Modeling, Analysis and Simulation of Homogenization Methods for Partial Differential Equations

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Abstract- The main interest is on Aysmptotic Analysis of partial differential equations. This is a technique to understand the macroscopic behaviour of a composite medium through its microscopic properties. The technique is commonly used for PDE with highly oscillating coefficients. The idea is to replace a given heterogeneous medium by a fictitious homogeneous one (the `homogenized' material) for numerical computations. The technique is also known as ``Multi scale analysis''. The known and unknown quantities in the study of physical or mechanical processes in a medium with micro structure depend on a small parameter \$\varepsilon\$. The study of the limit as \$ \varepsilon \rightarrow0 \$, is the aim of the mathematical theory of homogenization. The notion of \$G\$-convergence, \$H\$-convergence, two-scale convergence are some examples of the techniques employed for specific cases. The variational characterization of the technique for problems in calculus of variations is given by \$\Gamma\$-convergence. This paper presents a few examples. Given the complexity of these processes, the key to reliably simulate some relevant classes of such processes involves the construction of appropriate macroscopic (homogenized or effective) models. This is illustrated by studying a onedimensional model problem of oscillatory diffusion

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I. INTRODUCTION

Heterogeneous micro-structures on many non-separable scales and high contrast in physical properties of the constituents are key features for the superior behaviour of modern composite and multi-functional materials. However, these features cause major difficulties for their computer simulation. The resolution of all characteristic length scales is prohibitively expensive while the naive disregard of relevant microscopic information leads to questionable results, even on macroscopic scales of interest. Homogenization methods try to remedy this dilemma. They account for the relevant microscopic information in a hierarchical, concurrent and adaptive fashion so that a reliable simulation of multiscale problems eventually becomes feasible in state-of-the-art computing environments. This lecture concerns the design of the related numerical algorithms and, equally important, the mathematics behind them to foresee and assess their reliability and efficiency in engineering and scientific applications. Among the target applications of this lecture is the mechanical analysis of multiphase materials such as composite and multifunctional materials. The manipulation of characteristics and relative volumes of its constituents allows one to equip engineered multiphase materials with some targeted portfolio of physical properties (e.g. light-weight, stiffness, strong electric and magnetic order, energy conversion). The development of novel multifunctional materials for the next-generation of performance-tailored structures requires the topological optimisation of the microstructures and, hence, the understanding how certain material properties (conductivity, permeability, etc.) depend on controllable variables (thermal conductivities of the constituents, relative volumes, particles shapes, coating and

size). Transport processes in porous media, e.g. groundwater flow in unsaturated soils [16, 18], share the previous challenges in that the occurring permeabilities and hydraulic conductivities have rapidly changing features due to different types of soil, microscopic inclusions in the bottom or porous subsurface rock formations. Any meaningful numerical simulation of relevant physical effects has to account for these highly heterogeneous fine scale structures in the whole computational domain. If pore scale effects become relevant or if domains spread over kilometers, the computational load easily exceeds computer capacity when standard finite element or finite volume methods are used.



Numerical homogenization methods are techniques for finding numerical solutions of partial differential equations (PDEs) with rapidly oscillating coefficients (multiple scales) [26]. 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" [27]. These methods are also called multiscale methods as they typically combine numerical solvers on different scales.

II. MOTIVATION

The modeling of the physical processes in strongly heterogeneous medium motivates the study of partial differential equations with oscillating coefficients. The basic problem is this: a family of physical processes are assumed to solve A $\epsilon u\epsilon = f\epsilon$ (1.1) with appropriate initial and/or boundary conditions [28].

Here, $A\varepsilon$ is a differential operator, and the parameter ε stands for the period of oscillation. If the knowledge of small scale variation of the heterogeneous medium is only known to statistical extent, the medium is modeled as a random field. We are interested in deriving a homogenized equation that captures the effective properties of the heterogeneous medium, as the computational cost of solving the multi-scaled equation (1.1) is prohibitive [29]. Specifically, we would like to understand the following issues:

EXAMPLE

(1) Does the solution ue converge? If the limiting solution u solve the equation Au = f, (1.2) we call (1.2) a homogenized equation. (2) Which type of convergence do we have in (1)? Is it a L 2 convergence to a deterministic PDE, or is it a weak convergence to a stochastic PDE? (3) What is the rate of convergence? In other words, can we prove kue – $uk \le C\epsilon\gamma$ (1.3) for some $\gamma > 0$. 1.2 Example Let us see an example of the random homogenization problem:

$$\frac{\partial}{\partial t}u_{\varepsilon}(t,x) - \Delta u_{\varepsilon}(t,x) + \frac{1}{\varepsilon^{\alpha}}V(\frac{x}{\varepsilon})u_{\varepsilon}(t,x) = 0$$
$$u_{\varepsilon}(0,x) = u_{0}(x).$$
(1.4)

This equation can be seen as a continuous version of the parabolic Anderson model. The asymptotic behavior of this equation depends on the dimension d. For simplicity, we assume V to be a Gaussian field.

For d = 1 and α = 1/2, ue converges weakly to the stochastic PDE

$$\frac{\partial}{\partial t}u(t,x) - \Delta u(t,x) + \sigma u(t,x) \circ \dot{W} = 0,$$

$$u(0,x) = u_0(x), \quad (1.5)$$
where W[·] denotes spatial white noise.

• denotes Stratonovich product, and

$$\sigma^2 := \int_{\mathbb{R}^d} \mathbb{E}\{V(0)V(x)\}dx.$$
(1.6)

For d = 2 and $\varepsilon \alpha := \varepsilon |\log \varepsilon|$, or d > 2 and $\alpha = 1$, us converges in L 2 ($\Omega \times R$ d) to the deterministic PDE

$$\frac{\partial}{\partial t}u(t,x) - \Delta u(t,x) - \rho u(t,x) = 0,$$
$$u_{\varepsilon}(0,x) = u_0(x), \quad (1.7)$$

where

$$\rho := \begin{cases} c_d \hat{R}(0), & d = 2\\ \int_{\mathbb{R}^d} \frac{\hat{R}(\xi)}{|\xi|^2} d\xi, & d > 2. \end{cases}$$
(1.8)

Here, cd is the volume of unit sphere on (d–1)-dimensional hyperplane. $R^{(\xi)}$ is the Fourier transform of the covariance function

 $R(x) = E\{V(y)V(x + y)\}.$



Fig. 2 Modeling and Simulation

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 $\varepsilon : \Omega \longrightarrow R$, where Ω is an open subset of R d , $1 \le d \le 3$. 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) [30]. One can think of the solution as containing low O(1) frequency components and high O(1/ ε) frequency components. Solving numerically a given PDE of the above family using classical numerical approximations such as the finite element method (FEM) [31], 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 $O(\varepsilon - d)$, which can be prohibitive for small ε . If the family of solutions converges (in some appropriate sense) to a limit denoted u0 when the size of the heterogeneity $\varepsilon \rightarrow 0$ and if that limit is the solution of an averaged (homogenized) equation L0(u0) =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].

III. 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 Babu`ska [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(ue, v) = Z Ω a $\varepsilon \nabla u \varepsilon \cdot \nabla v dx = (f, v) \forall v \in V(\Omega), (1)$

where $(f, v) = R \Omega$ fvdx and V (Ω) is a Sobolev space that we choose to be H1 0 (Ω) (the space of square-integrable functions that vanishes on $\partial \Omega$ with square-integrable derivatives).

Here a ε is an oscillating tensor with fast $O(1/\varepsilon)$ and slow frequencies. The homogenized problem corresponding to the above equation reads: Find $u0 \in V(\Omega)$ such that

B0(u0, v) = Z Ω a $0\nabla u0 \cdot \nabla vdx = (f, v) \forall v \in V(\Omega).$ (2)

The solution us can be expected to behave as $u0 + \varepsilon u1$, with $ku1kL2(\Omega) = O(1)$ but $k\nabla u1kL2(\Omega) = O(1/\epsilon)$. A standard finite element (FE) approximation of (1) consists in 4 a solution uh of (1) in a finite dimensional space spanned by piecewise polynomials on a partition Th of Ω with mesh size h (see below). However, a good approximation of ue by uh (the FE solution) is usually obtained only if h ε in which case the complexity (DOF) scales as $O(\epsilon - d)$. 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 TH of $\Omega = \bigcup K \in TH K$, with elements K of diameter HK and $H = maxK \in TH$ 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

 $D = \cup T \in Th T$,

with elements T of diameter hT and a meshsize h that satisfies $h < \varepsilon$. We then consider the following FE spaces

 $VH(\Omega) = \{vH \in V (\Omega); vH|K \in P1 (K), \forall K \in Th\}, (3)$

 $Vh(D) = \{vh \in V (D); vh|T \in P1 (T), \forall T \in Th\}, (4)$

where P 1 (K) is the space of piecewise linear polynomials on K (resp. T).

For a cubic domain D = Y we also consider

 $Wh(D) = \{vh \in W1 \text{ per}(D);\$

 $vh|T \in P1 (T), \forall T \in Th\}, (5)$

where W1 per(D) is a Sobolev space of periodic functions (the closure of smooth periodic functions on D for the H1 norm, where functions differing by a constant are identified). We consider here piecewise linear polynomials and conformal meshes for simplicity but 5 emphasize that the methods described below have been generalized to higher order piecewise polynomial spaces and other types of FEs.

IV. HOMOGENIZATION OF PDES WITH GAUSSIAN COEFFICIENTS

Gaussian fields are unique among all random fields in that the first and second order moments (mean and covariance) completely determines the distribution. Without loss of generality, we assume Gaussian fields to have zero mean hereafter. For Gaussian fields, moments of all orders can be calculated in terms of the second order moments.

Definition 2.6. A Gaussian field is a random field involving only Gaussian distributed random variables.

Theorem 2.7. If $(Z1, \dots, Zn)$ is a zero mean multivariate Gaussian random vector, then.

$$\mathbb{E}[Z_1 \cdots Z_n] = \begin{cases} 0, & n \text{ is odd} \\ \sum \prod \mathbb{E}[Z_i Z_j], & n \text{ is even,} \end{cases}$$

where the notation P Q means summing over all distinct ways of partitioning $Z1, \dots, Zn$ into pairs.

V. SETTING OF THE PROBLEM

We consider a model problem of diffusion or conductivity in a periodic medium (for example, an heterogeneous domain obtained by mixing periodically two different phases, one being the matrix and the other the inclusions; see Figure 1.1). To fix ideas, the periodic domain is called Ω (a bounded open set in R N with N \geq 1 the space dimension), its period φ (a positive number which is assumed to be very small in comparison with the size of the domain), and the rescaled unit periodic cell Y = (0, 1)N . The conductivity in Ω is not constant, but varies periodically with period φ in each direction. It is a matrix (a second order tensor) A(y), where y = $x/\varphi \in Y$ is the fast periodic variable, while $x \in \Omega$ is the slow variable.

Equivalently, x is also called the macroscopic variable, and y the microscopic variable. Since the component conductors do not need to be isotropic, the matrix A can be any second order tensor that is bounded and positive definite, i.e., there exist two positive constants $\beta \le \alpha > 0$ such that, for any vector $\xi \in R$ N and at any point

$$\alpha |\xi|^2 \le \sum_{i,j=1}^N A_{ij}(y)\xi_i\xi_j \le \beta |\xi|^2.$$
(1.1)

At this point, the matrix A is not necessarily symmetric (such is the case when some drift is taken into account in the diffusion process). The matrix A(y) is a periodic function of y, with period Y, and it may be discontinuous in y (to model the discontinuity of conductivities from one phase to the other). Denoting by f(x) the source term (a scalar function defined in Ω), and enforcing a Dirichlet boundary condition (for simplicity), our model problem of conductivity reads

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

A periodic domain. where uq(x) is the unknown function, modeling the electrical potential or the temperature. Remark 1.1.1 From a mathematical point of view, problem (1.2) is well posed in the sense that, if the source term f(x) belongs to the space L 2 (Ω) of square integrable functions on Ω , then the Lax-Milgram lemma implies existence and uniqueness of the solution uq in the Sobolev space H1 0 (Ω) of functions which belong to L 2 (Ω) along with their first derivatives. Furthermore, the following energy estimate holds kuqkL2(Ω)

+ k ∇ uǫkL2(Ω) \leq C, where the constant C does not depend on ρ . The domain Ω , with its conductivity A x ρ , is highly heterogeneous with periodic heterogeneities of lengthscale ρ . Usually one does not need the full details of the variations of the potential or temperature u ρ , but rather some global of averaged behavior of the domain Ω considered as an homogeneous domain. In other words, an effective or equivalent macroscopic conductivity of Ω is sought. From a numerical point of view, solving equation (1.2) by any method will require too much effort if ρ is small since the number of elements (or degrees of freedom) for a fixed level of accuracy grows like $1/\rho N$. It is thus preferable to average or homogenize the properties of Ω and compute an approximation of u ρ on a coarse mesh.

Averaging the solution of (1.2) and finding the effective properties of the domain Ω is what we call homogenization. There is a difference of methodology between the traditional physical approach of homogenization and the mathematical theory of homogenization. In the mechanical literature, the socalled representative volume element (RVE) method is often used (see [8], or section 1 in [17]). medium, and averaging over it the gradient ∇u_0 and the flux A x o ∇u_0 . Denoting by ξ the average of the gradient and by σ that of the flux, the effective tensor of conductivity A* of this sample is defined by the linear relationship $\sigma = A \ast \xi$. It turns out that the averaged stored energy A x φ $\nabla u \varphi \cdot \nabla u \varphi$ is also equal to the effective energy A* $\xi \cdot \xi$. Although this type of definition is very intuitive, it is not clear whether it defines correctly an effective tensor A*. In particular, it may depend on the choice of source term f, sample size, or boundary conditions. The mathematical theory of homogenization works completely differently.

Rather than considering a single heterogeneous medium with a fixed lengthscale, the problem is first embedded in a sequence of similar problems for which the lengthscale o, becoming increasingly small, goes to zero. Then, an asymptotic analysis is performed as o tends to zero, and the conductivity tensor of the limit problem is said to be the effective or homogenized conductivity. This seemingly more complex approach has the advantage of defining uniquely the homogenized properties. Further, the approximation made by using effective properties instead of the true microscopic coefficients can be rigorously justified by quantifying the resulting error.

In the case of a periodic medium Ω , this asymptotic analysis of equation (1.2), as the period ρ goes to zero, is especially simple. The solution u ρ is written as a power series in ρ u ρ = $X + \infty$ i=0 ρ iui. The first term u0 of this series will be identified with the solution of the so-called homogenized equation whose effective conductivity A* can be exactly computed. It turns out that A* is a constant tensor, describing a homogeneous medium, which is independent of f and of the boundary conditions.

Therefore, numerical computations on the homogenized equation do not require a fine mesh since the heterogeneities of size φ have been averaged out. This homogenized tensor A* is almost never a usual average (arithmetic or harmonic) of A(y). Various estimates will confirm this asymptotic analysis by telling in which sense u φ is close to u0 as φ tends to zero. Remark 1.1.2 From a more theoretical point of view,

homogenization can be interpreted as follows. Rather than studying a single problem (1.2) for the physically relevant value of Q, we consider a sequence of such problems indexed by the period Q, which is now regarded as a small parameter going to zero.

The question is to find the limit of this sequence of problems. The notion of limit problem is defined by considering the convergence of the sequence (uq)q>0 of solutions of (1.2): Denoting by u its limit, the limit problem is defined as the problem for which u is a solution. Of course, u will turn out to coincide with u0, the first term in the series defined above, and it is therefore the solution of the homogenized equation. Clearly the mathematical difficulty is to define an adequate topology for this notion of convergence of problems as q goes to zero.

VI. IMPLEMENTATION OF PHYSICAL-STATISTICAL MODEL WITH HOMOGENIZATION

In terms of implementation, one can proceed as described in Section 1.2 where, depending on the type of observations that are made, a suitable statistical data model can be chosen along with an error distribution for the process model and prior for the parameters. Assuming that the data consist of observations of animal abundance (i.e., N(x,t), counts of animals; discussed in more detail in the following section) and we make the appropriate homogenization transformations, we can treat the harmonic mean as an operator using vector notation (i.e., $\delta \equiv \delta(\delta)$) in the following general hierarchical statistical model:

$$N(x,t) \sim [N(x,t) \mid u_0(x,t)], \quad \forall x,t$$
$$u_0(x,t) \sim [u_0(x,t) \mid f_h(\mathbf{u}_0(t-\Delta t), \bar{\boldsymbol{\delta}}(\boldsymbol{\delta}))], \quad \forall x,t$$
$$\boldsymbol{\delta} \sim [\boldsymbol{\delta}],$$

where the function fh represents the plain diffusion solver as a difference equation. Note that the process stage (2.9) of the hierarchical model could either be stochastic or a degenerate distribution implying no additional process uncertainty beyond that provided through the data model (2.8). Though perhaps possible, it would not be trivial to fit such a model and obtain uncertainty estimates for model parameters using maximum likelihood. Therefore, we describe a Bayesian approach to fit the model that uses an MCMC algorithm as described in recent literature pertaining to physical-statistical modeling (e.g., Wikle and Hooten 2010). The posterior distribution corresponding to the model specified in (1.8)– (1.10) can be expressed as

 $\left[\left\{\mathbf{u}_{0}(t)\right\}, \boldsymbol{\delta} \mid \left\{\mathbf{N}(t)\right\}\right] \propto \prod_{t} \left[\left[\mathbf{N}(t) \mid \mathbf{u}_{0}(t)\right] \prod_{t} \left[\mathbf{u}_{0}(t) \mid f\left(\mathbf{u}_{0}(t-\Delta t), \boldsymbol{\delta}\right)\right] \left[\boldsymbol{\delta}\right].$

It involves a product over the homogenized process distribution rather than the non-homogenized process. This model is completely non-conjugate, implying that full-conditional distributions cannot be found analytically, thus, a Metropolis–Hastings approach must be used to sample from the full-conditionals sequentially. The portion of an MCMC algorithm where the homogenization technique helps the most is when sampling the diffusion coefficients δ .

VII. RESULT AND DISCUSSION

Statistical models using partial differential equations (PDEs) to describe dynamically evolving natural systems are appearing in the scientific literature with some regularity in

recent years. Often such studies seek to characterize the dynamics of temporal or spatio-temporal phenomena such as invasive species, consumer-resource interactions, community evolution, and resource selection. Specifically, in the spatial setting, data are often available at varying spatial and temporal scales. Additionally, the necessary numerical integration of a PDE may be computationally infeasible over the spatial support of interest. We present an approach to impose computationally advantageous changes of support in statistical implementations of PDE models and demonstrate its utility through simulation using a form of PDE known as "ecological diffusion." We also apply a statistical ecological diffusion model to a data set involving the spread of mountain pine beetle (Dendroctonus ponderosae).

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