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Homogenization coarse graining (HCG) of the lattice discrete particle model (LDPM) for the analysis of reinforced concrete structures

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ABSTRACT

In this study, a coarse-graining framework for discrete models is formulated on the basis of multiscale homogenization. The discrete model considered in this paper is the Lattice Discrete Particle Model (LDPM), which simulates concrete at the level of coarse aggregate pieces. In LDPM, the size of the aggregate particles follows the actual particle size distribution that is used in experiment to produce concrete specimens. Consequently, modeling large structural systems entirely with LDPM leads to a significant number of degrees of freedom and is not feasible with the currently available computational resources. To overcome this limitation, this paper proposes the formulation of a coarse-grained model obtained by (1) increasing the actual size of the particles in the finescale model by a specific coarsening factor and (2) calibrating the parameters of the coarse grained model by best fitting the macroscopic, average response of the coarse grained model to the corresponding fine scale one for different loading conditions. A Representative Volume Element (RVE) of LDPM is employed to obtain the macroscopic response of the fine scale and coarse grained models through a homogenization procedure. Accuracy and efficiency of the developed coarse graining method is verified by comparing the response of fine scale and coarse grained simulations of several reinforced concrete structural systems in terms of both accuracy of the results and computational cost.

1. Introduction

Cementitious composites, such as concrete, are widely used in engineering applications. These materials are heterogeneous, are characterized by quasi-brittle mechanical behavior, and their mechanical response is strongly influenced by various phenomena such as crack initiation and propagation, interaction and coalescence of distributed micro-cracks into a localized macro crack, existence of confining pressure, and crack bridging effect of fibers. These phenomena occur at different spatial scales ranging from atomistic scale ($\sim 10^{-10}$ m) to the structural scale ($\sim 10^{1}$ m). Several micro-, meso-, and macro-constitutive models have been developed to simulate this complex behavior at various length scales. Most of the developed models are based on continuum mechanics which neglect the complex internal structure of the material, They are well suited to capture the global response of a structure, when inelastic behavior is distributed over a large volume of material. However, these models become inaccurate for complex loading conditions in which macroscopic mechanical behavior is heavily influenced by material heterogeneity and damage localization.

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Mini-scale models were proposed by several authors including Wittmann and coworkers [1] in 2D and Carol and coworkers [2–4] in 3D. They used the finite element method to discretize coarse aggregate pieces, mortar matrix, and aggregate-matrix interface. As an alternative to the use of continuum approaches, Schlangen modeled concrete through a discrete system of beams (lattice elements) [5]. In his approach, lattice meshes were used to create the internal structure of concrete, in which different material properties were assigned to the lattice elements corresponding to the various components such as matrix, aggregate, and interface. Bolander and coworkers [6,7] formulated a discrete mini-scale model based on the interaction between rigid polyhedral particles constructed through the Voronoi tessellation of the domain. Similar approach was employed by Nagai et al. [8] to simulate mortar and concrete in a 2D setting. Mini-scale models provide realistic simulations of concrete cracking, coalescence of several distributed cracks into a localized one, and fracture propagation. However, these models tend to be computationally intensive even to simulate laboratory test, and become untanable for 3D modeling which is necessary to capture correctly compressive failure and confinement effects.

The effect of the material internal structure on the macroscopic behavior can be analyzed efficiently by meso-scale model employing particle models in which only coarse aggregate pieces are simulated, and each particle corresponds to a single aggregate. This approach was applied successfully to geomaterials [9,10] as well as concrete [11–13]. Meso-scale models reduce considerably the size of the numerical problem, while they can capture the fundamental aspects of material heterogeneity along with damage localization and fracture processes even in the case of three-dimensional complex fracture phenomena.

Building upon earlier developments [12,14], Cusatis and coworkers developed an accurate meso-scale model for the simulation of concrete: the so-called Lattice Discrete Particle Model (LDPM) [15,16]. LDPM simulates concrete internal structure by modeling coarse aggregate pieces and approximating their interaction through the interaction of rigid polyhedral cells. LDPM successfully simulate concrete mechanical behavior by employing meso-scale constitutive relationships in which three major failure mechanisms are taken into account: fracture and cohesion in tension; compaction and pore collapse under compression; and frictional behavior in shear. LDPM provides a computationally efficient framework, which is able to model most aspects of concrete behavior such as uniaxial, biaxial, and triaxial responses.

Although the meso-scale modeling of various experiments on laboratory size concrete specimen has been performed successfully by particle models [16], numerical simulation of real size engineering structures using meso-scale models is impractical even with the use of parallel computing techniques. For instance, a concrete cylindrical specimen of 150 mm diameter and 300 mm height with maximum aggregate size of 10 mm simulated with LDPM includes approximately 8,500 particles. This yields to 51,000 degrees of freedom, given that each particle has 6 degrees of freedom. This clearly shows that the simulation of large concrete structures using LDPM is demanding computationally, as it requires solving a computational system characterized by billions of degrees of freedom [17]. Therefore, during the past few decades, researchers have developed multiscale computational methods, by which numerical simulation of large engineering problems is feasible within a reasonable amount of computational cost.

Among various multiscale models, computational multiscale homogenization methods have been studied extensively and employed sucessfully for the simulation of different heterogeneous materials. Multiscale homogenization method is a hierarchical approach, in which at least two length scales are considered simultaneously. At the lower scale, the heterogeneous structure of the material is simulated explicitly in a certain volume, the Representative Volume Element (RVE), which carries complete information of the internal structure [18–21]. At the macro-scale, the material is considered to be homogeneous, and during the analysis information flows between the two scales [22,19,23]. In this approach, the macroscopic material domain is discretized by finite elements, and a single RVE is assigned to each Gauss point of the macroscopic finite elements. At each computational step, strains at macro-level are imposed as essential boundary conditions to the corresponding RVE, and the solution of the RVE boundary value problem is then averaged for the calculation of the associated macroscopic stress tensor. The Asymptotic Expansion Homogenization (AEH) is a similar but more rigorous mathematically and it exploits the asymptotic expansion of the displacement field considering a length scale parameter representing the ratio of the material heterogeneity length scale to the macroscopic one [24,25]. Fish et al. [26] presented a generalized formulation for this approach and introduced the Generalized Mathematical Homogenization (GMH) for the homogenization of atomistic systems. Based on GMH, Rezakhani and Cusatis [27,28] derived a homogenization scheme for discrete models featuring both translational and rotational degrees of freedom.

Coarse Graining (CG) methods are another class of multiscale methods for reducing the computational cost of discrete fine-scale models. The method is based on converting a model with large number of degrees of freedom into a model with a reduced number of degrees of freedom but with the same mathematical and computational structure. The computational gain of CG is two fold: (1) the decrease of the number of degrees of freedom leads to fewer calculations per time step, and (2) the increase of the spatial resolution of the system allows larger stable time step in explicit solvers [29]. CG is widely used in the field of atomistic simulations and molecular dynamics [30,31]. CG models can be formulated relatively easily for homogeneous atomistic systems, consisting of a repetitive structure. Furthermore, heterogeneous atomistic models for materials such as protein-based materials, can be coarse grained if they are homogeneous at the meso-scale, which means that the local effects are negligible and they produce nearly homogeneous global behaviors [32]. There is a wide literature relevant to coarse-graining methods to which the reader is referred to for additional information [33–43].

In the study presented in this paper, multiscale homogenization and coarse-graining are combined, and a Homogenization Coarse Graining (HCG) framework is presented. The homogenization algorithm recently developed by Rezakhani and Cusatis [27,28] is employed to obtain the effective response of the fine-scale model with actual particle size as well as the CG model with enlarged particles. These effective responses of the fine-scale and CG RVEs are then used by an automatic parameter identification technique based on the nonlinear least square method to calibrate the CG LDPM parameters. Finally, several numerical examples are performed by the both LDPM and tCG LDPM to verify accuracy and effectiveness of the developed framework.