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Asymptotic expansion homogenization of discrete fine-scale models with rotational degrees of freedom for the simulation of quasi-brittle materials

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ABSTRACT

Discrete fine-scale models, in the form of either particle or lattice models, have been formulated successfully to simulate the behavior of quasi-brittle materials whose mechanical behavior is inherently connected to fracture processes occurring in the internal heterogeneous structure. These models tend to be intensive from the computational point of view as they adopt an "a priori" discretization anchored to the major material heterogeneities (e.g. grains in particulate materials and aggregate pieces in cementitious composites) and this hampers their use in the numerical simulations of large systems. In this work, this problem is addressed by formulating a general multiple scale computational framework based on classical asymptotic analysis and that (1) is applicable to any discrete model with rotational degrees of freedom; and (2) gives rise to an equivalent Cosserat continuum. The developed theory is applied to the upscaling of the Lattice Discrete Particle Model (LDPM), a recently formulated discrete model for concrete and other quasi-brittle materials, and the properties of the homogenized model are analyzed thoroughly in both the elastic and the inelastic regime. The analysis shows that the homogenized micropolar elastic properties are size-dependent, and they are functions of the RVE size and the size of the material heterogeneity. Furthermore, the analysis of the homogenized inelastic behavior highlights issues associated with the homogenization of fine-scale models featuring strain-softening and the related damage localization. Finally, nonlinear simulations of the RVE behavior subject to curvature components causing bending and torsional effects demonstrate, contrarily to typical Cosserat formulations, a significant coupling between the homogenized stress–strain and couple-curvature constitutive equations.

1. Introduction

Discrete fine-scale models, in the form of either particle or lattice models, have been formulated successfully in the literature to simulate the behavior of a variety of different materials. Their use has become more and more popular in the last few decades due to a number of appealing properties that make them advantageous compared to continuum based formulations.

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The geometry of discrete models is built with reference to the actual internal structure of the material of interest and it consists of "particles" connected through either "contact points" or "connecting struts" (also called "lattice elements"). This "a priori" discretization allows simulating material heterogeneity efficiently in the case of materials – such as concrete, rock, sea-ice, and toughened ceramics – characterized by hard and stiff inclusions embedded in a more compliant, weak, and brittle, matrix. In addition, the intrinsic particle/lattice spacing automatically provides the formulation with an internal characteristic length which can be made randomly variable if the discrete model is constructed according to the actual random distribution of material heterogeneity.

The degrees of freedom (displacements and rotations) are defined only at a finite number of points – referred also as "nodes" thereinafter – which, depending on the formulation, may or may not correspond to the particle center of mass or particle centroid. Strain and stress measures are defined at a finite number of points coinciding with the contact points or with some specified points along the connecting struts. The constitutive behavior is formulated through vectorial, as opposed to tensorial, stress versus strain relationships and stress tractions are supposed to be distributed over either a "contact area" or the cross sectional area of the connecting struts (in this paper, this area will be generically referred to as "facet"). Finally, the classical concepts of equilibrium and compatibility are formulated through algebraic equations, instead of partial differential equations typical of continuum mechanics. One of the main advantages of discrete models is that the discreteness of the formulation permits handling naturally displacement discontinuities arising during damage localization and fracture processes.

Rigid particle models, under the name of discrete element method (DEM), were first formulated to simulate both natural materials, such as geomaterials (Cundall, 1971; Serrano and Rodriguez-Ortiz, 1973; Cundall and Strack, 1979; Kawai, 1978), as well as man-made materials like concrete (Zubelewicz and Mroz, 1983; Plesha and Aifantis, 1983; Zubelewicz and Bažant, 1987). A somewhat similar model is the rigid-body-spring model (RBSM), which subdivides the material domain into rigid polyhedral elements interconnected by zero-size springs (Kawai, 1978; Bolander and Saito, 1998; Bolander et al., 1999, 2000).

Lattice models, pioneered by Hrennikoff (1941) to solve elastic problems in the pre-computers era, were later developed by many authors to model fracture in quasi-brittle materials in both 2D (Schlangen and van Mier, 1992) and 3D (Cusatis et al., 2003, 2003; Lilliu and van Mier, 2003; Berton and Bolander, 2006).

More recently, various discrete models, in the form of either lattice or particle models, have been quite successful in simulating concrete materials (Lilliu and van Mier, 2003; Cusatis et al., 2011a,b; Leite et al., 2004; Kim et al., 2008). For an extensive review of the currently available models for concrete the reader is directed to a recent special issue (Cusatis and Nakamura, 2011) collecting several papers covering a wide variety of concrete mechanics phenomena spanning several length scales, from the scale of cement particles to that of reinforced concrete structural members.

In most applications of interest in practice, fine-scale models lead to fairly large computational systems characterized by a huge computational cost making their practical use rather limited. For example, the full-scale computational analysis of an average concrete bridge would require millions of degrees of freedom or the simulation of a rock formation would require billions of degrees of freedom. The solution of such large problems, although possible in principle with large super computer clusters, is unimaginable in everyday engineering practice. For this reason, many studies have been devoted to finding optimal and rigorous approaches for multiscale computation.

Among different multiscale techniques available in the literature (Galvanetto and Ferri Aliabadi, 2009), the ones based on homogenization theory have been widely used over the past decades. The homogenization theory relies on two main assumptions. The first is the existence of a certain volume of material, the so-called representative volume element (RVE) or unit cell (UC), carrying a complete description of the internal material structure (Gitman et al., 2007; Kouznetsova et al., 2004). The second is that the size of such a volume is much smaller than the size of the overall solid volume under consideration. The latter is also known as the "scale separation" assumption.

Hill (1963) , Eshelby (1958), and Hashin and Strikman (1963) pioneered analytical homogenization techniques which were developed later by other authors (Christensen and Lo, 1979; Nemat-Nasser et al., 1993). Analytical homogenization is able to reasonably approximate material properties when the exact solution of the boundary value problem associated with the RVE problem can be obtained. However, in this approach, elastic behavior, small strains, and relatively simple internal structure are the limiting assumptions typically adopted. When complicated heterogeneous structures are considered, or constitutive behavior of constituents are nonlinear, other homogenization techniques (Lopez-Pamies et al., 2013, 2013) need to be considered.

To overcome these difficulties, computational homogenization is often used in the literature (Smit et al., 1998; Feyel, 2003; Kouznetsova et al., 2004; Miehe et al., 1999). In this approach, a single RVE is assigned to each calculation point (e.g. Gauss point in a finite element mesh) in the macro-domain and at each step of the nonlinear analysis, macro-strain increments are imposed as essential boundary conditions to the RVE. The solution of the RVE boundary value problem is then averaged for the calculation of the associated macroscopic stress tensor. Since no assumption is made for the macroscopic constitutive law, this method can be used for materials featuring extremely nonlinear behavior.

A somewhat similar but more mathematically rigorous homogenization technique is the so-called asymptotic expansion homogenization (AEH) that uses the asymptotic expansion of the displacement field based on a length parameter representing the ratio between the length scale of material heterogeneity and the macroscopic length scale. Starting from this expansion hierarchical boundary value problems are obtained at different scales. This approach can easily handle problems with multiple (more than 2) scales in both space and time (Fish et al., 2007); it does not make assumptions on the character