A. Abdulle and G. Vilmart. Coupling heterogeneous multiscale FEM with Runge-Kutta methods for parabolic homogenization problems: a fully discrete space-time analysis. *Math. Models Methods Appl. Sci.*, 22(6):1250002/1–1250002/40, 2012.
6. G. Allaire and M. Briane. Multiscale convergence and reiterated homogenisation. *Proc. Roy. Soc. Edinburgh Sect. A*, 126(2):297–342, 1996.
7. G. Allaire and R. Brizzi. A multiscale finite element method for numerical homogenization. *Multiscale Model. Simul.*, 4(3):790–812 (electronic), 2005.
8. I. Babuška. Homogenization and its application. Mathematical and computational problems. *Numerical solution of partial differential equations, III (Proc. Third Sympos. (SYNSPADE), Univ. Maryland, College Park, Md., 1975)*, pages 89–116, 1976.
9. I. Babŭska and J. Osborn. Generalized finite element methods: their performance and their relation to mixed methods. *SIAM J. Numer. Anal.*, 20:510–536, 1983.

10. A. Bensoussan, J.-L. Lions, and G. Papanicolaou. *Asymptotic analysis for periodic structures*. North-Holland Publishing Co., Amsterdam, 1978.

11. G. Beylkin, R. Coifman, and V. Rokhlin. Fast wavelet transforms and numerical algorithms. I. *Comm. Pure Appl. Math.*, 44(2):141–183, 1991.

12. M. E. Brewster and G. Beylkin. A multiresolution strategy for numerical homogenization. *Appl. Comput. Harmon. Anal.*, 2(4):327–349, 1995.

13. F. Brezzi and A. Russo. Choosing bubbles for advection-diffusion problems. *Math. Models Methods Appl. Sci.*, 4(4):571–587, 1994.

14. R. Du and P. Ming. Heterogeneous multiscale finite element method with novel numerical integration schemes. *Commm. Math. Sci.*, 8(4):863–885, 2010.

15. W. E. *Principles of multiscale modeling*. Cambridge University Press, Cambridge, 2011.

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

17. W. E, P. Ming, and P. Zhang. Analysis of the heterogeneous multiscale method for elliptic homogenization problems. *J. Amer. Math. Soc.*, 18(1):121–156, 2005.

18. Y. Efendiev and T. Y. Hou. *Multiscale finite element methods. Theory and applications*, volume 4 of *Surveys and Tutorials in the Applied Mathematical Sciences*. Springer, New York, 2009.

19. Y. R. Efendiev, T. Y. Hou, and X.-H. Wu. Convergence of a nonconforming multiscale finite element method. *SIAM J. Numer. Anal.*, 37(3):888–910, 2000.

20. B. Engquist and O. Runborg. Wavelet-based numerical homogenization with applications. *Multiscale and multiresolution methods*, 20:97–148, 2002.

21. M. Geers, V. Kouznetsova, and W. Brekelmans. Multi-scale computational homogenization: Trends and challenges. *J. Comput. Appl. Math.*, 234:2175–2182, 2010.

22. A. Gloria. Reduction of the resonance error. Part 1: Approximation of homogenized coefficients. *Math. Models Methods Appl. Sci.*, 21(8):1601–1630, 2011.

23. V. H. Hoang and C. Schwab. High-dimensional finite elements for elliptic problems with multiple scales. *Multiscale Model. Simul*, 3(1):168–194, 2005.

24. T. Hou, X. Wu, and Z. Cai. Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients. *Math. Comp.*, 68(227):913–943, 1999.

25. T. J. R. Hughes. Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods. *Comput. Methods Appl. Mech.*

Engrg., 127(1-4):387–401, 1995.

26. V. Jikov, S. Kozlov, and O. Oleinik. *Homogenization of differential operators and integral functionals*. Springer-Verlag, Berlin, Heidelberg, 1994.
27. P. Kanouté, D. Boso, J. Chaboche, and B. Schrefler. Multiscale methods for composites: A review. *Arch. Comput. Meth. Eng.*, 16:31–75, 2009.
28. F. Murat and L. Tartar. H-convergence, topics in the mathematical modeling of composite materials. *Progr. Nonlinear Differential Equations Appl.*, 31:21–43, 1997.
29. G. Nguetseng. A general convergence result for a functional related to the theory of homogenization. *SIAM J. Math. Anal.*, 20(3):608–623, 1989.
30. J. T. Oden and K. S. Vemaganti. Estimation of local modeling error and goal-oriented adaptive modeling of heterogeneous materials. I. Error estimates and adaptive algorithms. *J. Comput. Phys.*, 164(1):22–47, 2000.
31. H. Owhadi and L. Zhang. Localized bases for finite-dimensional homogenization approximations with nonseparated scales and high contrast. *Multiscale Model. Simul.*, 9(4):1373–1398, 2011.
32. G. Sangalli. Capturing small scales in elliptic problems using a residual-free bubbles finite element method. *Multiscale Model. Simul.*, 1(3):485–503 (electronic), 2003.

Recent publications :

MATHEMATICS INSTITUTE OF COMPUTATIONAL SCIENCE AND ENGINEERING
Section of Mathematics
Ecole Polytechnique Fédérale
CH-1015 Lausanne

45.2012 B. BECKERMANN, D. KRESSNER, C. TOBLER:
An error analysis of Galerkin projection methods for linear systems with tensor product structure

46.2012 J. BECK, F. NOBILE, L. TAMELLINI, R. TEMPONE:
A quasi-optimal sparse grids procedure for groundwater flows

47.2012 A. ABDULLE, Y. BAI:
Fully discrete analysis of the heterogeneous multiscale method for elliptic problems with multiple scales

48.2012 G. MIGLORATI, F. NOBILE, E. VON SCHWERIN, R. TEMPONE:
Approximation of quantities of interest in stochastic PDES by the random discrete L^2 projection on polynomial spaces

01.2013 A. ABDULLE, A. BLUMENTHAL:
Stabilized multilevel Monte Carlo method for stiff stochastic differential equations

02.2013 D. N. ARNOLD, D. BOFFI, F. BONIZZONI:
Tensor product finite element differential forms and their approximation properties

03.2013 N. GUGLIELMI, D. KRESSNER, C. LUBICH:
Low-rank differential equations for Hamiltonian matrix nearness problems

04.2013 P. CHEN, A. QUARTERONI, G. ROZZA:
A weighted reduced basis method for elliptic partial differential equations with random input data

05.2013 P. CHEN, A. QUARTERONI, G. ROZZA:
A weighted empirical interpolation method: a priori convergence analysis and applications

06.2013 R. SCHNEIDER, A. USCHMAJEW:
Approximation rates for the hierarchical tensor format in periodic Sobolev spaces

07.2013 C. BAYER, H. HOEL, E. VON SCHWERIN, R. TEMPONE:
On non-asymptotic optimal stopping criteria in Monte Carlo simulation.

08.2013 L. GRASEDYCK, D. KRESSNER, C. TOBLER:
A literature survey of low-rank tensor approximation techniques

09.2013 M. KAROW, D. KRESSNER:
On a perturbation bound for invariant subspaces of matrices

10.2013 A. ABDULLE:
Numerical homogenization methods