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PARTICLE MODEL FOR FRACTURE AND STATISTICAL MICRO-MACRO CORRELATION OF MATERIAL CONSTANTS

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Abstract

The paper presents a brief overview of several recent studies at Northwestern University. An efficient type of random particle model, representing a special case of the discrete element method, is presented, used to determine the correlation between micro and macro fracture characteristics, and applied to the simulation of quasibrittle fracture. The particle locations are generated randomly and the mechanical behavior is characterized by a triangular softening force-displacement diagram for the interparticle links. An efficient solution algorithm based on replacement of stiffness changes by inelastic applied forces is formulated. The size effect method is used to determine the dependence of the mean values of the macroscopic fracture energy and macroscopic effective fracture process zone length on the dominant particle spacing, microductility, and the mean value and standard deviation of microstrength. In closing, an application of the dynamic version of the model to the breakup of a plate caused by in-plane impact is described.

1 Introduction

The discrete element approach based on the particle representation of mechanical systems was initiated by Cundall (1971). His distinct element method was extended to the study of microstructure and crack growth in geomaterials with finite interfacial tensile strength by Zubelewicz (1980) and Plesha and Aifantis (1983). Zubelewicz and Bažant (1987) studied a particle model equivalent to a lattice whose links transmit not only axial forces but also shear forces proportional to joint rotations, and showed such a model can simulate a wide fracture process zone and gradual post-peak softening. Their approach was modified and refined by Bažant et al. (1990), who used it to study the size effect on the nominal strength and on the post-peak slope of load-deflection diagrams. Observing that the macro-fracture energy can hardly be determined by summing up the energies dissipated by fractured interparticle links, they showed this is possible by the size effect method. In contrast to Zubelewicz and Bažant, the particles were assumed to have only axial interactions as in a truss. A variant of the lattice model whose links transmit not only axial forces but also shear force proportional to joint rotations was successfully used by Schlangen and van Mier (1992) in simulations of various failure modes in concrete. In that variant, the shear transmission capability of the links was achieved by considering the links to be beams subjected to bending. The particle model was shown to be also effective for dynamic fracture problems, e.g., for large-scale simulations of an ice floe impact on a cylindrical obstacle (Jirásek and Bažant, 1995b).

The present paper extends the size effect method (Bažant, 1987) to the determination of the effective fracture process zone size in a particle system and analyzes the effect of interparticle link characteristics and microstrength randomness on the macrofracture properties. It also reviews an efficient numerical method which permits repeated analysis of large particle systems (Jirásek, 1993). This is especially important for the present random particle model, for which a large number of simulations is needed in order to obtain reliable results. A dynamic version of the model is applied to an impact problem. All calculations are performed in two dimensions but an extension to three dimensions would be straightforward.

2 Description of the model

Any regular particle arrangement necessarily results into directional bias affecting the direction of crack propagation. To construct an unbiased model, the coordinates of particle centers are randomly generated using a uniform probability density over the specimen

area with a restriction of a certain minimum distance L_{min} between any two particle centers. L_{min} is empirically chosen such that an excessive local concentration of particles be suppressed. Interaction between two particles is assumed to take place only if their centers are closer than a certain interaction distance L_{max} , reflecting particle size. This form of the interaction rule, also used by Bažant et al. (1990), is easy to implement and it generates reasonable link structures when, after some trials, a proper value of L_{max} is found.

Values of L_{min} and L_{max} should be related to some intrinsic length of the model, e.g., to the interparticle distance in a regular square array of the same particle density $L_0 = \sqrt{A_s/n}$ where A_s is the specimen area and n is the total number of particles. It is very difficult to generate random particle systems with L_{min} close to L_0 but $L_{min} = 0.8L_0$ is feasible and leads to an acceptable macroscopic uniformity of the particle arrangement. Reasonable link structures are generated with L_{max} around $1.6L_0$ (Fig. 1a).

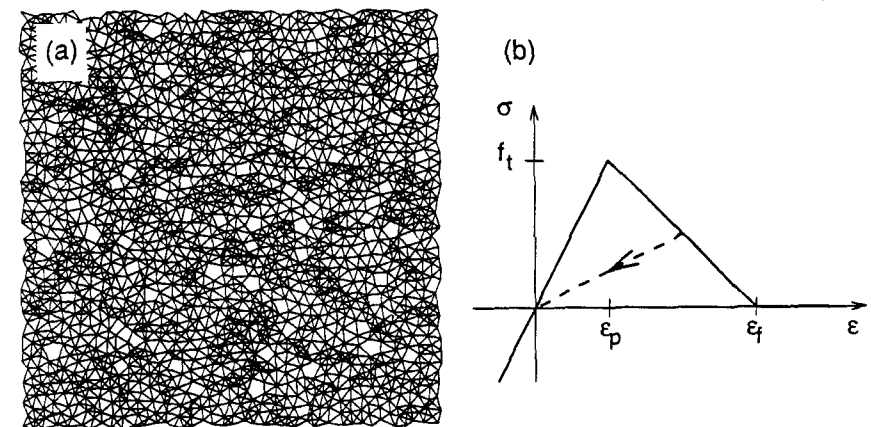


Figure 1: (a) Random lattice, (b) bilinear stress-strain diagram

The most important ingredient of a particle model used for fracture simulation is no doubt the microscopic constitutive equation, i.e., the nonlinear stress-strain law (or, equivalently, force-extension law) for an individual link. This law must be kept as simple as possible to ensure numerical efficiency and at the same time it must reflect the essential mechanical properties of the material. The simplest description of quasibrittle fracture is given by a bilinear stress-strain law with a linear elastic part and a linear softening part (Fig. 1b), which can be defined by the microscopic strength, f_t , strain at peak stress, ϵ_p , and strain at complete failure, ϵ_f .

3 Size effect method

One of the fundamental problems in micromechanical modeling of materials is the relationship between the micro- and macro-level properties. The present study focuses on two material characteristics essential for modeling of fracture processes in quasibrittle materials—the fracture energy and the effective length of the fracture process zone.

The micro-level parameter having the strongest influence on the overall ductility of the particle model is no doubt the fracture energy of the particle links, which is affected by the microstrength, f_t , and the microductility, $\gamma_f = \varepsilon_f/\varepsilon_p$.

It is important to realize that the macroscopic fracture energy G_f can by no means be evaluated by simply cutting the specimen by a straight line, counting the total energy needed to break all the links intersected by the cut and dividing it by the length of the cut. A real quasibrittle specimen never breaks along a sharp straight cut but rather develops a certain fracture process zone which propagates across the ligament. Even if we determine which links enter the inelastic range by a numerical simulation, it is questionable whether one should count the energy dissipated by all the links, or only by the links located in the fracture process zone. Moreover, it is often very difficult to simulate the fracture process up to the formation of a complete macroscopic crack passing across the entire ligament. Another problem with this definition of fracture energy is that it is not independent of the size of the specimen, its geometry and crack length.

An objective definition of the fracture energy can be given in the limit for an infinitely large body (Bažant, 1987). Bažant and Kazemi (1988) proposed an effective method to evaluate the fracture energy based on the size effect law, $\sigma_N = Bf_u[1 + D/D_0]^{-1/2}$, where σ_N = nominal strength, D = size of the specimen, and Bf_u and D_0 are adjustable parameters of the law. If the peak loads are known for several different sizes, the size effect parameters Bf_u and D_0 can be evaluated by regression analysis. The size-independent and shape-independent fracture energy G_f and effective length of the fracture process zone c_f are calculated as

$$G_f = (Bf_u)^2 \frac{D_0}{E'} g(\alpha_0), \quad c_f = D_0 \frac{g(\alpha_0)}{g'(\alpha_0)} \quad (1)$$

where $g(\alpha)$ = nondimensional function characterizing the specimen geometry, $\alpha_0 = a_0/D$ = nondimensional length of stress-free crack or notch, and $E' = E$ = Young's modulus (assuming plane stress).

4 Method of inelastic forces

The peak load for a particle system with a random particle arrangement and a random microstrength is itself a random variable. Reliable results can be obtained only if the distribution of this variable is known with sufficient accuracy. The size-effect based analysis of random particle systems is therefore feasible only if an effective static solver is available. An approach specifically designed for the analysis of particle systems with a piecewise linear micro-level constitutive law was proposed by Jirásek (1993). This approach combines an event-controlled selection of incremental step sizes with the so-called method of inelastic forces (MIF), which makes it possible to calculate the exact displacement increments in each step without iterations and using only the elastic stiffness matrix.

The MIF is in detail explained in Jirásek and Bažant (1995a). Briefly, the incremental equations of equilibrium $\mathbf{K}\dot{\mathbf{d}} = \dot{\lambda}\mathbf{f}^{ref}$, where \mathbf{K} = tangential stiffness matrix, \mathbf{d} = displacement vector, λ = load multiplier and \mathbf{f}^{ref} = reference loading vector, are transformed to

$$\mathbf{K}_0\dot{\mathbf{d}} = \dot{\lambda}\mathbf{f}^{ref} - \hat{\mathbf{B}}^T\dot{\mathbf{s}} \quad (2)$$

where \mathbf{K}_0 = elastic stiffness matrix, $\hat{\mathbf{B}}$ = reduced geometric matrix, and $\dot{\mathbf{s}}$ = vector of rates of inelastic forces. This vector is defined as

$$\dot{\mathbf{s}} = \hat{\mathbf{D}}\hat{\mathbf{B}}\dot{\mathbf{d}}, \quad (3)$$

where $\hat{\mathbf{D}}$ = diagonal matrix containing the differences between current and elastic link stiffnesses for all the links that have entered the inelastic range. The solution of (2) is expressed as

$$\dot{\mathbf{d}} = \dot{\lambda}\mathbf{d}^{ref} + \hat{\mathbf{R}}\dot{\mathbf{s}} \quad (4)$$

where \mathbf{d}^{ref} is the solution of $\mathbf{K}_0\mathbf{d}^{ref} = \mathbf{f}^{ref}$ and $\hat{\mathbf{R}}$ is the solution of $\mathbf{K}_0\hat{\mathbf{R}} = \hat{\mathbf{B}}^T$, and substituted into (3). This yields the fundamental equations of MIF,

$$(\mathbf{I} - \hat{\mathbf{D}}\hat{\mathbf{B}}\hat{\mathbf{R}})\dot{\mathbf{s}} = \hat{\mathbf{D}}\hat{\mathbf{B}}\mathbf{d}^{ref}\dot{\lambda} \quad (5)$$

The rates of inelastic forces are solved from (5), which typically is a very small set of equations as compared to (2), and then substituted into (4) to get the displacement rates. Hence, the solution of the incremental equations of equilibrium can be found without assembling and decomposing the tangential stiffness matrix—the knowledge of the initial elastic stiffness matrix, assembled and decomposed only once and used throughout the entire analysis, is sufficient. It should be emphasized that the *exact* solution is found and *no iterations* are involved.

5 Calculation of fracture characteristics

The MIF is perfectly suited for fracture simulations of large particle systems with a bilinear micro-level constitutive law. Three-point bending beam geometry was chosen for the present study. In all the calculations, the specimen had a span-to-depth ratio 2.5 : 1, and a notch was created at midspan by deleting all the links intersected by a line from the beam bottom up to 0.4 of the depth. Four different sizes scaled as 1 : 2 : 4 : 8 were considered. To take into account also the local variation of strength, the microstrength was treated as a random variable with a log-normal distribution characterized by the mean value \bar{f}_t and coefficient of variation ω_f .

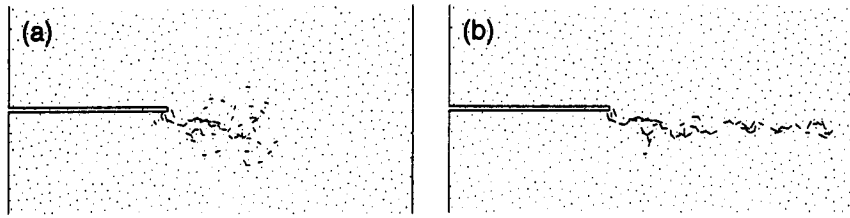


Figure 2: Fracture process zone: (a) microductile material, (b) microbrittle material

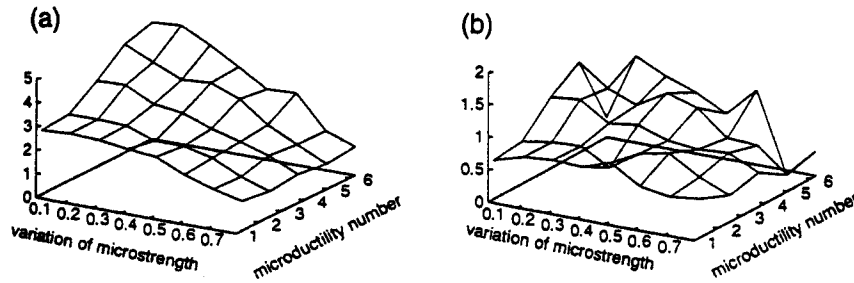


Figure 3: (a) Normalized fracture energy and (b) process zone size as functions of the microductility and coefficient of variation of microstrength

Typical results are illustrated by the plots of the fracture process zone in Fig. 2. Fig. 3 shows three-dimensional graphs of the normalized fracture energy $\bar{G}_f = E'G_f/L_0\bar{f}_t^2$ and the relative process zone size $\bar{c}_f = c_f/L_0$ as functions of the coefficient of variation ω_f and the microductility γ_f . This figure summarizes the results obtained by running 30 simulations with 4 sizes for each of 40 different combinations of ω_f and γ_f . The coefficient of variation was varied between 0 % and 70 % and the microductility between 1.25

and 6.25. The large number of simulations helped to limit the scatter due to randomness and to get fairly consistent results, at least for \bar{G}_f . As a first approximation, the dependence of \bar{G}_f and \bar{c}_f on ω_f and γ_f can be described by bilinear functions

$$\bar{G}_f = 2.16 - 1.08\omega_f + 0.48\gamma_f - 0.71\omega_f\gamma_f, \quad (6)$$

$$\bar{c}_f = 0.64 + 0.08\omega_f + 0.09\gamma_f - 0.19\omega_f\gamma_f, \quad (7)$$

Analysis of the results led to the following conclusions:

1. The ratio of macro-fracture energy to the fracture energy of idealized square lattice of particles for straight-line fracture parallel to a lattice line varies approximately from 1 to 3. The effective process zone size varies approximately from 0.5 to 2 times the average interparticle distance.
2. At constant average microstrength and microductility, the macroscopic fracture energy is proportional to the average particle spacing. It decreases with increasing coefficient of variation of microstrength (or micro-fracture energy) and increases with increasing microductility. The latter increase however weakens with increasing coefficient of variation of microstrength.

6 Impact simulations

The present particle model was also implemented in an explicit dynamic code and its performance was tested through the simulation of an in-plane impact of a square plate on a rigid cylindrical obstacle. The simulations were run as part of a project focusing on fracture of sea ice floes but the general approach is applicable to other quasibrittle materials as well. It turned out that good results can be obtained only if the compressive part of the stress-strain law is not linear elastic but has a partial drop followed by a plateau. It is interesting that in spite of the strong influence of the compressive part of the stress-strain law on the overall performance of the model, the number of links damaged by crushing is usually very small.

Various stages of a typical impact event are documented in Fig. 4. This example refers to a floe of 400 × 400 m in size, hitting an obstacle with radius $R = 100$ m at initial velocity $v = 1$ m/s.

Fig. 5 presents a comparison of the contact force histories for four different sizes of the floe, again with $R = 100$ m and $v = 1$ m/s. Note that not only the peak force but also the total duration of the contact increases with the size of the floe. This trend is especially important with regard to model verification, because the observed impact events for large floes (many square kilometers in size) often extend over a period of several minutes.

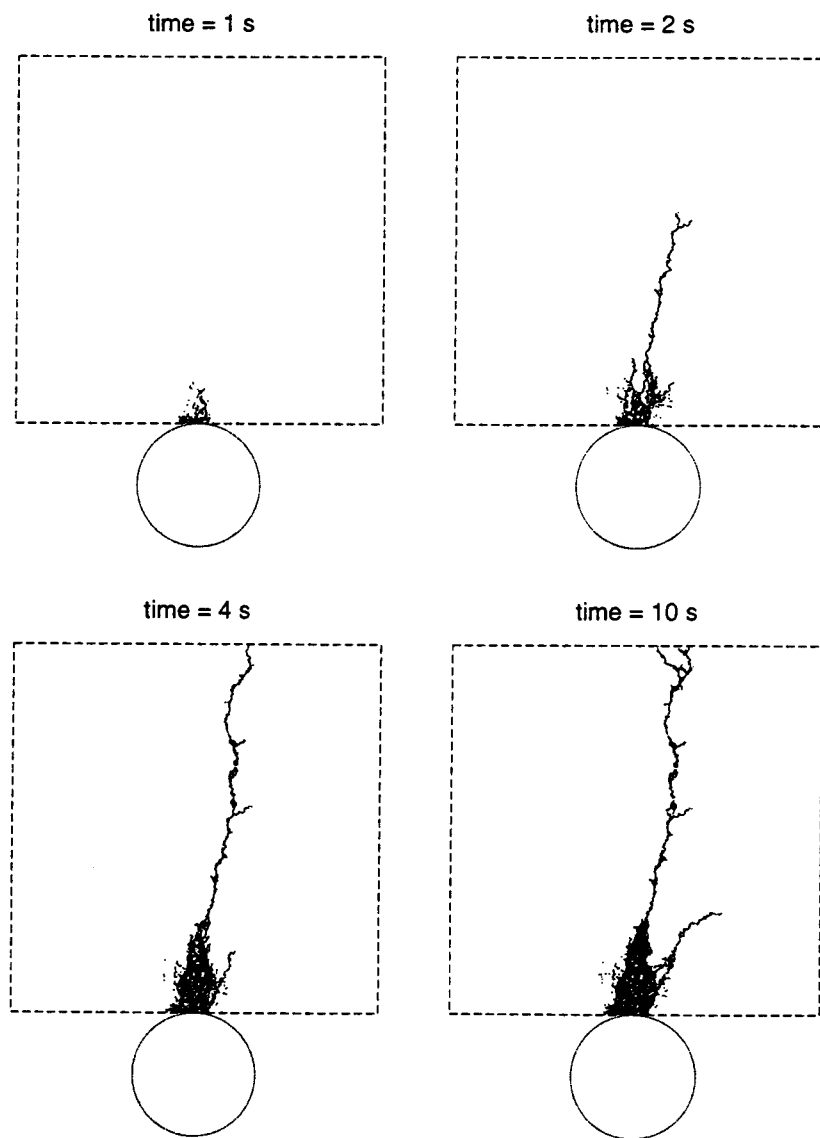


Figure 4: Evolution of fracture pattern during impact

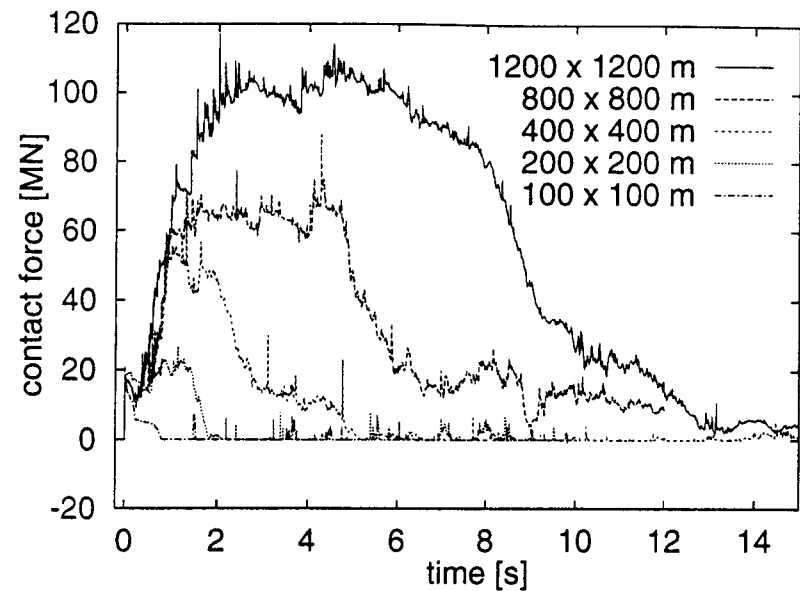


Figure 5: Contact force histories for different sizes

7 Future work

A possible area of future application of the particle model could be a micromechanical analysis of damage localization in heterogeneous materials with special attention to the correspondence between the microscopic processes and nonlocal macroscopic models. Such a study could provide suitable forms of the nonlocal averaging operator not only inside the body of interest but also in the vicinity of its boundary.

The MIF can be extended to other types of models with a piecewise linear behavior, most notably to elastoplastic frames. This will be the subject of a forthcoming publication (Jirásek, 1995). The basic idea of the MIF could also be exploited when constructing the initial directions of various branches of the equilibrium diagram after a bifurcation. The tangential stiffness matrices corresponding to individual branches often differ only by the contribution of a few materials points which change their status, e.g., from softening to unloading. Such a situation could be efficiently handled by an MIF-like technique.

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