Homogenization of Coupled Phenomena in Heterogenous Media

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Contents

Main notations

Operators

$\otimes$	tensor product
$:$	doubly contracted tensor product
$\cdot$	scalar product
$\times$	vector product
$\triangle, \triangle_x$	Laplacian, Laplacian with respect to the variable $\mathbf{x}$
$\mathrm{div}, \mathrm{div}_x$	divergence, divergence with respect to the variable $\mathbf{x}$
$\mathbf{grad}, \mathbf{grad}_x$	gradient, gradient with respect to the variable $\mathbf{x}$
$\mathbf{curl}, \mathbf{curl}_x$	curl, curl with respect to the variable $\mathbf{x}$
$\langle a \rangle$	mean of a over the period Ω
$\langle a \rangle_{\Omega_\alpha}$	mean of a over the domain Ω_α

Dimensions, bases, spatial variables

Ω	period
Ω_α	domain occupied by constituent α
$\partial\Omega$	boundary of the period
Γ	interface between two constituents
l	microscopic length [m]
L	macroscopic length [m]
$\varepsilon = l/L$	separation of scales parameter
$\mathbf{e}_i$	unit vector – orthonormal basis
$\mathbf{n}$	unit vector normal to the interface Γ
$\mathbf{X} = X_i\ \mathbf{e}_i$	physical spatial variable [m]
$\mathbf{x}^* = \mathbf{X}/L_c = x_i^*\ \mathbf{e}_i$	macroscopic dimensionless variable [-]
$\mathbf{y}^* = \mathbf{X}/l_c = y_i^*\ \mathbf{e}_i$	microscopic dimensionless variable [-]

Dimensionless numbers

$\mathcal{B}$	Biot number [-]
$\mathcal{K}n$	Knudsen number [-]
$\mathcal{P}e$	Péclet number [-]
$\mathcal{R}e$	Reynolds number [-]
$\mathcal{R}t$	transient Reynolds number [-]
$\mathcal{S}$	Strouhal number [-]

Properties and physical quantities

$\mathbf{a} = a_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$	elastic tensor [MPa]
c	concentration [-]
c_α	volume fraction of constituent α [-]
C_α	heat capacity of constituent α [J/(Kg.K)]
$\mathbf{c} = c_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$	effective elastic tensor [MPa]
$\mathbf{D}(\mathbf{v}) = D_{ij}(\mathbf{v})\, \mathbf{e}_i \otimes \mathbf{e}_j$	strain rate tensor [s^{-1}]
$\mathbf{D}^{\mathrm{dif}} = D^{\mathrm{dif}}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	effective diffusion tensor [m^2/s]
$\mathbf{D}^{\mathrm{dis}} = D^{\mathrm{dis}}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	effective dispersion tensor [m^2/s]
$\mathbf{D}^{\mathrm{mol}} = D^{\mathrm{mol}}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	molecular diffusion tensor [m^2/s]
$\mathbf{e}(\mathbf{u}) = e_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	strain tensor [-]
E	Young's modulus [MPa]
h	inverse of the thermal contact resistance
$\mathbf{H} = H_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	inverse of the intrinsic permeability tensor [m^2]
$\boldsymbol{\mathsf{H}}(\omega) = \mathsf{H}_{ij}(\omega)\, \mathbf{e}_i \otimes \mathbf{e}_j$	inverse of the dynamic permeability tensor $\boldsymbol{\mathsf{K}}$ [m^{-2}]
$\boldsymbol{\mathsf{H}}^{\mathrm{R}}, \boldsymbol{\mathsf{H}}^{\mathrm{I}}$	real and imaginary parts of the $\boldsymbol{\mathsf{H}}$ tensor
$\mathsf{H}(\omega) = \mathsf{K}^{-1} = \mathsf{H}^{\mathrm{I}} + i\mathsf{H}^{\mathrm{R}}$	inverse of the dynamic permeability of an isotropic medium
$\mathbb{H}(\omega) = \mathbb{H}_{ij}(\omega)\, \mathbf{e}_i \otimes \mathbf{e}_j$	inverse of the dynamic hydraulic conductivity tensor $\boldsymbol{\Lambda} = \eta\boldsymbol{\mathsf{K}}(\omega)$
$\mathbf{H}^{\mathrm{k}} = H^{\mathrm{k}}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	Klinkenberg tensor [m^2]
$\mathbf{I}$	identity tensor
$\mathcal{K}$	intrinsic permeability of an isotropic medium [m^2]
$\mathbf{K} = K_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	intrinsic steady state permeability tensor [m^2]
$\mathbf{K}^{\mathrm{k}} = K^{\mathrm{k}}_{ij}\, \mathbf{e}_i \otimes \mathbf{e}_j$	Klinkenberg permeability tensor [m^2]
$\mathsf{K}(\omega) = \mathsf{K}^{\mathrm{R}} + i\mathsf{K}^{\mathrm{I}}$	dynamic permeability of an isotropic medium [m^2]
$\boldsymbol{\mathsf{K}}(\omega) = \mathsf{K}_{ij}(\omega)\, \mathbf{e}_i \otimes \mathbf{e}_j$	dynamic permeability tensor [m^2]
$\boldsymbol{\mathsf{K}}^{\mathrm{R}}, \boldsymbol{\mathsf{K}}^{\mathrm{I}}$	real and imaginary parts of the $\boldsymbol{\mathsf{K}}$ tensor
M	form factor
p	fluid pressure [Pa]
t	time [s]
T_α	temperature of constituent α [°K]
$\mathbf{u}_{\mathrm{s}} = u_{\mathrm{s}i}\, \mathbf{e}_i$	solid displacement [m]

$\mathbf{v} = v_i \, \mathbf{e}_i$	fluid velocity [m/s]
$\boldsymbol{\alpha}$	Biot tensor [-]
δ	boundary layer thickness (thermal, diffusion...)
η	dynamic fluid viscosity [Pa.s]
λ_α	thermal conductivity of constituent α [W/(m.°K)]
$\boldsymbol{\lambda}^{\text{eff}} = \lambda_{ij}^{\text{eff}} \, \mathbf{e}_i \otimes \mathbf{e}_j$	effective thermal conductivity tensor [W/(m.°K)]
λ	Lamé coefficient [MPa]
Λ_v	viscous length
$\boldsymbol{\Lambda}(\omega) = \Lambda_{ij}(\omega) \, \mathbf{e}_i \otimes \mathbf{e}_j$	hydraulic conductivity tensor
μ	shear modulus [MPa]
ν	Poisson's ratio [-]
ρ	fluid density [kg/m^3]
$\boldsymbol{\sigma} = \sigma_{ij} \, \mathbf{e}_i \otimes \mathbf{e}_j$	Cauchy stress tensor
τ_0, τ_∞	low- and high-frequency tortuosity
ϕ	porosity [-]
ω	pulsation (angular frequency) [rad/s]

Subscripts

α_c	characteristic value of α
α^*	dimensionless quantity ($\alpha = \alpha_c \alpha^*$)
$\mathcal{Q}_l$	dimensionless number $\mathcal{Q}$ estimated from the microscopic viewpoint
$\mathcal{Q}_L$	dimensionless number $\mathcal{Q}$ estimated from the macroscopic viewpoint

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Introduction

The result of a fusion of mathematical and physical concepts, homogenization has established itself as a method of overcoming the usual framework based on a description of elementary phenomena in a homogenous medium, to achieve the objective of a global description of coupled phenomena in heterogenous media. This book aims to present the key methodological points and their relevance to engineering science in a pedagogical format.

What is the nature of the problem? Even brief observation of natural or industrial materials reveals that they often consist of a combination of different constituents in various structures, and they are therefore heterogenous.

For example, take the behavior of civil engineering materials. The descriptions of the properties that they exhibit – and consequently the design rules for structures built using these materials – are, for the most part, issues related to the mechanics of continuous media applied to homogenous media. This theory has been widely proven, and a huge number of constructions designed using these principles can attest to its success, as can the accuracy of modeling performed using this approach. This simple observation leads us to believe that heterogenous materials can, at least subject to certain constraints, be treated similarly. But why and to what extent is this concept useful?

Furthermore, although the heterogenous nature of the material may not be obvious for this apparently continuous medium, it is on the other hand clear that its behavior depends on the characteristics of the heterogenities. How then do we proceed if we are to account for the properties of the constituents when defining the behavior of an equivalent continuous homogenous medium?

These two points are of great practical importance. On one hand, understanding of the limits of a method is an important safety consideration, and on the other hand determination of the equivalent continuous medium allows us to better understand the parameters that govern its behavior (for a natural material) or to adapt the constituent parts to achieve the desired performance (for an artificial material).

The homogenization methods have been developed to answer these questions. They make it possible – under well-specified conditions – to obtain a description of the behavior of heterogenous materials starting from the behavior of the heterogenities.

A condition essential for the existence of an equivalent continuum is that the physical mechanism under study should vary on a length scale which is very large compared to the scale of the heterogenities. This requirement for a difference in length scales gives rise to the expressions "upscaling method" and "method of multiple scales". The term "homogenization" also arises from this, because considering the heterogenities to be of infinitessimal size compared to the effects under study naturally leads us to consider the medium as a homogenous or, more precisely, homogenized continuum.

Linking the large-scale observable behavior to microscopic mechanisms is an age-old preoccupation of physicists.

One famous example is that of elasticity, where Navier (1821) and Poisson (1829) obtained a single macroscopic isotropic elastic coefficient from a particular molecular model: the two Lamé coefficients are equal. Cauchy (1828) obtained a two-coefficient isotropic elastic model starting from a more sophisticated molecular model. From among these well-known names we also draw attention to the preliminary work of Rayleigh (1892) on the conductivity of media containing impurities present in a parallelopiped lattice, and that of Einstein (1906) on the viscosity of suspensions and sedimentation rates.

These attempts remained intermittent until the 1950s when the needs of industrial development demanded a detailed understanding of the behavior of natural materials (the oil industry), manufactured materials (in particular steels and alloys), and the design of new materials (mainly for aeronautics). In order to understand the significance of small scale mechanisms on global behavior, scientific approaches at the time involved phenomenological micromechanical models built on thermodynamic principles. The pioneering works of Biot (1941) and of Hill (1965) took this approach.

It was in the 1970s that a new school of thought was born, started by Keller who used a rather different angle to tackle the question of the change of scales. This involved the method of asymptotic expansions at multiple scales. Initially built on an approach which was more mathematical than mechanical, this method was a true conceptual leap forwards in terms of its rigor and formalism. The works of Bensoussan *et al.* (1978) and Sanchez-Palencia (1980) are still important references on this subject, with similar ideas developed in Russia by Bakhvalov and Panasenko (1989).

Initially confined to very specialist circles, these methods blossomed considerably in the 1990s. During this period their fields of application were broadly diversified across all traditional engineering fields, and also in life sciences, particularly biomechanics. This undeniable success is thanks to the effectiveness of asymptotic methods for treating complex physics on a microscopic scale, and their ability to include coupling between different phenomena.

However, while their use has become almost routine for some research groups, it remains poorly documented at present in a form suitable for engineers and researchers working in related fields. These considerations convinced us there was a demand for a book which would set out a coherent picture of these approaches, and render them accessible to a wider audience than just specialists in this research area.

Rather than be exhaustive (which would not be an easy task), we have chosen to pick a few problems where the main points can be presented in a simple manner. The aim is also – using a unified treatment – to illustrate the common thought processes connecting the issues addressed in this book. In keeping with this approach, the bibliography does not attempt to be exhaustive, but shows the reader the seminal works in the field, and the references corresponding to the main steps of the problems we consider.

This volume, which has grown out of the Mechanics of Heterogenous Media course taught at the University of Grenoble by J.L. Auriault, is intended to be a basic course in upscaling methods, aimed at advanced students, engineers and graduate students. With this pedagogical aim, we have used a progressive approach to each subject, starting out with traditional problems and then following them with recent developments. We also thought it useful to illustrate the potential applications of the results of homogenization. With this in mind, for each of the themes we treat, the theoretical results are followed by an example of the development through homogenization which provides a concrete example of the advances in a particular field of application.

This book is divided into four parts.

Part 1 is an introduction to the philosophy of homogenization methods. We discuss methods aimed at periodic and random materials while emphasizing their physical significance and their potential applications to real materials, which are often neither perfectly periodic or perfectly random.

The basic examples given in Chapter 1 give an understanding of the fundamental tools underlying both methods. Chapter 2 goes into more detail on the techniques and discusses connections between them and the details which distinguish them. There is a detailed discussion of conditions for their application, delineating the range of validity of these approaches. This overview of methods underlines the power of the asymptotic method at multiple scales for the treatment of complex physics with many coupled effects in materials with simple or heirarchical morphologies. Combining rigorous formalism and intuitive reasoning, Chapter 3 presents the methodology of the multiple scale approach which will be used throughout the rest of the book. The emphasis is on the systematic use of dimensional analysis combined with the separation of length scales. We also detail the means of expressing a practical problem involving real materials in the context of homogenization. This methodological basis is applied in the following sections where we specifically treat the physical mechanisms involved in coupled phenomena.

Part 2 presents a first field of application of homogenization. We study the physics of transport by diffusion, convection and advection, phenomena which allow us to apply the basic tools of upscaling methods to engineering problems.

Chapter 4 focuses on thermal transfer in heterogenous media. Going beyond the classical model of thermal transfer in a composite, we find a diverse range of macroscopic models depending on the level of contrast in the conductive properties of the constituents and their interfaces. In particular, memory effects arise from the presence of local non-equilibrium of a very weakly conducting phase, and two-temperature models can be developed for quasi-insulating interfaces. The transport of solutes in porous media is examined in Chapter 5. We highlight the different descriptions associated with the local physics of pure diffusion and then with diffusion-advection. This second situation, which is reached at high transport rates, results in a macroscopic dispersion. The range of validity of each of these models is explicitly specified. Chapter 6 makes use of, and extends, these results, focusing on specific materials. The numerical procedure of periodic homogenization is illustrated by determining the coefficients for fibrous and granular materials. By way of comparison, we recall the classical self-consistent analytical estimates. Finally, comparison with experimental results enables us to judge the appropriateness of these models for describing the properties of materials.

Part 3 is dedicated to the modeling of Newtonian fluid flows in rigid porous media.

Chapter 7 discusses incompressible fluids using multiple-scale asymptotic expansions. It starts with the canonical problem of Darcy's law (in the regime of steady-state laminar flow). It continues taking into account inertial effects, both in the dynamic linear regime which leads to memory effects through visco-inertial coupling, and in the steady-state advective regime, where the correction due to weak non-linearities is established. The flow in porous media of compressible fluids such as gases is the subject of Chapter 8. Using the asymptotic method, we treat in succession high pressure steady-state flows, wall slip effects in rarefied gases and, in the dynamic regime, the acoustic description under weak pressure perturbations with thermal coupling. The transfer of theoretical results for homogenization to their numerical formulation is illustrated in Chapter 9. The solution to local problems derived by periodic homogenization is given for calculation of the Darcy permeability of granular and fibrous materials. Finally, Chapter 10 returns to the same problems, which are discussed in the context of a self-consistent approach. We use this to establish analytical estimates and bounds for steady state and dynamic permeabilities, thermal effects, wall slip corrections and – by analogy – for the trapping constant.

Part 4 focuses on the behavior of deformable saturated porous media.

Chapter 11 considers the behavior in the quasi-static regime, first examining that of the empty porous medium (a specific case of an elastic composite) and then that of the saturated medium, introducing the fluid-solid coupling. Depending on the level of contrast between the shear properties of the fluid and the solid, the asymptotic method of multiple scales leads to three distinct behaviors whose properties are discussed.

The study of poroelastic behavior is extended to the dynamic regime in Chapter 12. The characteristics of the three possible behaviors – including the Biot biphasic model – are analyzed in detail, particularly properties of the effective coefficients. The range of validity of each of the descriptions is specified. Chapter 13 puts the homogenization results to numerical use in order to carry out a parametric analysis of the elastic and coupling coefficients in the biphasic model. At the same time these results, obtained for cohesive granular media, are compared to traditional self-consistent estimates and to bounds. In Chapter 14, the homogenized biphasic behavior is used with the aim of describing the propagation of waves in saturated porous media. After specifying the properties of the three propagation modes, the transmission of waves across a poroelastic interface is examined. We also establish the expression for Green's functions in the context of poroelasticity, the integral formulation, and the fields radiated by abrupt dislocations.

To complete our summary of this text, it is worth mentioning certain important subjects which are not treated here (or only discussed briefly).

One of these subjects is complex microstructures. In fact, we will only consider media whose local geometry is sufficiently simple that it can be characterized by a typical length scale of the heterogenity, and whose local problems can be formulated in terms of continuous media. This choice means that we omit:

– Media whose architecture involves very different characteristic sizes (such as double porosity media). These can give rise to various interacting physical effects on each length scale. These many possible couplings vastly increase the diversity of the possible macroscopic behaviors, with some behaviors only being possible in such media as;

– Microstructure whose behavior can be reduced to that of various interacting points within the material (for example the nodes in trellis structures). For these it is preferable to use a locally discrete description, and to move to a continuum description through homogenization. This alternative approach will not be discussed here.

A second aspect only outlined is that of the corrections to macroscopic descriptions which have been established to first order. Indeed, for the most part, the results presented here are restricted to the first significant term, and lead to descriptions involving a continuous medium which is materially simple, and descriptions valid in the bulk of the heterogenous medium. There are two corrections which can usefully be applied to these descriptions:

– those which appear on the boundary of the medium. They lead to a boundary layer with a thickness of the order of the size of the representative elementary volume. This makes it possible to reconcile local boundary conditions and boundary conditions used at the macroscopic scale;

– those which make it possible to treat situations with weak separation of scales, obtained by including higher-order terms within the homogenized descriptions. These correctors to simple continuum models introduce non-local effects whose spatial extent is of the order of the size of the representative elementary volume.

Finally, we will not discuss the taking into account of non-linearities. All the cases that we present involve linear effects, or sometimes weakly non-linear ones where the non-linearity can be treated as a perturbation of the linear solution. Whether they have material or geometric origins, non-linearities introduce considerable theoretical difficulties compared to linear situations. While the establishment of criteria through local limit analysis – the rheology of elastic composites with a non-linear power law, or the flow of non-Newtonian power-law fluids in porous media – has been successfully achieved, in general non-linearities present a real challenge to upscaling methods.

These three omitted themes – complex microstructures, corrections and non-linearities – are very rich and interesting, and they deserve further discussion on their own. We hope that this volume will offer a sufficiently clear and solid basis to guide the reader who may wish to explore these fields.

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Part one

Upscaling Methods