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Particle discretization techniques for fracture simulation of concrete materials

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ABSTRACT: The fracture behavior of concrete depends on the properties and distributions of its primary phases (cement-based matrix, aggregate inclusions, and matrix-inclusion interfaces). The quality of fracture simulations at the material mesoscale, at which these phases are explicitly modeled, depends largely on the discretization strategy. This paper describes a Voronoi-based discretization procedure for fracture simulations of particulate materials such as concrete. Attention is given to the discretization of individual particles, assumed to be convex polyhedra, within the material domain. Explicit modeling of the matrix-inclusion interface enables more realistic simulations of inclusion debonding. The dependence of interface fracture on particle shape is demonstrated using a lattice-based simulation approach.

1 INTRODUCTION

The fracture behavior of concrete is strongly related to geometrical and mechanical properties of the aggregates and their interface with the surrounding matrix. At subcritical load levels, fracture in ordinary concrete consists mainly of debonding along the interfacial zones. This microcracking sets the stage for the various toughening mechanisms that become active in the post-peak stages of loading.

For mesostructural models of concrete, the size, shape, and distribution of aggregates are drawn directly from the physical structure of the material. This is in contrast to conventional continuum models, in which material heterogeneity is represented in an average sense. Capable simulation models are needed to study the mechanism of interface debonding amidst multiple cracking, as well as the toughening mechanisms caused by interactions between neighboring particles. Such simulations rely on an appropriate level of discretization and controllable degree of heterogeneity within the modeling framework.

Starting with Le Béton Numérique (Roelfstra et al. 1985), various simulation models have been developed to study fracture behavior at the concrete mesoscale (Schlangen & van Mier 1992, Cusatis et al. 2003). Developments in computing technology have enabled, in recent years, three-dimensional simulation of mesoscale fracture. Carol et al. (2001) and Caballero et al. (2007) used zero-thickness interface elements to investigate the fracture patterns of concrete materials with angular particles. Yip et al. (2006) studied the toughening mechanisms of concrete using a lattice model of spherical particles embedded within a mortar matrix. Recent calculations of the authors have shown that the sphere and angular shape inclusions exhibit quite different debonding behaviors.

This paper describes a novel Voronoi-based approach for discretizing concrete at the mesoscale, where the material is regarded as a three-phase composite composed of a mortar matrix, aggregate inclusions, and matrix-inclusion interfaces. Fracture simulations are based on an irregular lattice model of the three-phase composite, in which the Voronoi tessellation serves to define both the lattice topology and properties of the lattice elements. Interface debonding is simulated for an angular particle embedded within a material subjected to far-field tension. As a step toward studying the interaction of developing cracks within particulate materials, the mesostructure of concrete is discretized as sets of multiple particles.

2 STRUCTURE GENERATION

2.1 *Voronoi discretization*

Voronoi tessellation of a set of points is an increasingly popular means for partitioning a domain into a collection of cells. In this research, points are inserted in the problem domain by the process of Random Sequential Addition (RSA) (Widom 1966). Point insertion relies on knowing the domain dimensions and a minimum allowable distance l_m between neighboring points. With an increasing number of trial points, the problem domain eventually becomes saturated with points (i.e., no additional points can be inserted). Figure 1 shows an internal view of Vo-

ronoi cells produced from a saturated point set. The motivations for pursuing point saturation include the ability to:

- economize on the number of points needed for accurate solutions of the elastic problem;
- effectively grade nodal point density by setting l_m as a function of the spatial coordinates;
- maximize the degree of uniformity of the cell volumes; and
- effectively discretize nonconvex domains of elementary geometry.

2.2 *Polyhedra generation*

The Voronoi diagram can be used to generate a variety of shapes and sizes of particles, each of which is a convex polyhedron. Uniform distributions of spatial points form mono-shape/size Voronoi cells, whereas a variety of shapes/sizes can be obtained by changing the degree of regularity of point allocation. As seen in Figure 1, the characteristic of irregular angularity, which is exhibited in crushed rock, becomes available. Such polyhedra are henceforth used to define aggregate geometry for the purpose of simulation. While the generation of such polyhedra is computationally inexpensive, other important aspects of the shape of actual rock (e.g., concavity, surface texture) are not considered by this simple treatment of geometry.

Within morphology-based approaches, the geometric features of the actual materials should be reflected in the models. Aggregate shapes can be surveyed using data acquisition systems. Figure 2 shows three representations of a granite aggregate. The surface points and their triangle network (obtained using a three-dimensional, non-contact laser scanner) show the typical complexity of actual aggregate (e.g., irregular shape, local concavity). The construction of Voronoi-based representations for such shapes is not straightforward. This is ongoing work of the authors.

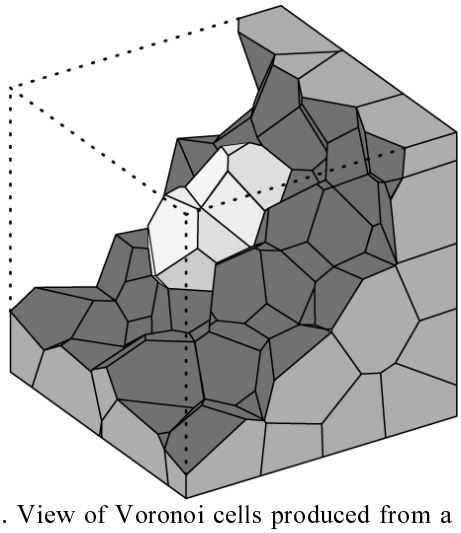

Figure 1. View of Voronoi cells produced from a saturated point set.

2.3 *Particle subdivision*

The procedure described in section 2.1 can be used to discretize a spherical particle of radius r embedded in a matrix material. The point insertion process involves:

- defining the particle-matrix interface by introducing *ij* point pairs along the radial direction, as shown in Figure 3a. Point i (representing the particle) is positioned at a distance $r - t/2$ from the center of the particle, whereas point j (representing the matrix) is positioned at a distance $r + t/2$, where t is the interface thickness. Such pairs of points are randomly inserted to discretize the interface. Here, too, point saturation is accomplished by maintaining a preset l_m between neighboring pairs of points. The l_m constraint is not enforced between the points forming each pair. The collection of resulting Voronoi facets tiles the interface with controllable thickness t (Fig. 3b).
- randomly inserting points both inside and outside the spherical region, maintaining distance l_m between neighboring points.

This technique can be extended to discretizing polyhedral particles, such as that shown in Figures 1 and 4a. A process of sequential point insertion defines the geometry of each polyhedron. First, sets of four points are inserted to define each vertex of the polyhedron. These (one interior and three exterior) points define the three planes that meet at a polyhedron vertex. Next, each edge of the polyhedron is defined by sets of three (one interior and two exterior) points positioned along the edge using the process of RSA. Similarly, each face of the polyhedron is constructed with randomly placed pairs of (one interior and one exterior) points. Random filling of the polyhedron interior and the surrounding

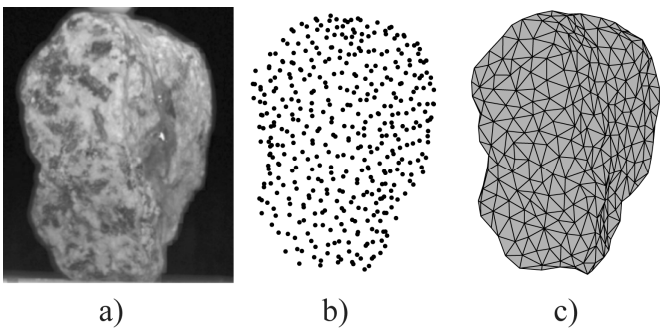

Figure 2. Aggregate surface representations: a) digital image; b) point cloud; and c) corresponding surface triangulation.

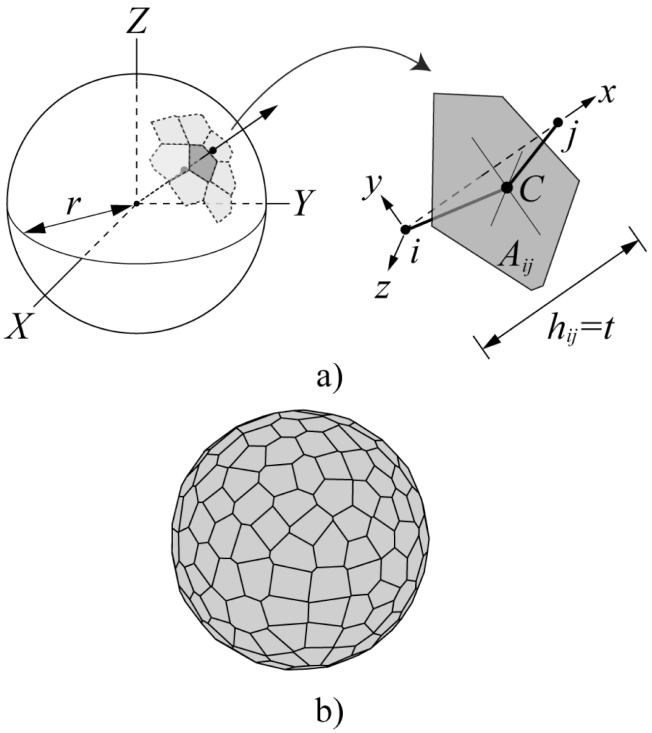

Figure 3. Point generation of surface of a spherical particle and its corresponding Voronoi facet with enlarged view of basic lattice element at the interface; b) Voronoi discretization produced from a saturated point set.

matrix occurs only after the sequence of features (vertex, edge, and face) construction has been completed. Details of this process will be described in a forthcoming paper.

3 ANALYSIS METHOD: LATTICE MODEL

Topology of the lattice network is defined by the dual Delaunay tessellation of the nodal points. Each lattice element *ij* is composed of a zero-size spring set located at the area centroid *C* of the corresponding Voronoi facet (Fig. 3a). Each node has three translational and three rotational degrees of freedom. The spring set (not shown in the figure) is composed of three uniaxial springs, oriented normal and tangential to the Voronoi facet, and three rotational springs about the same local axes. Due to the Voronoi (A_{ij}/h_{ij}) scaling of the spring constants, the lattice is elastically homogeneous under uniform modes of straining. This Voronoi-based lattice also provides energy conserving, grid size insensitive representations of tensile fracture. Details and indications of model accuracy are given elsewhere (Bolander & Saito 1998, Berton & Bolander 2006, Yip et al. 2006).

4 APPLICATION EXAMPLES

4.1 *Debonding of matrix-particle interface*

Consider the angular particle shown in Figure 4a, which is assumed to be embedded within a cubic domain under uniaxial tension in the vertical direction. Both the particle and surrounding matrix materials are discretized via the aforementioned Voronoi-based procedure. The simulation considers a three-phase material (i.e., the particle-matrix interface is also discretized). A weak interface is assumed for representing this porous interfacial transition zone (ITZ); the inclusion is treated as a relatively stiff material, as is the case for normal strength concrete.

Debonding of the angular particle is shown in Figure 4b. The sequence of breaking elements is indicated by the darker gray shading of corresponding Voronoi facets. Interface fracture initiates within the upper part of the particle and then propagates downward toward the particle mid-region. This failure pattern is similar, yet different in the local stress conditions causing fracture, to that of a spherical particle (Asahina et al. 2009).

4.2 *Representing multi-particle systems*

The discretization approach is extended to modeling multiple particles within the material domain. Particles are first discretized by the procedure discussed in section 2.3, then a process of random insertion is carried out without overlapping previously positioned particles and the domain boundaries. A constant l_m is used for all particles so that nodal density is fairly uniform regardless of particle size. For comparison purposes, spherical and polyhedral particles are considered.

The size distribution of spherical aggregate can be set by a grading curve, such as the Fuller curve. Defining the sieve size of the polyhedral aggregates is less straightforward, since the cross-section area through the polyhedron centroid depends on particle shape and orientation. For the sake of expediency,

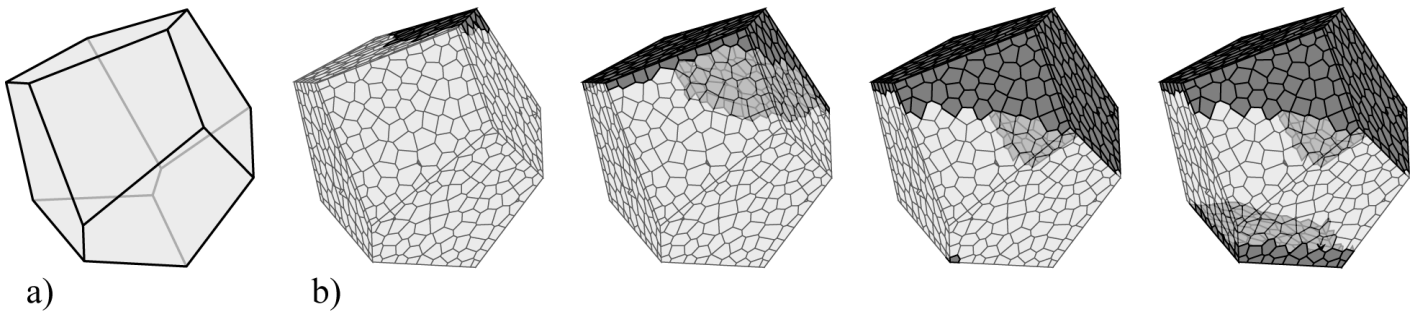

Figure 4. a) Referenced polyhedral particle, and b) evolution of debonding along the particle-matrix interface.

the effective diameter of a polyhedral particle is set equal to the diameter of a sphere of equivalent volume.

Figure 5 shows graded distributions of subdivided aggregates for both cases without depicting the discretized matrix phase. Repetitive use of a single polyhedron, at different orientations, has been used in the construction of Figure 5b. The gray shading reflects the size of polyhedron, in which darker grays have been used for larger size particles. This differential shading adds depth perception to the figures. The mortar cube dimension is 40mm and the largest sphere has diameter d_{max}= 20mm. The distribution of sphere diameters in the Fuller curve is discretized as follows: d=20, 16, 12, 10, 8, 6, and 5mm. The resulting volume fractions are 51.2% and 45.7% for the spherical and polyhedral particles, respectively. In both cases, the target volume fraction of the Fuller curve can not be achieved due to the restricted nature of the process of fixing particle position. A number of methods have been studied to achieve denser packings of the aggregates. Dynamic mixing processes have been used to obtain concrete mesostructures with a dense random-packing (Stroeven 1999). Effective search with a common plane algorithm is used to accelerate the detection of the contact with neighboring angular particles (Nezami et al. 2004). Digital approaches have been employed to avoid the difficulties of collision search (Jia & Williams 2001). Such approaches could be applied here.

In this research, discretized particles are sequentially introduced into the domain prior to random serial insertion of mortar matrix nodes. This approach is convenient for discretizing regions around fairly dilute concentrations of particles for which the ITZ of neighboring particles does not overlap. However, percolation clusters are formed in higher density packings, for which additional detailing of the overlapping ITZ of contiguous particles is required. Such details have been established for the simulation of interface flow through spherical particulate media, where the percolated ITZ acts as a channel for moisture transport (Bolander et al. 2007). Current efforts involve discretization of the intersections and overlapping of ITZ of different angular particles, in which, more geometrical features (e.g., corners, edges) exist.

5 CONCLUSIONS

This paper discusses the development of versatile techniques for discretizing convex particles, which are used in the representation of concrete mesostructure. Voronoi-based strategies subdivide the particle and provide an explicit representation of the particle-matrix interface. In particular, interface thickness is an adjustable model parameter. Two applications, where such Voronoi-based discretization is applied, are presented to demonstrate potential improvements in the quality of fracture simulations at the concrete mesoscale. Inclusion geometry affects the local progression of debonding along the particle-matrix interface. In extending this work to modeling actual concrete systems, several difficulties are anticipated. These include the meshing of densely packed inclusions, for which the ITZ of different particles can overlap in a complicated manner, especially for the

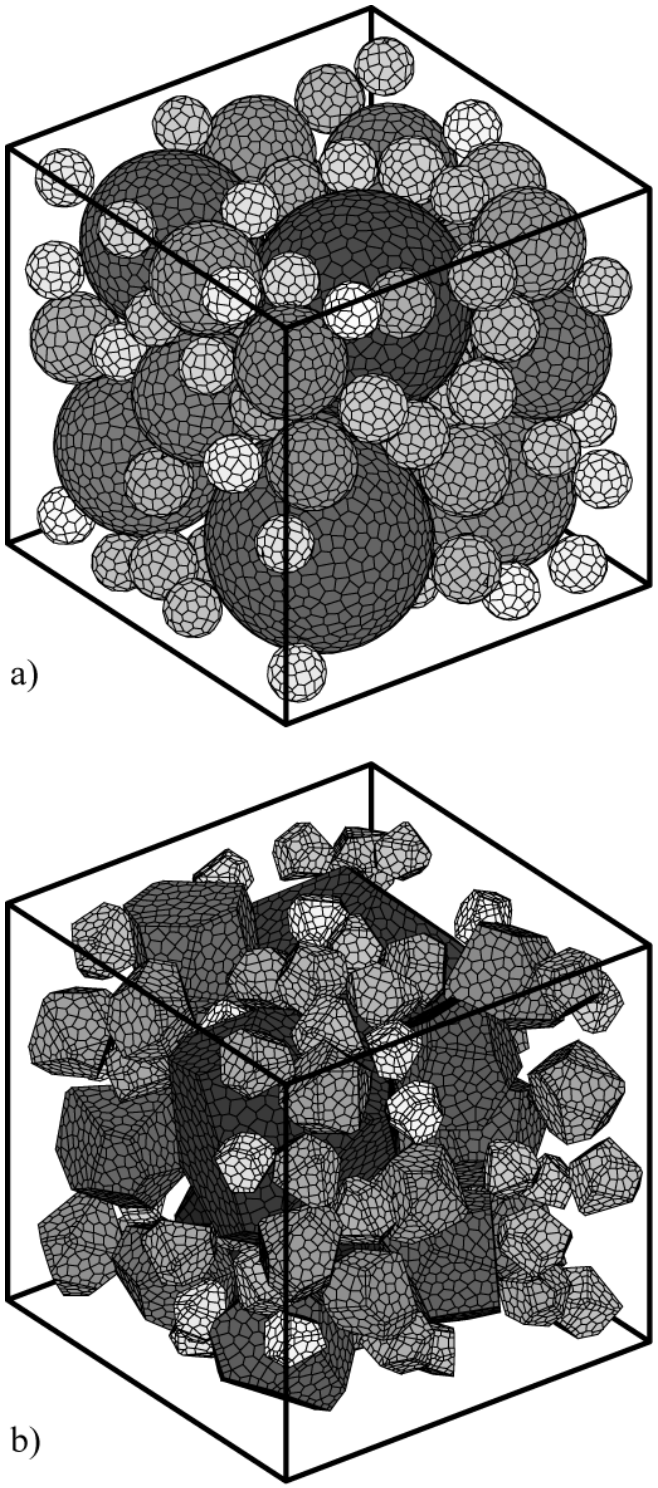

Figure 5. Graded distribution of: a) spherical; and b) convex polyhedral inclusions.

general case of non-spherical particles. The computational expense associated with large three dimensional simulations is also an issue.

ACKNOWLEDGEMENT

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