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Multi-scale computational homogenization: Trends and challenges

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ABSTRACT

In the past decades, considerable progress had been made in bridging the mechanics of materials to other disciplines, e.g. downscaling to the field of materials science or upscaling to the field of structural engineering. Within this wide context, this paper reviews the state-of-the-art of a particular, yet powerful, method, i.e. computational homogenization. The paper discusses the main trends since the early developments of this approach up to the ongoing contributions and upcoming challenges in the field.

1. Introduction

Multi-scale methods have contributed to a considerable progress in bridging the field of mechanics of materials to the field of materials science. This is mainly due to a fruitful combination of micromechanics and mathematical approaches, with a steadily increasing multi-disciplinary character. Several improved micromechanical theories and associated numerical models have been proposed and implemented, where a lot of interaction with materials science is involved. The developed understanding of single phases and complex interfaces in materials is optimally used in multi-scale homogenization techniques, where it is aimed to predict the collective multi-phase response of materials. Large deformations, damage and cracking, phase transformations, etc. can thereby be taken into account.

There are various ways to classify multi-scale methods in a general setting [1]. In this paper, however, attention is restricted to a particular method that falls in the category of homogenization methods based on integration over short length scales [1]. This category of methods is also called 'coarse graining' in the physics community [2]. Among the various homogenization techniques proposed, a *computational homogenization* scheme is probably one of the most accurate techniques in upscaling the nonlinear behaviour of a well-characterized microstructure. This method is essentially based on the construction of a micro-scale boundary value problem, that is used to determine the local governing behaviour at the macro-scale. In case the macro-scale boundary value problem is solved simultaneously, a fully nested solution of two boundary value problems is obtained, one at each scale. Though computationally expensive, the procedures developed allows one to assess the macroscopic influence of microstructural parameters in a rather straightforward manner. The first-order technique is by now well-established and widely used in the scientific and engineering community. Departing from this case, this paper briefly focuses on some recent trends and development in the past years on computational homogenization techniques and applications. Within this context, several topics are addressed:

- First-order computational homogenization: historical overview and key principles.
- Second-order computational homogenization: to resolve some intrinsic shortcomings of the first-order scheme, incorporating the size of the underlying microstructure.

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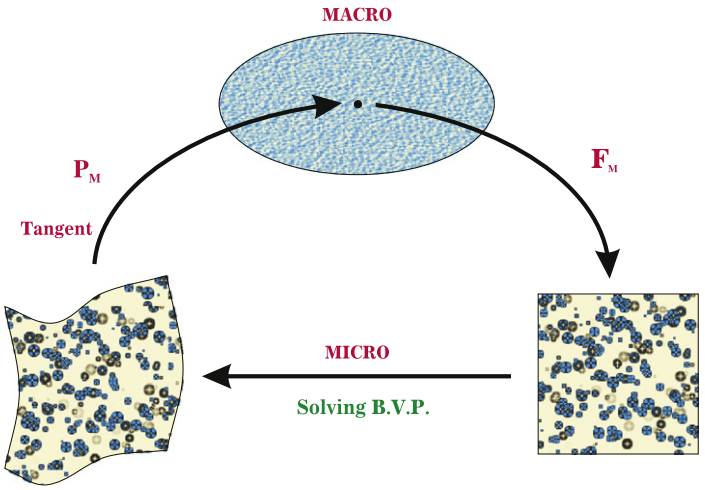

Fig. 1. First-order computational homogenization of continua.

- Continuous–discontinuous multi-scale approach for damage: the coarse scale is modelled discretely or with a discrete band (weak discontinuity), whereas the fine scale is modelled with a continuum.
- Computational homogenization of multi-physics problems, focusing on the homogenization of the thermal (heat conduction) problem, and its coupling to a mechanical homogenization scheme.
- Computational homogenization of structured thin sheets and shells: application of second-order homogenization principles to through-thickness representative volume elements, enabling its application to shell-type continua.
- Computational homogenization of interface problems, which is now emerging.

The most important issues are commented for each of the topics addressed, with a particular emphasis on the applicability, and possible limitations of each. The paper concludes with some general remarks on the added value of computational homogenization techniques as stand-alone tools or in development of alternative multi-scale methods. Finally, some open issues and challenges are summarized.

2. First-order homogenization for mechanical problems: The basis

The first-order method was first addressed in [3], about 20 years ago, even though some elements on coupling constitutive equations across the scales were already in place earlier [4]. The major developments that have led to the completion of this method took place about 10 years later, through a number of contributions [5–16]. Whereas some of the published work was initially restricted to small deformations and/or linear material behaviour, the method is fully general and has been elaborated over time for large deformations with arbitrary nonlinear material behaviour at the fine scale. The basic principle of the method is highlighted in Fig. 1, where the scale transitions between two scales are indicated. The governing macroscopic kinematical quantities (the deformation gradient tensor $\mathbf{F}_M$ in this case) are transferred to the micro-scale, in order to define a boundary value problem (BVP) on a representative volume element (RVE). The micro-scale boundary value problem can be solved in a standard manner, leading to a deformed RVE with boundary displacements and surface tractions. Using standard mathematical averaging equations, the macroscopic stress tensor $\mathbf{P}_M$ can be extracted. In case a macroscopic BVP is to be solved in parallel, tangents can be obtained directly from the RVE stiffness matrix through a static condensation process. In case the finite element method is used at both scales to solve the entire problem as a nested BVP, a true FE^2 method results, a name which is also quite often used to denote computational homogenization methods [12].

The scale bridging in the first-order scheme naturally relies on the classical linearization of the macroscopic nonlinear deformation map, $\vec{x} = \phi(\vec{X})$, applied to a material vector $\Delta\vec{x}$ in the deformed state:

$$\Delta\vec{x} = \mathbf{F}_M \cdot \Delta\vec{X} + \vec{w} \tag{1}$$

with $\vec{x}$ and $\vec{X}$ associated position vectors in the deformed and reference state, respectively, and in which $\mathbf{F}_M = (\vec{\nabla}_{0M}\vec{x})^T$. The local fine scale contribution that differs from the macro-scale deformation is identified as the micro-fluctuation field $\vec{w}$. Eq. (1) is valid in every point at the fine scale. The scale transitions are commonly complemented by two averaging equations: (1) volume averaging of the deformation $\mathbf{F}_M$ or the stress $\mathbf{P}_M$; (2) the Hill–Mandel macro-homogeneity condition, which essentially reflects volume averaging of the virtual work. Using these averaging equations allows one to construct a boundary value problem that can be schematically expressed through the prescribed displacements $\vec{u}^\star$ of some characteristic boundary points of the RVE.

$$\vec{u}^\star = \vec{f}(\vec{X}, \mathbf{F}_M). \tag{2}$$