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An efficient morphology generation and level set representation of cementitious microstructures with arbitrarily shaped aggregates and cracks via extended finite elements

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ABSTRACT

Concrete has a random and complex microstructure, the mesh generation of which could be challenging and time-consuming. This research presents a numerical procedure for morphology generation and level set representation of realistic cementitious microstructures without meshing the internal material interfaces. Central to the proposed numerical method is the exploitation of a vector level set function in the description of arbitrarily shaped aggregate inclusions, which allows bypassing the orthogonal projection operation on the inclusion interface as well as the determination of the outward normal. The proposed level set method is then coupled to the extended finite element method to simulate crack propagation in cement-based materials. To realistically simulate the microstructure of concrete, an improved approach that is capable of reproducing the complex geometric shape and surface texture of aggregates is proposed. To enhance the computational efficiency, a packing algorithm that mimics the settling of soil particles and enables dense aggregate packing patterns is developed to speed up the process of placing the generated aggregates into representative volume elements. After that, a series of numerical experiments are conducted to evaluate the accuracy and efficiency of the new technique. The evaluation demonstrates the effectiveness and potential of the proposed method.

1. Introduction

Concrete plays a pivotal role in the construction industry. As one of the most durable and versatile building materials in the world, it furnishes the built structures with the resistance to diverse natural and manmade forces. With the advancement of computing capabilities, it is now possible to zoom in and take a closer look at the microstructural deformation and evolution of the concrete material in complex mechanical, chemical, and thermal environments and study the physical mechanisms underlying many phenomena of the concrete material that are hard to be experimentally explored. The development of robust and reliable numerical methods for better characterization and simulation of the concrete material thus becomes increasingly important. Commonly, such characterization and simulation is carried out by performing micromechanical analyses of concrete on a representative volume element (RVE) using numerical methods such as the finite element method (FEM). The FEM is a powerful computational technique that has been extensively utilized for obtaining approximate solutions to partial differential equations (PDE). The technique solves the problem by dividing a complex and irregular model into smaller and regular subdomains called finite elements. However, despite its appealing features and capabilities, the FEM also have weaknesses and pitfalls. One of the major shortcomings pertaining to the FEM in modeling concrete and cementitious composites is that the traditional finite element mesh is generated such that the element boundary has to conform to the mortar-aggregate interface. However, as shown in Fig. 1b, since cementitious composites normally contain a large number of randomly distributed aggregates of complicated shape, generating the mesh for such a complex problem could be rather cumbersome. Moreover, as illustrated in Fig. 1a, due to the presence of the really thin region of the interfacial transition zone (ITZ) between the aggregate and the cement paste, an extremely dense mesh is usually needed around this thin region, which may involve an enormous amount of computation. In recognition of the importance of the ITZ, Dunant and co-authors [1,2], Guidoum and Navi [3] have developed numerical and experimental methods to study the effects of the ITZ on the mechanical behavior of concrete.

In light of the above limitations of the FEM, various automatic mesh generation techniques have been developed (e.g., among others, [4–8]). More recently, in a series of research works, Fries

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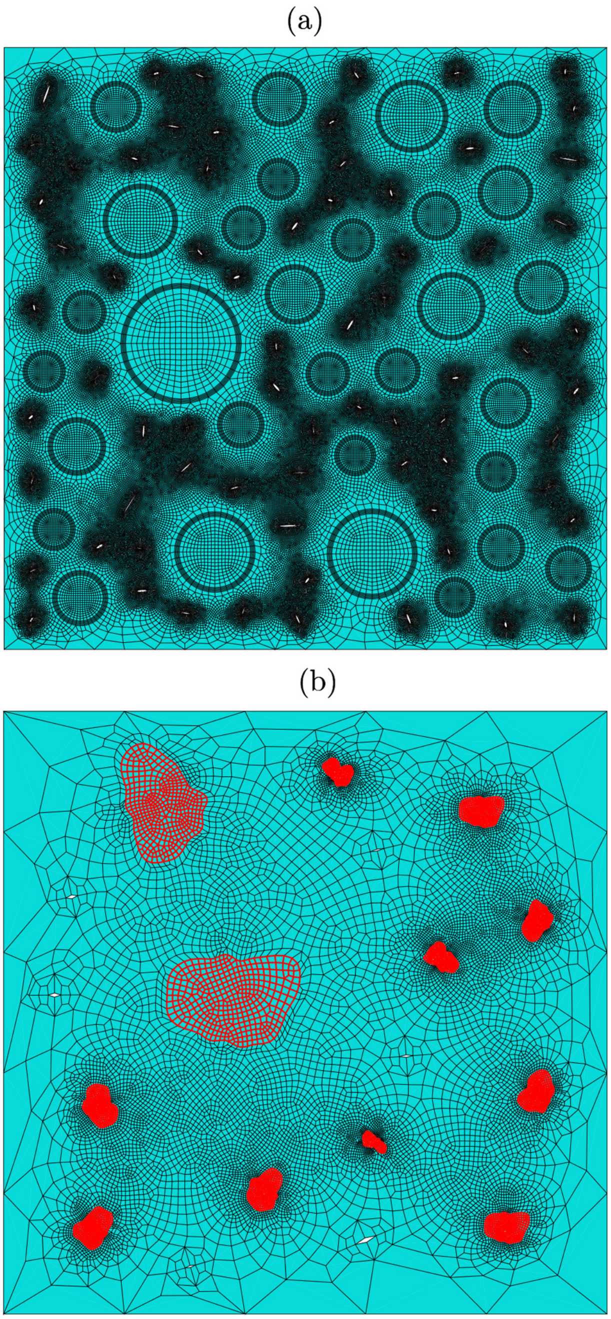

Fig. 1. Illustration of finite element meshes of cementitious microstructures with mortar, aggregates, ITZs, and voids: (a) circular aggregates generated using simplified modeling approaches. (Note that in the figure, the thin layer on the periphery of a circular aggregate is ITZ.) (b) Arbitrarily shaped aggregates generated using advanced modeling approaches. (Note that in the figure, the aggregates are highlighted in red.) (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

and co-authors [11–15], Moumnassi [16] proposed higher-order meshing of implicit geometries using the level set method. In [15], a new conformal decomposition method was also proposed. A thorough review of such method was presented by Dunant et al. in [9] and by Bordas et al. in [10]. However, it should be noted that although these mesh generation techniques provide a most valuable tool for meshing two dimensional (2D) and three dimensional (3D) domains, they could still face significant challenges for complex cementitious microstructures. Under such circumstances, the finite element mesh can be extraordinarily difficult to generate. If inappropriately handled, poor or distorted elements may occur, leading to erroneous and divergent results during the solution process. In order to successfully mesh geometrically complicated configurations and ensure smooth transition at the material interfaces, significant computational efforts and care are needed. Motivated by the aforementioned challenges, a number of new numerical techniques addressing the meshing issues posed by the FEM have appeared in the literature. One of the alternatives that can reduce the burden of mesh generation in the FEM is the boundary element method (BEM) (e.g., among others, [17,18]). Compared to domain discretization techniques such as the FEM, in the BEM, only the boundary of the domain has to be discretized, thus significantly trimming down the computational cost. But this advantage could be lost in handling nonlinear problems, where domain discretization might still be needed. Following a different route, meshless methods (MM) that are intended to bypass the mesh generation process have been developed to remedy the meshing issues posed by the FEM. Examples include, but are not limited to: the smoothed particle hydrodynamics (SPH) [19,20], the element free Galerkin method [21], the meshless local Petrov-Galerkin method [22], the meshless Hp-cloud method [23,24], the partition of unity finite element method (PUFEM) [25], the method of finite spheres [26]. In addition to BEM and MM, other novel numerical methods have also been proposed, which include the scaled boundary finite element method [27], the natural neighbor Galerkin method [28], the isogeometric analysis (IGA) [29], the finite cell method [30], and the extended finite element method (XFEM) [31–38].

In particular, by integrating the FEM and the PUFEM, the XFEM offers an attractive option for numerical modeling of cementitious microstructures. The XFEM has also been applied to many diverse fields for a variety of problems. For instance, recovery approaches for error estimation [39,44,45], residual approaches [40–42,46], and original a posteriori error treatments for the generalized FEM [47,48] have appeared in the literature. Within the framework of recovery based approaches, the role of statical admissibility of the fields was examined in [43]. On the other hand, goal oriented error measures were considered in [50–54]. A summary and comparison of these approaches is referred to [49]. The capability of the XFEM is further extended by the coupling with the level set method (LSM) [55]. A number of level set functions have been proposed in the literature for the representation of inclusions and voids (e.g., among others, [35–38]). In addition to the conventional level set methods, multiple level set modeling approaches have also been reported. For instance, significant developments were made by Moumnassi and co-authors [56,57] on the representation of sharp edges and corners in 3D by utilizing multiple level set functions that are capable of representing complex geometrical features directly extracted from computer aided design (CAD). In [36], Sukumar et al. proposed a numerical methodology to model polygonal inclusions using the LSM within the framework of the XFEM. The methodology decomposes a polygonal interface into line segments. A level set method based on the use of signed distance function is then employed to describe the polygonal interface, which involves the determination of the minimum distance between the sample point and the polygon as well as the outward normal to the interface. In case of intricate concrete microstructures with aggregates of complex shape, the minimum distance and outward normal calculation can be computationally intensive. Hence, fast and reliable level set representation methods that work for complex microstructural geometries are needed.

In addition to the difficulties faced in meshing complex concrete microstructures, the realistic representation and simulation of concrete microstructures also requires the consideration of a number of essential issues. First, the shape and surface texture of the aggregates can exert substantial impact on the strength and material properties of concrete (e.g., among others, [58–69]). For

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