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Computational homogenization of structures and materials

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Abstract — This presentation briefly focuses on some recent trends and development in the past years on computational homogenization techniques and its applications. Within this context, several topics are addressed: (1) first-order computational homogenization: historical overview; (2) second-order computational homogenization: how to incorporate the size of the underlying microstructure; (3) continuous-discontinuous multi-scale approach for localization problems; (4) multi-physics and coupled problems: heat conduction & thermo-mechanically coupled problems; (5) thin structures, shells and beams with a complex through-thickness architecture; (6) computational homogenization towards cohesive zones.

Keywords — homogenization, multi-scale, coarse graining, strain gradients, localization, shells, heat conduction

1 Introduction

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. 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 allow 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.

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: (1) first-order computational homogenization: historical overview and key principles; (2) second-order computational homogenization: to resolve some intrinsic shortcomings of the first-order scheme, incorporating the size of the underlying microstructure; (3) 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; (4) computational homogenization of multi-physics problems, focusing on the homogenization of the thermal (heat conduction) problem, and its coupling to a mechanical homogenization scheme; (5) computational homogenization of substructured thin sheets and shells: application of second-order homogenization principles to through-thickness representative volume elements, enabling its application to shell-type continua; (6) computational homogenization of interfacial mechanics and separation problems. 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 concluding comments on open issues and challenges are given.

2 First-order computational homogenization

About 20 years ago, Renard [3] established the basic ingredients of the first-order computation homogenization method, 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, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 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 figure 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

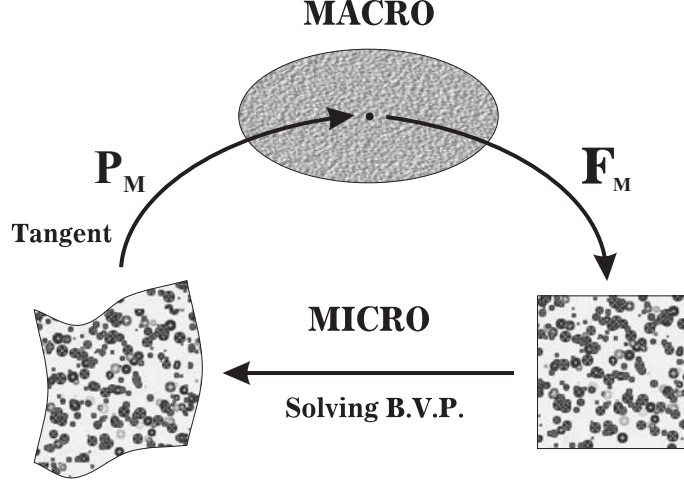


Figure 1: First-order computational homogenization of continua

macroscopic nonlinear deformation map, $\vec{x} = \phi(\vec{X})$, applied to a material vector $\Delta\vec{x}$ in the deformed state:

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

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} . Equation (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 to construct a boundary value problem that can be schematically expressed through the prescribed displacements \vec{u}^* of some characteristic boundary points of the RVE.

$$\vec{u}^* = \vec{f}(\vec{X}, \mathbf{F}_M) \quad (2)$$

This equation clearly highlights that the macroscopic deformation enters the micro scale BVP through the boundary conditions at the RVE. Various types of boundary conditions can be derived, all resulting from the micro-macro averaging relation adopted (e.g. volume averaging of the microscopic deformation gradient \mathbf{F}_m at the RVE scale resulting in \mathbf{F}_M at the macro scale). Among these, periodic boundary conditions have proven to be most versatile, both for periodic and non-periodic underlying microstructures. They are therefore mostly used nowadays for RVE analyses, for more details see [14, 17].

There is one key assumption that requires additional comments in terms of the adopted linearization in equation (1), which is the principle of separation of scales. This principle is best formulated as follows: “*The microscopic length scale is assumed to be much smaller than the characteristic length over which the macroscopic loading varies in space*”. In most cases this implies that the governing length scales are well separated, i.e.

$$\ell_{discrete} \lll \ell_{micro} \lll \ell_{macro} \quad (3)$$

The proper interpretation of the principle of separation of scales for the first-order method results from (1). This equation implicitly assumes that the macroscopic deformation gradient \mathbf{F}_M is constant over the spatial length scale associated to the RVE size.

Whereas the first-order method has now grown towards a standard tool in computational homogenization [18, 19, 20, 21, 22], it should be emphasized that the method has its limitations:

- The method complies with the principle of local action and the material point concept and is therefore in a non-modified form limited to a standard continuum mechanics theory at the macro-scale
- The aforementioned principle of separation of scales clearly sets limits for the first-order case. As a consequence, large spatial gradients at the macro-scale cannot be resolved. The method is therefore not suited for the analysis of localization problems.
- The principle of local action mathematically assigns an infinitely small size to the RVE, which only satisfies the right inequality in equation (3). The real physical size ($\ell_{discrete}$ and ℓ_{micro}) is therefore not accounted for. Size effects affecting the macro scale behaviour can therefore not be properly studied.

Unfortunately, some of these limitations are sometimes ignored and the method has already been applied in the literature beyond its limits of applicability.

3 Second-order computational homogenization

Inspired by the limitations that restricted the use of the first-order method, a full second-order extension has been developed in the literature [23, 24, 25, 26, 27, 28]. Departing from a second-order Taylor series expansion of the nonlinear deformation map, truncated after the second term, the macroscopic kinematics becomes of the full gradient type.

$$\Delta\vec{x} = \mathbf{F}_M \cdot \Delta\vec{X} + \frac{1}{2} \Delta\vec{X} \cdot {}^3\mathbf{G}_M \cdot \Delta\vec{X} + \vec{w} \quad (4)$$

Using this Taylor series expansion, the macroscopic (coarse scale) kinematics is determined through the deformation gradient tensor \mathbf{F}_M and its Lagrangian gradient ${}^3\mathbf{G}_M = \vec{\nabla}_{0M} \mathbf{F}_M$. The key point in the second-order two-scale framework, resides in applying relation (4) to a representative part of the microstructure, such that a classical boundary value problem is obtained at the micro scale (or fine scale).

The macro-micro scale transition essentially translates the macroscopic kinematics towards proper boundary conditions on an RVE, i.e.

$$\vec{u}^* = \vec{f}(\vec{X}, \mathbf{F}_M, {}^3\mathbf{G}_M) \quad (5)$$

The second-order method is schematically represented in figure 2, where the averaging leads to the macroscopic stress tensor \mathbf{P}_M and the higher-order stress tensor ${}^3\mathbf{Q}_M$. The boundary value

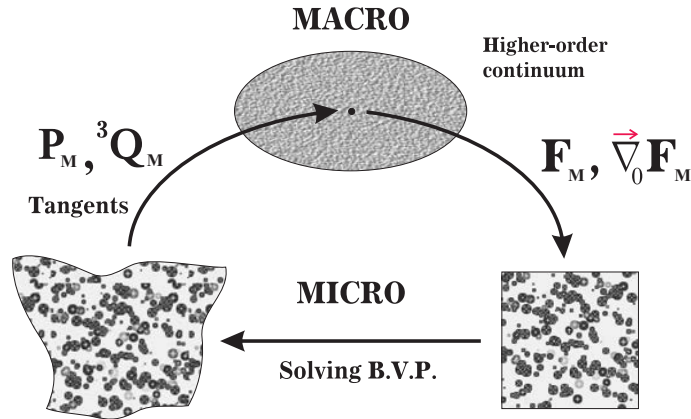


Figure 2: Second-order computational homogenization of continua

problem at the micro-scale remains a classical (first-order) one (though alternative approaches are possible here as well), and can be solved with a standard solution technique. The micro-macro scale transition relies on extended averaging relations, departing from a second-order extension of the Hill-Mandel macro-homogeneity condition. The resulting equilibrium at the macro scale is of Mindlin's type (full second gradient), along with its typical higher-order boundary conditions. Like for the first-order problem, a homogenized consistent tangent operator can be easily retrieved through static condensation of the underlying micro-scale stiffness matrix (of the discretized FE-problem). The main change with respect to the first-order method, is the incorporation of a length scale, which is essentially defined by the size of the RVE. The latter raised a number of questions on the exact role of the RVE size, along with its physical significance and its impact on the solution [26]. The classical concept of the first-order representative element does not apply anymore. The proper size of the second-order RVE is fully governed by two bounds:

- The upper bound: the separation of scales for the extended homogenization scheme allows for linear variations of the macroscopic strain fields over the size of the RVE (or quadratic in the displacements), see equation (4). The size of the RVE may not be larger than the macroscopic spatial length scale characterizing these linear variations at the macro-scale.
- The lower bound: this bound is identical to the first-order case and is dictated by the statistical representativeness of the RVE (along with its boundary conditions).

The optimal size is the smallest RVE that is still statistically representative (within the desired limits of accuracy) and still complies with the assumed scale separation.

The key characteristics that make the second-order approach superior to the first-order one are:

- It allows for a proper assessment of second-order constitutive equations emanating from a lower scale. Even for the linear case, all Mindlin's stiffness tensors can be rigorously reconstructed. For the nonlinear case, this would be completely out of reach with other, analytically based methods.
- It accounts for a micro-scale length scale, even though care must be taken in transporting this length scale across the scales (through the RVE size, see above).
- It naturally passes deformation gradients to an RVE, which allows for the study of gradient-sensitive materials at the micro scale (e.g. geometrically necessary dislocations in metallic crystals). Without this second-order approach, macroscopic deformation gradients (e.g. in bending) are not passed to the RVE boundaries, and hence not resolved.
- It resolves the ill-posedness of the macroscopic problem in the presence of moderate localization, along with the characteristic mesh dependency on that scale. A full parallelism with conventional higher-order constitutive equations used as localization limiters exists in this sense.

In spite of these positive characteristics, the principle of separation of scales also dictates a limit here. The method cannot properly resolve macroscopic localization bands beyond a quadratic nature in the displacements. Sharper localization regions will naturally violate this condition. The method can therefore not be used for a complete softening analysis at the macro-scale. In spite of this concern, the second-order generalization well tackles moderate localization bands and the second-order macro-micro kinematics turned out to be particularly useful for its application to shells and beams, see section 5.

4 Continuous-discontinuous computational homogenization

At present, a lot of research efforts are concentrated on the proper multi-scale handling of problems involving damage and fracture, i.e. intense localization. As advocated in the sections 2 and 3, the continuous homogenization schemes are not applicable to this limit case. Inspired by the success of different types of embedded localization band models used in constitutive modeling of engineering materials, attention is focusing on the development of a continuous-discontinuous homogenization scheme.

The first approach in this category was developed in the context of masonry cracking, but the methodology is far more generic [29, 30]. It essentially relies on the proper incorporation of a localization band at the macro-scale, along with a two-fold first-order homogenization scheme to resolve the response in the damaging ($\mathbf{F}_M^b, \mathbf{P}_M^b$) and unloading material ($\mathbf{F}_M^s, \mathbf{P}_M^s$), see figure 3 for a sketch of principles. In here, \mathbf{F}_M^b and \mathbf{P}_M^b are the deformation gradient tensor and the first Piola-Kirchhoff stress tensor in the localization band respectively. Likewise, \mathbf{F}_M^s and \mathbf{P}_M^s are the same quantities in the adjacent unloading volume surrounding the localization band. This has to

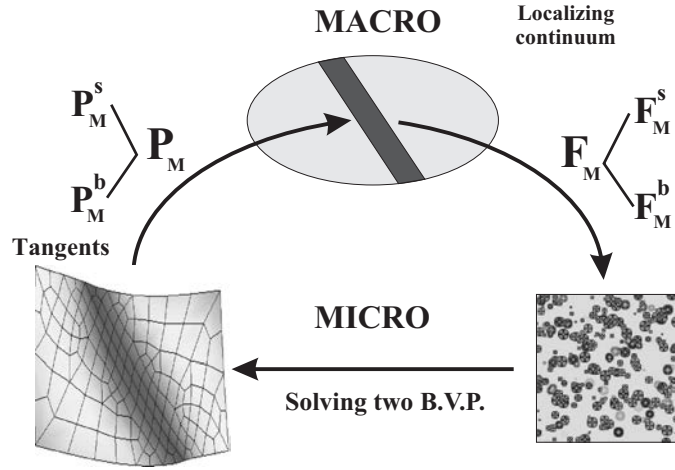


Figure 3: Continuous-discontinuous computational homogenization for localizing continua

be complemented by a proper numerical scheme to couple the length scales between the micro and macro-domain. Nevertheless, it remains a true homogenization scheme whereby only small parts of the physical domain are resolved to extract the full structural response. Several technical issues come into play: detecting the onset of localization, handling the macro-volume with the embedded localization band (compatibility and traction continuity), snap-back at the level of finite size macro-domain, path following within the RVE, etc. A solution scheme with a fixed size of the localization band has been developed on this basis, which is adequate for many cases. Alternative approaches aimed to establish a rigorous coupling between a macroscopic finite element size and the damaging RVE [31]. However, this solution essentially steps off from the key ideas and benefits of homogenization and much more resembles a domain decomposition approach with an embedded scale refinement.

Recent developments that are obviously related to the proposed continuous-discontinuous homogenization scheme can be found in [32, 33], where advantage is taken of a X-FEM approach to incorporate the discontinuity at the macro scale. The more general case, were localization bands can steadily evolve in width, is still open and several research groups are currently working on this difficult challenge.

5 Computational homogenization for shells and beams

The second-order computational homogenization methodology and its mathematical principles particularly paid off in the homogenization of 3D volume elements towards shells [34] (or beams in a simplified version, partially addressed in earlier work see [35, 36]). The computational homogenization of shells is mainly useful if complex substructures exist, which cannot be captured in a layered-wise composite shell approach. Many such practical examples exist, complemented by an in-plane periodic nature of the substructure: flexible electronics, sandwich panels, ship hull core structures, etc. The shell homogenization problem is sketched in figure 4. Like for

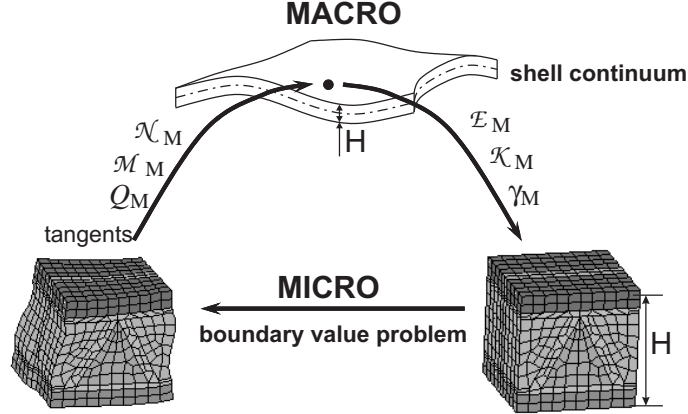


Figure 4: Two-scale homogenization of shells with a through-thickness RVE

the other computational homogenization schemes, macroscopic kinematical quantities (in-plane membrane strains \mathcal{E}_M , curvature \mathcal{K}_M and transverse shear γ_M are passed to the micro scale to construct the boundary value problem.

$$\vec{u}^* = \vec{f}(\vec{X}, \mathcal{E}_M, \mathcal{K}_M, \gamma_M) \quad (6)$$

The formulation developed in literature, relies on a through-thickness representative volume element where the top and bottom surface of the shell are physically incorporated at the RVE level. A particular loading case has been investigated, excluding external tractions acting on the top and bottom face of the shell. The resulting homogenization scheme directly combines a planar homogenization (in the reference plane of the shell) with a full integration through the thickness. The shell kinematics is second-order and naturally transferred to a 3D RVE on the basis of the kinematics developed in [24]. The macroscopic generalized stress resultants, i.e. moments \mathcal{M}_M , transverse forces \mathcal{N}_M and shear forces \mathcal{Q}_M follow from the homogenization process. Like for all other cases, a fully consistent tangent operator can be extracted through static condensation of the RVE stiffness matrix. The macroscopic shell formulation does not need an additional layered integration scheme, since the thickness is entirely resolved. At this stage, the Kirchhoff-Love and Mindlin-Reisner cases were treated. Intrinsic well-known shortcomings of the shell theory in passing from a 3D continuum to a shell have to be resolved in setting up the scale transition. Extensions to more general shell theories (e.g. solid-like shells) and other loading conditions (non-zero tractions on the top or bottom face) are open.

6 Computational homogenization of multi-physics problems

A computational homogenization enables the coupling of two boundary value problems in a nested numerical setting, which justified the frequently used term FE^2 . Beyond mechanical problems,

several other physical phenomena may be dealt with through this method. Not too many attempts have been made in this direction at this stage. In this section, emphasis is put on some developments in thermo-mechanics.

6.1 Heat conduction in solids

Many problems are characterized by severe temperature variations that may affect structural and material performance at different scales. Engineering examples of such thermal loading conditions include thermal coatings, refractories in furnaces, microelectronics components and engines. The computational homogenization of the heat conduction problem that couples the thermal problem at two scales has been addressed in [37, 38], and is schematically shown in figure 5. A transient

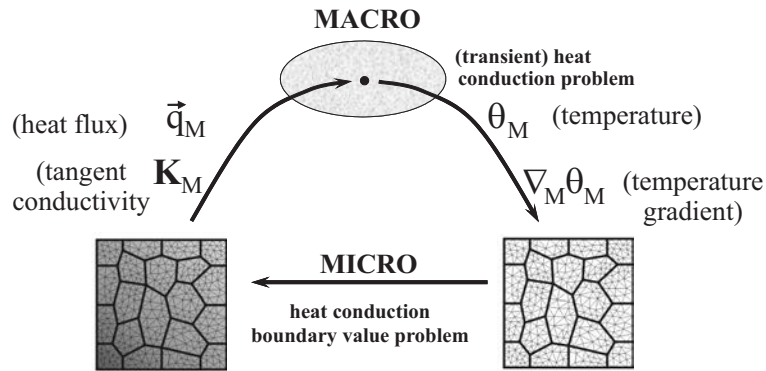


Figure 5: Two-scale homogenization of heat conduction

heat conduction problem is considered at the macro scale, for which the heat flux \vec{q}_M and conductivity \mathbf{K}_M are not formulated explicitly, but determined through the computational homogenization procedure. The macroscopic temperature θ_M and temperature gradient $\nabla_M \theta_M$ are transferred to the micro scale and used to define the boundary conditions on the thermal RVE. The micro scale heat conduction boundary value problem is solved, after which the macroscopic heat flux \vec{q}_M is obtained by volume averaging the resulting heat flux field over the RVE. The macroscopic (tangent) conductivity \mathbf{K}_M is extracted from the (discretized) microstructural conductivity matrix. Although the development of the computational homogenization framework for the heat conduction problems follows the same philosophy as its mechanical counterpart, some fundamental differences have to be tackled [37]. These differences mainly reside in the physics of the equations to be homogenized and the fact that an average temperature has to be resolved in the scale transitions as well. The principle of separation of scales allows to couple a transient macro scale problem to a steady-state micro scale problem. Extensions towards a transient analysis at both scales are possible here as well [39].

6.2 Coupled thermo-mechanics

Combining the thermal problem with the mechanical problem allows to construct a fully coupled two-field and two-scale homogenization scheme. From a practical point of view, this can be solved in different ways, among which an operator-split routine is most convenient [40]. Anisotropy, nonlinearity and temperature dependence of both mechanical and thermal material characteristics can be introduced at the micro scale with various morphologies enabling an effective structure-property analysis. Dealing with these coupled nonlinearities in other homogenization techniques is an almost infeasible task.

7 Computational homogenization of interfacial separation

A recent extension that is gaining interest, is the computational homogenization of interfacial volumes towards cohesive zones [41]. Unlike the standard first-order technique, this scheme can properly handle localization at the macroscopic scale. An interfacial macroscopic model (traction-opening $\vec{t}_M(\vec{\Delta})$ for a cohesive zone) is coupled to an interfacial RVE of finite dimensions (i.e. a finite volume with a small thickness that models the interface domain as a continuum with all its geometrical details, phases, defects and bonds). The macro scale kinematics (interfacial opening vector $\vec{\Delta}_M$) is used to construct the boundary conditions at the level of the interfacial RVE (which has a finite physically motivated initial thickness).

$$\vec{u}^* = \vec{f}(\vec{X}, \vec{\Delta}_M) \quad (7)$$

The RVE boundary value problem is solved and the resulting RVE tractions are averaged to identify the macroscopic interfacial traction vector \vec{t}_M . Complex mixed-mode interfacial loading conditions can be easily investigated. Again, tangents can be extracted in a straightforward manner.

8 Concluding comments

Bridging scales from materials science to mechanics of materials and further to structural mechanics, takes a lot of benefit from what computational homogenization has to offer as a reference solution. It is a powerful technique that has demonstrated its potential in a number of cases throughout the literature. It is, however, a computationally expensive technique that naturally calls for an adaptive and parallelized solution strategy. It may not be considered as a tool that replaces other homogenization techniques in general. Whenever a closed-form macroscopic equation can be derived, this should remain the first choice. However, when this is not possible or when the validity of a macroscopic constitutive equation needs to be assessed, then computational homogenization provides a natural reference solution to compare with. This is, without any doubt, one of the main applications of the method. Note that the quality of the solution obtained through a computational homogenization method entirely depends on the quality of the description of materials, phases and interfaces at the micro scale. The scale transition is properly dealt with, but this cannot remedy any shortcomings that may be present in the micro scale description. Nevertheless, adequately characterizing single phases and interfaces seems a lot more realistic and feasible than characterizing the complexity in multi-phase systems.

Undoubtedly, considerable progress has been made since the introduction of the early concepts of computational homogenization about 20 years ago. Nevertheless, many open issues are yet to be resolved in the coming years:

- computational homogenization of emerging and evolving localization bands, coupled to enriched finite element descriptions on the macro scale
- extended shell formulations
- more complex loading conditions for shells and beams
- extended interfacial descriptions
- optimal use of different BVP solution strategies at both scales (e.g. [42])
- other multi-physics and coupled field problems (electro-mechanical, thermo-electrical, fluid-structure interaction, magneto-electro-elasticity, acoustics, etc.)
- elaborate handling of spatial-temporal and kinetics aspects in upscaling

- dynamic problems, including inertia effects and/or propagating waves
- problems related to nonconvexity and micro-structure evolution emanating from the micro scale
- integration of phase field models across the scales

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