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Homogenization and micromechanics

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Abstract

In this paper we present a survey on homogenization theory and related techniques applied to micromechanics, some perspectives of technological importance and a list of related references. The points of interest are the validation of homogenization results, the characterization of composite materials and the optimal design of complex structures, and are viewed here as a combination of mathematical and mechanical homogenization. Multiscale micromechanics methods and the classical as well as the emerging analytical and computational techniques are presented. Moreover, selected applications of novel homogenization techniques are outlined.

1. A survey

Composites are present everywhere, from the geomaterials to the engineered materials: common metals, some rocks, such as sandstone or granite, construction materials such as wood and concrete, bone, fiberglass and lightweight carbon fiber composites, are all examples of composites. Composites are heterogeneous materials that have inhomogeneities much larger than the atomic scale, with a statistically homogeneous behavior at macroscopic length scales. We study composites for their usefulness and for the implications of the related knowledge in many fields of science. One more compelling reason is the many beautiful mathematical questions begging for answers ([1]).

Mathematical homogenization in periodic materials consists in setting the problem as a sequence of equations describing the heterogeneous material when the heterogeneities become smaller and smaller. This method, of course, assumes that the mathematical problem, for fixed size of heterogeneities, is well posed, or at least that one is able to prove the existence of (at least) one solution of the problem and an a priori estimate for it (independent of the size of heterogeneities) in some functional space. The problem of passing to the limit as the size of heterogeneities tends to zero is difficult since weak topologies are involved and since it is a nonlinear process. In random media the analog of periodicity is statistical homogeneity.

The works by [2] and [3] offered the functional analysis techniques for continuum mechanics problems. [4] presented the limit solution for the linear elasticity periodic model and the explicit form of effective coefficients. A particular conclusion was that, generally, isotropy of constituents is not stable by homogenization. The interest of mathematicians on engineering applications was the basis of important works during the next five years ([5], [6], [7], [8]). Meanwhile, Tartar and Murat ([9], [10]) presented the compensated compactness technique, the most important technique in deterministic homogenization problems.

In the next five years, Murat, Tartar, Francfort and Suquet published fundamental works on homogenization of mechanical processes: non-linear PDE's ([11]), plasticity [12], [13]), linear thermoelasticity ([14]), linear viscoelasticity ([15]), linear elasticity ([16]), thermoviscoelasticity ([17]). In the early 1980s, the main extension of the Hill's micromechanics ([18], [19], [20]) to homogenization techniques for composites is accomplished. Moreover, optimal bounds and rigorous theories of design have been derived ([21]).

In the early 1990s, new homogenization-induced effects, such as the stability by homogenization introduced previously by Tartar, or the loss of convexity of the homogenized energy and the commutability between homogenization and linearization ([22]), have been developed and new results in non-linear elasticity and plasticity have been derived ([23], [24], [22], [25], [26], [27], [28].

In micromechanics, homogenization aims at "tailoring" new materials with enhanced properties by averaging simple phases. ([15], [29], [30], [12], [16], [31], [32], [33], [34], [35], [36], [37], [1], [38], [39], [40], [41], [42]), [43], [44], [35], [45], [46], [47], [48], [49]). In particular, the concept of "homogeneous equivalent continuum" has been used to simulate the macroscopic response from microscopic considerations by replacing the heterogeneous medium, represented by the representative volume element, by a continuum model.

Computational methods based on mathematical homogenization have been applied to micromechanics. New methods, competitive with the finite elements method, have also been proposed. They are based either on a multilevel finite element method or on an explicit coupling of the microstructural responses with the macroscopic ones, or on emerging theoretical approaches. Some of them use locally exact elastic solutions of the unit cell problem.

In the next section, we will present some applications and related perspectives of homogenization techniques concerning the design of composite materials and structures, the computational homogenization of complex structures, the homogenization with microstructure effect for determining effective dynamical properties of composites, the homogenization in the context of strain-gradient elasticity, the wave propagation in composites, and the kinetic techniques, homogenization and propagation of oscillations in non-linear elastic geomaterials.

2. Perspectives

The first perspective of homogenization is still to complete the mechanical characterization of elastic heterogeneous materials and structures. The effective elastic coefficients can, of course, be defined by solving the corresponding partial differential equations problem. However, there are some happy exceptions, such as the homogeneity transformations, duality transformations, translations, in which one may start from a known solution and then create by 90^o rotations new solutions which are stable by homogenization provided that the transformation is based on weakly continuous bilinear functions. Moreover, variational inequalities and principles needed to determine the necessary and sufficient conditions satisfied by the material characteristics of the phases, in order that the strain energy is weakly continuous, can be used. One extension of this research is the systematic classification of special cases of non-linearly elastic composites on the basis of variational principles, instead of constitutive relations and by using Legendre transformations in the same role with matrix inversion in linear elasticity ([9], [50]). It is worth noticing that sufficient conditions for exact relations between effective tensors for arbitrary structure of the composite (not only coated laminate) are already available ([51]).

In the same context, a second perspective of homogenization is the thermomechanical characterization of inelastic heterogeneous materials. In almost all cases (even in the linear-ones), the assumptions concerning the properties of the constituents (for instance, the elastic or plastic isotropy), are no more valid for the effective material ([48]). Additionally, the non-linear constitutive laws do not conserve their type in the effective medium. This is particularly unpleasant since many non-linear (for instance power law) constitutive laws have been established in mechanics literature and they are used for the mechanical characterization of these (homogeneous) constituents by comparing with experimental results. Moreover, the effective properties depend on the initial and boundary conditions and so every non-linear problem is a particular case. The related homogenization techniques aim at formulating necessary conditions for the stability by homogenization of the equations describing the problem and more specifically of the constitutive law.

Modeling and homogenization of epoxy plates reinforced by fibers and nanotubes are based on the multiple scale methods. Composites made of epoxy with carbon nanotubes, that exhibit excellent thermomechanical and electrical properties, and carbon fibers are very popular in aerospace engineering, mechanical engineering, computer construction etc. Adding more selected constituents, for instance shape memory alloys ([52]) gives additional properties, such as large reversible deformations and larger energy absorbtion. A multi scale homogenization starts from the nanostructure, where the atomic scale is simulated with the help of molecular dynamics analysis, and results to the characterization of the behavior matrix-carbon nanotubes (interfacial strength, cracks, pull-up). This information goes from the molecular dynamics analysis to the microstructure level (mesoscale), where appropriate homogenization techniques are applied to complete the macroscopic characterization of these materials. These techniques combine classical micromechanical methods (method of composite cylinder, Mori-Tanaka method, self-consistent method) with the method of asymptotic expansion and take on account of the elastic and/or the inelastic response of the constituents.

Recently, mathematical homogenization provided the framework for the optimal design of heterogeneous materials and complex structures. In structural design, the related mathematical theory (compensated compactness, variational principles) allows for determining bounds for the effective properties by using the elastic energy of the heterogeneous and of the homogenized material. Optimization in materials applies inverse homogenization for determining ideal materials with prescribed elastic properties ([53]). Optimization in structures applies shape or topology optimization, resulting to structures with optimal behavior with respect to prescribed functions (acting stresses, or deformations or absorbed energy or desirable geometry), under different loads. The shape optimization, introduced in [54], [55], [34], [56], [57], [58], [59], looks for solutions minimizing the sum of elastic compliance and weight of a structure under known loading.

Another promising field of interest is the computational micromechanics simulation of complex structures. Alternatively to the prevalent finite-element approach, there are recently developed techniques that are attractive and potentially more efficient. The parametric finite volume micromechanics ([41], [60], [61], [47]) has to affront serious difficulties in applying the required boundary conditions in a subvolume, whose response is representative of the whole material. Nevertheless, this method can be applied with accuracy in situations requiring very good estimations of both the microscopic and the macroscopic response of elastic and inelastic materials and structures. Combining this approach with the locally exact homogenization can be a reliable and easily applicable technique thanks to the easy way of introduction of the data, its efficiency, the relatively modest computational cost and the fast convergence of the solution.

Homogenization techniques are also useful for the computational evaluation of the dynamical properties of a composite material. Under harmonic loading, the effective elastic tensor and the damping coefficient depend on the frequency and thus carry multiple information on both the structure and the integrity of the composite. However, homogenization techniques cannot capture the size-effects of the microstructure. In other words, they predict the same effective coefficients for all composites having the same volume fraction and different size of inclusions. This problem can be faced by considering generalized elasticity theories ([62], higher order gradient elasticity ([63]), micropolar elasticity ([64]), non-local elasticity ([37])), that assume that the microstructure effect in the constitutive equations may be expressed in terms of internal variables. These theories can also support successfully new scattering techniques of homogenization of fiber-reinforced and particulate composites, where the dynamical properties can be approximated by iterative methods based on wave dispersion and attenuation predictions in these materials.

In Biomechanics, the homogenization based on higher order strain-gradient theories ([65]) provided some new results. Tissues exhibit important porosity and high heterogeneity and can be considered as a three-dimensional periodic truss. Several attempts of simulating the behavior of these tissues have been made by different researchers in the framework of classical elasticity. The framework of higher order continuum medium, as, for instance, the Cosserat continuum, seems to form a basis for a more consistent approximation of these materials under homogenization.

Additionally, homogenization could contribute to the preservation of the monuments, since ancient structures are made of discrete dry stones. The technique under consideration has interesting results regarding the mechanical behavior of ancient masonry structure or columns. Some applications can be found in [66], [44], on two- and three-dimensional block structures.

Another perspective of technological interest is the imaging problem in random media, systematically developed by Papanicolaou and coworkers ([67], [68], [69], [70]) since 2002, with a methodology (coherent interferometry) in which heterogeneities are modeled as random media and stochastic analysis methods are applied. This problem is very difficult and needs methods completely different than the homogeneous or the known deterministic methods. The challenge is to obtain statistically stable results, even if one knows only some statistical properties of the heterogeneities. It is expected that this methodology can be extended to the mathematical and numerical solution of new applications in sea acoustic imaging and to the study of its applicability limits in terms of perturbations, isotropy of the random medium and distance. Moreover, new mathematical techniques in seismic inverse problems are expected, together with the above imaging techniques. The simulation of seismic response in a city-like environment and the interaction source-city in weak soils is of particular interest ([71]). The phenomenon is characterized by enhancement and prolongation of seismic waves due to guided waves.

Compensated compactness applied to the study of oscillations of hyperbolic systems gives only a "static" information at a fixed point and time. On the contrary, the kinetic formulation for the elasticity system ([72]), give evolutionary equations for "kinetic functions" which in principle should capture information on propagation of oscillations. [73] are focusing on problems of periodic homogenization involving the transport of oscillating fine scales in order to develop the connection between homogenization problems and kinetic limits. This approach offers some novel insights when compared with the well known hyperbolic homogenization results obtained in [74], [75], [76](using the double-scale limit).

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