FRACTURE IN MULTIPHASE PARTICULATE MATERIALS: LATTICE MODELING ISSUES

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ABSTRACT

An irregular lattice model is developed to simulate fracture in softening materials with multiphase mesostructure. Lattice elements are defined on the edges of the Delaunay tessellation of an irregular set of points positioned in the material domain. The dual Voronoi tessellation is used to scale the elemental stiffness terms, in a manner that renders the lattice model elastically homogeneous. A cohesive description of fracture is introduced to obtain energy conserving, grid-insensitive descriptions of cracking in homogeneous materials. These fundamental, essential requirements of the model are verified, in preparation for simulating fracture in multiphase particulate materials, such as cement-based composites.

1 INTRODUCTION

Lattice models are composed of simple, one-dimensional mechanical elements connected on a set of nodal points that is either regularly or irregularly distributed in space. The primary justification for such models comes from the discontinuous structure of matter at a very small scale, where material can be regarded as a collection of particles held in equilibrium through forces of interaction. Lattice models are also useful in studying the behavior of various materials at coarser length scales, with interest in the effects of disorder and breakdown under loading [1-5].

Some fundamental aspects of lattice models are most evident when studying their abilities to represent a homogeneous continuum. For this reason, the lattice model presented in this paper is first applied toward modeling the elasticity and fracture of homogeneous materials. The lattice model, which is based on the concept of a Rigid-Body-Spring Network (RBSN) [6,7], is elastically homogeneous under simple modes of straining and provides grid insensitive representations of fracture in softening materials. These results serve as a starting point for modeling fracture in multiphase particulate materials.

2 IRREGULAR LATTICE MODEL

2.1 Domain discretization and lattice element description

Connectivity of the lattice elements is defined by the Delaunay tessellation of an irregular set of points, which are distributed within the material domain (Fig. 1). These points act as the lattice sites or nodes. The Voronoi diagram, of the same point set, partitions the domain into a collection of cells, each of which is a convex polyhedron. The geometry of the cell facets serves to define the elastic and fracture properties of the lattice elements.

Lattice element *ij* is composed of a zero-size spring set, located at the area centroid (point *C*) of the Voronoi facet common to nodes *i* and *j*, and rigid arm constraints that link the spring set with the nodal degrees of freedom (Fig. 2a). This concept of a rigid-body-spring model was first developed by Kawai [8]. In this three-dimensional setting, each node has three translational and

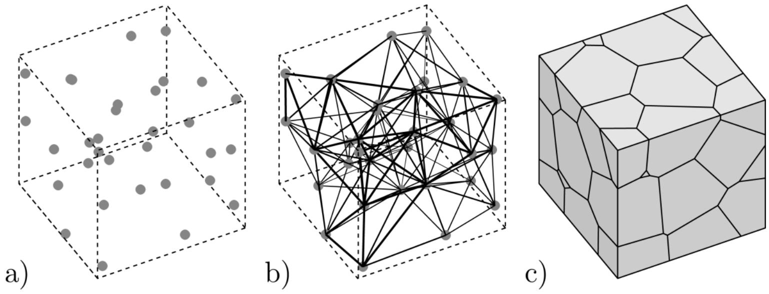


Figure 1 – Lattice model construction sequence: a) irregular point set; b) Delaunay tessellation; and c) Voronoi diagram

three rotational degrees of freedom. The spring set (not portrayed in the figure) consists of three uniaxial springs, oriented normal and tangential to the facet, and three rotational springs about the same local axes. The uniaxial and rotational springs are assigned stiffness coefficients:

$$k_n = k_s = k_t = E\frac{A_{ij}}{h_{ij}}, \quad k_{\phi n} = E\frac{J_p}{h_{ij}}, \quad k_{\phi s} = E\frac{I_{11}}{h_{ij}}, \quad k_{\phi t} = E\frac{I_{22}}{h_{ij}} \tag{1}$$

where A_{ij} is the facet area; h_{ij} is the element length; E is the elastic modulus; J_p is the polar moment of inertia; and I_{11} and I_{22} are the two principal moments of inertia of the facet area.

2.2 Fracture model

The RBSN modeling of fracture is based on the crack band concept of Bazant and Oh [9]. In general, loading of an element will be skew to the element axis ij. The normal and tangential springs are activated and, for tensile loading of the material, the normal spring will be in tension (Fig. 2b). The fracture criterion is based on the following measure of stress

$$\sigma_R = \frac{F_R}{A^p_{ij}} \tag{2}$$

where F_R is the resultant of the spring forces acting on the element facet and A^P_{ij} is the projection of the facet area on a plane perpendicular to the direction of F_R (Fig. 2b). Within each computational cycle, the ratio $\sigma_R/\sigma(w)$ is computed for all of the elements, where the cohesive stress $\sigma(w)$ is a bilinear function of the crack opening displacement w (Fig. 2c). A prismatic crack band develops within the element with $\max(\sigma_R/\sigma(w)) > 1$. The width of this crack band is $h_{ij}\cos\theta$, where θ is the angle between the facet normal and the resultant force F_R. Crack opening displacement is related to the fracture strain ε_R over the crack band:

$$\varepsilon_R = \frac{w}{h_{ij}\cos\theta} \tag{3}$$

For a critical element, fracture involves an isotropic reduction of the spring stiffnesses and an associated release of spring forces, so that σ_R follows the material softening relation. The release of spring forces causes an imbalance between the external and internal nodal force vectors, which is corrected through conventional equilibrium iterations. A maximum of one element spring set is modified per iteration cycle, as is common for lattice models [1]. The modeling of fracture differs from that of conventional lattice models in several respects: 1) fracture can form at angle θ to the element axis; and 2) element breaking is a gradual process that conserves energy in association with a cohesive softening relation.

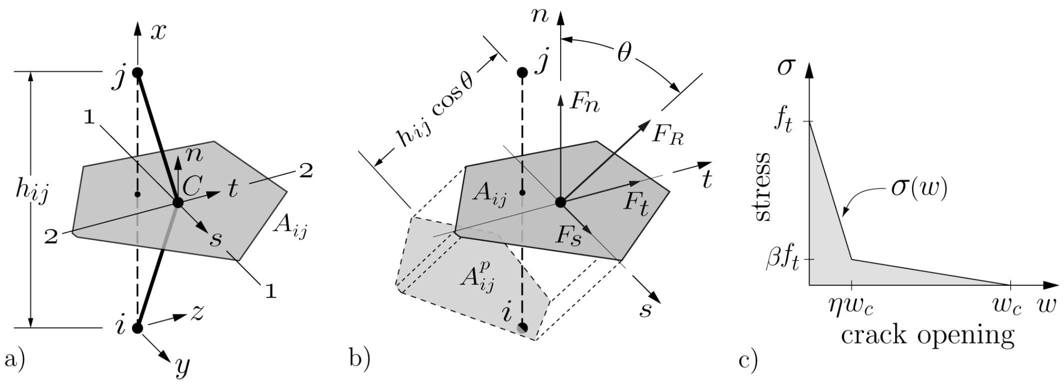


Figure 2: a) Lattice element *ij*; b) resultant force on element facet; and c) cohesive crack relation

3 MODELING FRACTURE OF HOMOGENEOUS MATERIALS

Some basic properties of lattice models are evident when studying their application to modeling the elasticity and fracture of homogeneous materials. Consider a rectangular prism of homogeneous material under uniaxial tensile loading. The prism has cross-section area A and tension softening properties as shown in Fig. 2c. Prior to cracking or other nonlinear behavior, the axial displacement of any point in the prism is $u = \varepsilon X$, where X is the position of the point in the direction of the prism axis and ε is the axial strain, which is constant over the prism length. Figure 3a shows an irregular lattice model of the prism, where the nodes associated with the $+X$ and $-X$ faces of the Voronoi diagram have been assigned displacement the boundary condition $u = \varepsilon X$. The model strains uniformly, so that the unconstrained nodes within the midsection of the model displace accordingly, with relative error $e_r = 7.02\text{x}10^{-8}$ where

$$e_r = \frac{\|u - u^h\|_2}{\|u\|_2}\ , \qquad \|u - u^h\|_2 = \sqrt{\sum_{I=1}^{N} \left(u(X_I) - u^h(X_I)\right)^2}. \tag{4}$$

Displacement u^h is the numerical solution and N is the number of unconstrained lattice nodes. The small relative error indicates the irregular lattice, based on the Voronoi scaling of the stiffness coefficients given in eqn (1), provides an elastically homogeneous representation of the material for this simple mode of straining. The stress σ_R is uniform throughout the specimen model and, for increasing axial load, reaches the tensile strength f_t in all elements simultaneously. A small reduction of the tensile strength value in any one element initiates fracture within that element.

From the point of fracture initiation, fracture propagates through the cross-section and the material separates (Fig. 3b). In Fig. 3c, average stress σ and axial displacement δ have been normalized to better indicate that the cohesive softening curve, used as input to the model, is manifested at the structural scale. The separation process involves only two nodes per element; this facilitates the transition from continuous to discontinuous behavior and avoids significant stress locking.

If the crack band is constrained to form normal to the element axis (σ_n criterion), as would be the case for a central force spring lattice, the model response is not a direct reflection of the softening curve. There are two main sources of error: 1) the magnitude of the stress component aligned with the element axis, σ_n, is less than the average axial stress $\sigma = P/A$, unless the element is aligned with the direction of tensile loading; and 2) after fracture initiation, the component of

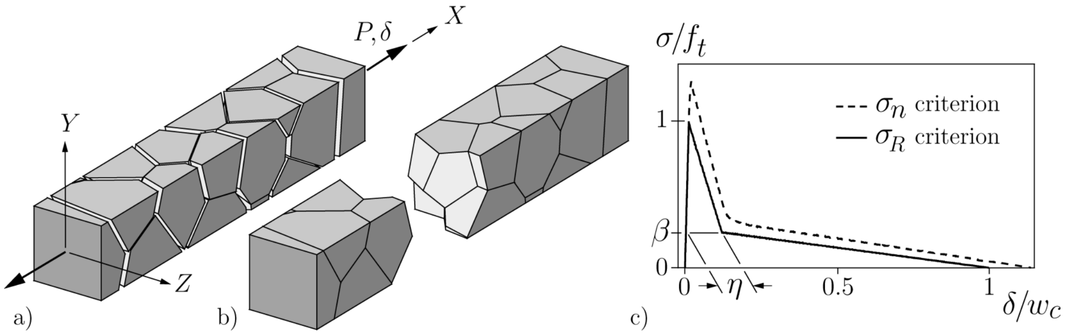


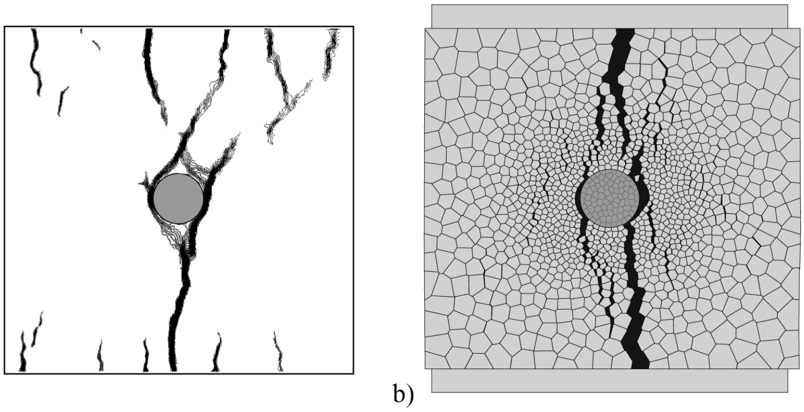
Figure 3 - Uniaxial tension test simulation: a) uniform straining; b) traction free crack condition; and c) load-displacement response curves

crack opening in the direction of the element axis is smaller than that in the direction of loading. These two sources of error combine to produce excess strength and energy consumption, as seen in Fig. 3c, which can be viewed as a form of stress locking. Even for the classical lattice approach (where element softening is not considered), the first of these sources of error would still be present. A third source of error involves the possible use of non-Voronoi scaling of the stiffness terms. If each of the lattice elements is assigned a constant area, then the relative error in displacement expressed by eqn (4) becomes $e_r = 1.83 \times 10^{-1}$. In general, irregular lattices exhibit this type of artificial heterogeneity [10], which can strongly affect the modeling of fracture. Under this condition, fracture initiates in the model well below the load level given by $\sigma = f_t$.

4 MULTIPHASE MATERIALS - MODELING ISSUES

At the mesoscale of cement based composites, for example, three phases are evident: a mortar matrix, aggregate inclusions, and the matrix-inclusion interface. In the lattice modeling of such multiphase materials, the common approach is to map the material mesostructure, or its statistical equivalent, onto the lattice so that each element is associated with a particular material phase [2,5]. The matrix and inclusion phases are often assumed to be homogeneous and isotropic, so that the results of the previous section are directly applicable; the lattice representation of the interface is generally coarse and should have directional properties to reflect local material structure.

Stress distributions around the inclusions are significantly influenced by Poisson ratio effects, particularly when there is a strong mismatch in the elastic properties of the inclusion and matrix phases [7]. Due to the one-dimensional nature of lattice elements, lattice models are at a disadvantage in modeling Poisson effects. A limited range of macroscopic Poisson ratio can be modeled by the regular arrangement of lattice elements or the adjustment of element stiffness coefficients, but a local realization of Poisson effect is not obtained. The RBSN is able to model a range of Poisson ratio, but at the expense of introducing artificial heterogeneity into the material model. An alternative hybrid approach, which combines the RBSN and finite element technology, has been developed to exactly model both elastic constants [7], although the modeling of fracture becomes more complicated. Figure 4 compares experimental and numerical crack patterns developed in a mortar panel with a stiff cylindrical inclusion. In the experimental program [11], the specimen was subjected to uniaxial compression by displacement controlled loading, with minimal lateral restraint due to the load platen surfaces. The failure pattern observed during testing was measured using Digital Image Correlation (DIC), which provides high-resolution mappings of



a) b)

Figure 4 – Vertical splitting of mortar panel with stiff inclusion: a) localization of surface displacements measured using Digital Image Correlation [11]; and b) planar lattice simulation

specimen surface displacements. In Fig. 4a, only the closely spaced contour lines, indicating surface displacement localization, are shown. In the lattice model of the specimen, fracture initiated along the weak interface and ultimately exhibits a pattern similar to that witnessed during testing, including the shear cones that develop above and below the stiff inclusion.

Softening at the macroscale is the result of various toughening mechanisms active in the fracture process zone, which extends over a finite volume of the mesostructure. Such toughening mechanisms were first demonstrated with planar lattice models [2]. However, it is clear that three-dimensional models are necessary for realistic modeling of both the material structure and the toughening mechanisms [4,5]. At the mesoscale, fracture events are thought to be brittle, so that the conventional lattice approach (in which fractured elements are removed from the lattice) is applicable. However, most of the modeling issues discussed in section 3 are still relevant.

With adequate resolution of the mesostructure model, various phenomena can be simulated, including those related to the geometry and distribution of the phases. For simulations where the crack direction is known in advance, a finer mesh can be used in that region (Fig. 5). However, the degree of model refinement is limited by several factors, including available computing resources and our abilities to measure properties at small scales.

5 CONCLUSION

This paper examines the performance of an irregular lattice model for arguably the most basic of material types and loading conditions: isotropic, homogeneous materials subjected to uniaxial tensile loading. Nonetheless, the fundamental properties of lattice models are most evident under such conditions. For the lattice model described here, the scaling of element stiffness terms is based on a Voronoi discretization of the material domain and provides an elastically uniform description of the material under uniform modes of straining. The energy dissipation mechanisms active at finer scales are lumped into a macroscopic cohesive crack relation. In contrast to classical lattice models, element breaking is gradual and governed by rules that provide an energy conserving representation of fracture through the irregular lattice. The objective representation of fracture in homogeneous materials is prerequisite for modeling fracture of multiphase particulate materials, which is ongoing work of the authors.

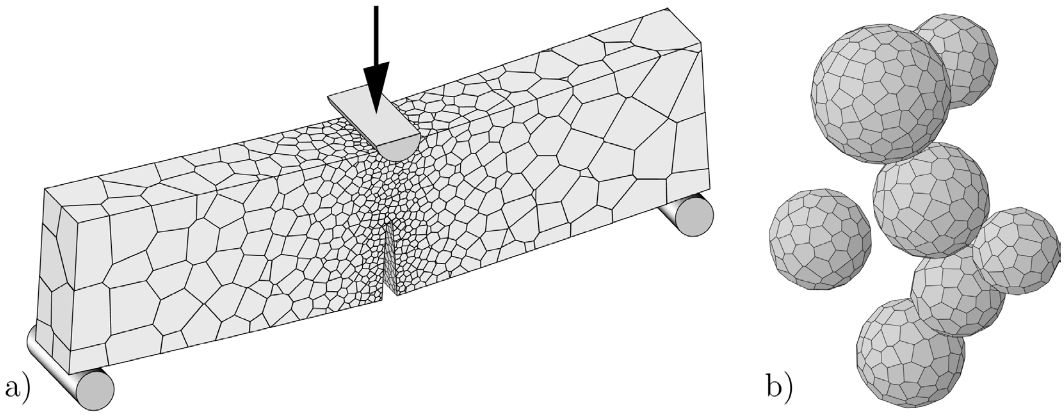


Figure 5: a) Three point bend test of notched concrete beam; b) modeling of spherical inclusions

ACKNOWLEDGEMENT

This work is part of an ongoing research project on modeling overlay systems made of fiber-reinforced cement composites, supported by the US National Science Foundation through grant (CMS-0201590) to the University of California at Davis.

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