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A mortar based approach for the enforcement of periodic boundary conditions on arbitrarily generated meshes

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ABSTRACT

A new approach for the enforcement of periodic boundary conditions on representative volume element (RVE) problems is presented. The strategy is based on a mortar formulation and considers two and three dimensional problems in the finite deformation frame. The mortar discretization is combined with the *Lagrange* multiplier method for the enforcement of periodicity constraints at each pair of corresponding boundaries of the RVE in a weak integral sense. The interpolation of the *Lagrange* multipliers is undertaken with dual shape functions, which can be locally eliminated from the RVE system of equations by static condensation, avoiding an increase on the system size. The numerical treatment within a Newton-based finite element solution procedure for the RVE equilibrium problem is discussed in detail. The resulting method is able to efficiently enforce periodic configurations over complex RVEs at finite strains with arbitrarily generated finite element meshes. Several numerical examples are presented to demonstrate the robustness of the method and the quality of results.

1. Introduction

The design of new materials is one of the most challenging tasks in engineering science that has been continuously fostered by the increasing requirements of novel applications. Since the response of the material at the macroscopic level is a direct consequence of the material microstructural geometry and evolution, the establishment of relationships between the microstructure and the macroscopic properties of materials has attracted considerable research efforts. In recent years, a general modeling framework, the so-called multilevel finite element framework (ML-FEM) or FE^2 [1–5], has been developed to capture the behavior of heterogeneous materials. The underlying idea of the method is to extract the quantities required for the macro-scale by solving a micro-scale problem over a statistically representative volume element (RVE). This modeling framework allows an effective description of complex microstructural geometries, arbitrary constitutive material behavior and microstructural evolution. Nevertheless, some disadvantages have also been associated with the ML-FEM such as the computational cost that the solution of multi-scale problems incurs [6–10] or the loss of representativeness of the RVE when softening regimes are reached [11,12].

In the ML-FEM framework, the definition of the size of the RVE problem is extremely important since it should be large enough to statistically represent the microstructure of the material. In contrast, as the size of the RVE problem increases, memory storage and computational requirements can become prohibitive. This is due to the fact that in the ML-FEM

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framework the macroscopic equilibrium problem is solved simultaneously with one microscopic RVE problem for each point of the macroscopic mesh. Another important feature of this technique is the definition of the boundary condition to apply for the RVE problem. There are three classic kinematical constraints: linear boundary displacements, uniform boundary tractions and periodic boundary fluctuations. Several numerical studies have shown [13,14] that the periodic boundary condition (PBC) is the one that converges faster to the theoretical/effective solution when the RVE size increases. This means that for the same RVE size, the PBC delivers a better estimation of the effective properties. Therefore, due to its representativeness and computational efficiency, this contribution focuses on the enforcement of PBCs for randomly generated meshes.

The classical approach for applying the PBC consists on the enforcement of an identical displacement fluctuation field for each pair of corresponding boundaries of the RVE. This forces the RVE to be discretized with a conform mesh on opposite boundaries, i.e. the finite element mesh topology has to be such that a one-to-one correspondence exists between nodes of opposing sides of the RVE boundary [3,15]. Although for some simple RVE geometries this requirement may be easily met using commercial pre-processors or even dedicated mesh generation algorithms [16], this is not generally the case. For instance, if the microstructure does not have geometrical periodicity, which is the most frequent case for microstructures obtained from real image processing, the mesh will not probably be conform. Furthermore, this requirement is also quite restrictive within the context of the finite element method. In particular, it is extremely challenging to develop an adaptive remeshing strategy, which employs an unstructured mesh generator, that always generates a conform mesh. In addition, the introduction of discontinuities at the RVE level, which is a rapidly expanding topic [17–21], would also be very difficult to accommodate.

In order to circumvent the requirement of having conform meshes, several solutions have been proposed. A surface-to-surface constraint has been suggested in [22,23], which can be found in some commercial finite element codes. In this case, the boundary of the RVE is split into master and slave parts where the nodes embedded in the slave domain are prescribed and defined by the closest nodes on the opposite edge/surface (master domain) by interpolation. Despite its simplicity, this approach suffers from lack of robustness when the master and slave edges/surfaces have a different node density. A slightly different approach was proposed in [24] and recently enhanced and optimized in [25]. In this approach, the displacement field at two opposite sides of the RVE is interpolated by linear combinations of shape functions which need to satisfy some constraints. A different solution was proposed in [26] by introducing an independent finite element discretization of the boundary tractions.

In this work, a different strategy is proposed to enforce PBCs on RVE problems with an arbitrary finite element mesh discretization. This approach is inspired on the mortar method [27], which was originally introduced in the context of domain decomposition techniques. This method is able to efficiently enforce interface constraints over interacting non-conform domains in a variationally consistent way based on the *Lagrange* multiplier method. An essential feature of the method is the introduction of interface conditions in an integral (weak) form instead of strong, point wise constraints. Furthermore, the mortar method is able to preserve optimal convergence rates from the finite element methods as long as appropriate mortar spaces are chosen. The use of the so-called dual *Lagrange* multipliers spaces [28] allows for an efficient local elimination of the discrete *Lagrange* multipliers by static condensation. These advantages have led to the application of the mortar method in different computational fields such as contact problems [29–34] and recently in fluid–solid interaction problems [35].

The present contribution is structured as follows. In Section 2 we briefly review the basic ingredients of the formulation of homogenization based multi-scale models. The new strategy to enforce PBC is introduced in Section 3. Spatial discretization of the RVE equilibrium problem based on standard and dual bases is presented in this Section, followed by details on the evaluation of the integrals, for both two and three dimensional problems. Two distinct schemes are obtained: a force–displacement and fully-displacement based scheme. Finally, in order to demonstrate the efficiency of the method, Section 4 presents several numerical examples to assess the results followed by some conclusions.

2. Homogenization based multi-scale modelling

This section provides a brief summary of the basic concepts of homogenization based multi-scale models at finite strains (also known as ML-FEM or FE^2 multi-scale models). A more detailed description can be found in references [3,36–39,15] among others. For the sake of clarity, all variables defined at the macro-scale will be identified by $*\{\boldsymbol{x}\}$, where $\boldsymbol{x}$ denotes an infinitesimal point at the macroscopic domain. Conversely, the microscopic variables will be associated to an infinitesimal point at the microscopic domain, denoted by $\boldsymbol{y}$. For example, following this notation, $\boldsymbol{A}\{\boldsymbol{x}\}$ and $\boldsymbol{A}\{\boldsymbol{y}\}$ denote a generic parameter, field or tensor respectively defined at the coarse and fine scales. In turn, capital letters $\boldsymbol{X}$ and $\boldsymbol{Y}$ denote coordinates of a generic point at the undeformed macro and micro domains respectively.

2.1. Homogenization theory

The main assumption of the present family of multi-scale theories is that at a generic macroscopic point and at an instant in time t, the macroscopic deformation gradient, $\boldsymbol{F}\{\boldsymbol{x},t\}$, is defined as the volume average of its microscopic counterpart, $\boldsymbol{F}\{\boldsymbol{y},t\}$, over the undeformed configuration of the RVE

$$\boldsymbol{F}\{\boldsymbol{x},t\} = \frac{1}{V_0}\int_{\Omega_0} \boldsymbol{F}\{\boldsymbol{y},t\}dV = \boldsymbol{I} + \frac{1}{V_0}\int_{\Omega_0} \nabla_{\boldsymbol{p}}\boldsymbol{u}\{\boldsymbol{y},t\}dV. \tag{1}$$