Simulation of Dynamic Failure Evolution in Brittle Solids without Using Nonlocal Terms in the Strain-Stress Space

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Abstract: To simulate the dynamic failure evolution without using nonlocal terms in the strain-stress space, a damage diffusion equation is formulated with the use of a combined damage/plasticity model that was primarily applied to the case of rock fragmentation. A vectorized model solver is developed for large-scale simulation. Two-dimensional sample problems are considered to illustrate the features of the proposed solution procedure. It appears that the proposed approach is effective in simulating the evolution of localization, with parallel computing, in a single computational domain involving different lower-order governing differential equations.

keyword: Brittle failure, damage diffusion, multi-physics, parallel computing

1 Introduction

There exist two different approaches to model the evolution of material failure, i.e., continuous and discontinuous ones, after the onset of failure is identified. Decohesion models and fracture mechanics models are representative of discontinuous approaches, in which strong discontinuities are introduced into a continuum body such that the mathematical model is wellposed for given boundary and/or initial data. On the other hand, nonlocal (integral or strain gradient) models, Cosserat continuum models and rate-dependent models are among the continuous approaches proposed to regularize the localization problems, in which the higher order terms in space and/or time are introduced into the strain-stress relations so that the mathematical model is well-posed in a higher order sense for given boundary and/or initial data. As demonstrated for different problems, there are certain kinds of applicability and limitation for different approaches, depending on the scale of the problem and the degrees of discontinuity considered [Bazant and Chen (1997); Chen (1996)]. If the initiation and orientation of localized failure mode is identified via the bifurcation analysis, either a continuous or a discontinuous approach could be used to model and simulate the evolution of failure, depending on the degree of discontinuity and the scale considered.

If a continuous approach is of interest, the use of higher order terms in space makes it difficult to perform large-scale computer simulation, due to the limitation of current computational capabilities. As can be found by reviewing the existing nonlocal models, the nonlocal terms are usually included in the limit surface so that a single higher order governing equation will appear in the problem domain. Can we find an alternative approach to replace the single higher order equation with two lower order equations? If we can, parallel computing might be used for the large-scale simulation of localization problems.

As shown in the previous research [Chen and Sulsky, (1995)], the evolution of localization might be equally well characterized by the formation and propagation of a moving material surface of discontinuity. With the use of a moving material surface, a partitioned-modeling approach has been proposed for localization problems. The basic idea of the approach is that local constitutive models are used inside and outside the localized deformation zone with a moving boundary being defined between different material domains. As a result, the extrapolation of material properties beyond the limitations of current experimental techniques might be avoided in modeling the evolution of localization. An attempt has also been made to investigate the use of the jump forms of conservation laws in defining the moving material surface. By taking the initial point of localization as that point where the type of the governing differential equations changes, a moving material surface of discontinuity can be defined through the jump forms of conservation laws across the surface. Because the transition from a hyperbolic equation to an elliptic one could be represented by a parabolic one which governs a diffusion process, an analytical solution has been obtained for a dynamic softening bar with the use of a similarity method for the transition involving a weak discontinuity. To obtain a closed-form solution, the diffusion speed of the moving material surface was assumed to be constant [Xin and Chen (2000)].

In reality, the motion of the material surface depends on the stress state and internal state variables, so that the constant diffusion speed can be thought as a special case of diffusion, i.e., the time average of a real diffusion process. Due to the limitation of current experimental facilities, it is still a challenging task to quantitatively determine how the internal energy diffuses in real-time associated with the evolution of localization. As will be shown in this paper, however, the use of different governing differential equations, after localization occurs, makes it possible to replace the single higher order equation with two lower order equations so that parallel com-

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puting might be used for the large-scale simulation of localization problems.

To predict the evolution of localization without the assumption of a constant diffusion speed, a damage diffusion equation is formulated with the use of a combined damage/plasticity model. As a result, lower order wave and diffusion equations will appear in a single computational domain. Twodimensional sample problems are then considered to illustrate how the dynamic evolution of localization can be simulated without using nonlocal terms in the strain-stress space.

2 Constitutive Modeling

To estimate stress-wave-induced fracturing, a combined damage/plasticity model has evolved over a number of years, which was primarily applied to the case of rock fragmentation [Chen (1993); Taylor, Chen and Kuszmaul (1986); Thorne (1990) and (1991)]. Within the loading regime of the model, an isotropic elasticity tensor governs the elastic material behavior, a scalar measure of damage is active through the degradation of the elasticity tensor if the confining pressure $P \ge 0$ (tensile regime), and a pressure-dependent perfectly plastic model is used if P < 0 (compressive regime).

Based on the previous work, the evolution of tensile damage can be described by the following equations:

$$C_d = \frac{5k}{2} \left(\frac{K_{IC}}{\rho c \dot{\varepsilon}_{max}}\right)^2 \varepsilon_v^m \tag{1}$$

$$\overline{\mathbf{v}} = \mathbf{v} \left(1 - \alpha C_d \right) \tag{2}$$

$$D = \frac{16(1-v^2)}{9(1-2\overline{v})}C_d$$
(3)

$$\overline{K} = (1 - D)K \tag{4}$$

in which C_d is a crack-density parameter, K_{IC} the fracture toughness, ε_v the mean volumetric strain, $\dot{\varepsilon}_{max}$ the maximum volumetric strain rate experienced by the material at fracture, c the uniaxial wave speed $\sqrt{E/\rho}$ with E being Young's modulus, ρ material density and D a single damage parameter. Also, K and v are the original bulk modulus and Poisson's ratio, respectively, for the undamaged material, and the barred quantities represent the corresponding parameters of the damaged material. The model parameters k and m can be determined by using the fracture stress versus strain rate curve. To obtain consistent unloading/reloading moduli, the assumption of $\alpha = 16\beta/9$ is employed with β being the fraction of damage.

With the use of

$$f_1(\overline{\mathbf{v}}) = \frac{1 - \overline{\mathbf{v}}^2}{1 - 2\overline{\mathbf{v}}}$$
 and (5)

$$f_2(\overline{\mathbf{v}}) = \frac{2\left(1 - \overline{\mathbf{v}} + \overline{\mathbf{v}}^2\right)}{\left(1 - 2\overline{\mathbf{v}}\right)^2} = \frac{\partial f_1(\overline{\mathbf{v}})}{\partial \overline{\mathbf{v}}} \tag{6}$$

the rate forms of Eqs. 1-4 can be found to be

$$\dot{C}_{d} = \frac{5km}{2} \left(\frac{K_{IC}}{\rho c \dot{\epsilon}_{max}}\right)^{2} \varepsilon_{\nu}^{m-1} \dot{\varepsilon}_{\nu} = F_{1}(\varepsilon_{\nu}) \dot{\varepsilon}_{\nu}$$
(7)

$$\dot{\overline{\mathbf{v}}} = -\alpha \mathbf{v} F_1(\boldsymbol{\varepsilon}_{\nu}) \, \dot{\boldsymbol{\varepsilon}}_{\nu} = F_2(\boldsymbol{\varepsilon}_{\nu}) \dot{\boldsymbol{\varepsilon}}_{\nu} \tag{8}$$

$$\dot{D} = \frac{16}{9} \left(f_1 \dot{C}_d + f_2 C_d \dot{\overline{\mathbf{v}}} \right) = F_3 \left(\boldsymbol{\varepsilon}_{\boldsymbol{\nu}} \right) \dot{\boldsymbol{\varepsilon}}_{\boldsymbol{\nu}} \tag{9}$$

$$\dot{\overline{K}} = -K\dot{D} = -KF_3\left(\varepsilon_{\nu}\right)\dot{\varepsilon}_{\nu} \tag{10}$$

with F_i denoting functionals. As can be seen, the damage evolution can be determined for given $\dot{\varepsilon}_v$, based on the load-ing/unloading condition. It has been assumed in the above derivation that the effect of strain rate is history-independent. As a result, the condition of $\ddot{\varepsilon}_{max} = 0$ can be used. As can be seen from Eqs. 7-10, a one-step vectorized model solver can be designed for large-scale computer simulation.

The fundamental assumption of the above damage model is that the material is permeated by an array of randomly distributed microcracks which grow and interact with one another under tensile loading. Hence, the constitutive model does not treat each individual crack; rather it predicts the growth of the microcracks as an internal state variable, *D*, which determines the accumulation of material damage. However, only the evolution of damage with time at a given material point, instead of the evolution of damage both with time and in space, is considered in the model. In other words, the model is local in nature. As a result, the simulation results are mesh-dependent. To remedy this defect, nonlocal terms have been included in the model at the cost of more CPU time and difficulty in vectorizing the code.

Based on a recent study on the failure wave phenomenon [Chen and Xin (1999); Feng and Chen (1999)], it appears that, in the dynamic failure process of certain engineering materials, microfissuring at one location induces local deformation heterogeneity that in turn initiates microfissuring in the adjacent material and so on, if a critical state is reached. Hence, a diffusion equation governing the progressive percolation of heterogeneous microdamage appears to capture the essence of the dynamic failure evolution in certain engineering materials, as verified with the experimental data available. The use of jump conditions could also result in a diffusion equation governing the failure wave speed, through a mathematical argument [Chen and Xin (1999)]. However, a well-defined constitutive model is required to be incorporated into the damage diffusion equation.

To simulate the dynamic failure evolution of a class of brittle solids, it is proposed that a strain-based damage diffusion equation be combined with the above tensile damage model without the use of nonlocal terms in the strain-stress space, as shown next.

3 Damage Diffusion

If the bifurcation analysis of acoustic tensor identifies the onset of localization based on the continuum tangent stiffness tensor, a surface of discontinuity will be driven by the heterogeneity and stress concentration, with \mathbf{n} being the vector normal to the surface. The law of damage diffusion is assumed to be

$$\mathbf{J} = -d\frac{\partial C}{\partial \mathbf{n}} \tag{11}$$

in which *C* is the concentration of microcracks (the number of microcracks per unit volume), **J** the flux of microcracks (the number of microcracks diffusing down the concentration gradient per unit time per unit area), and *d* the damage diffusivity function. If the damage diffusion is assumed to be isotropic, a damage diffusivity function of mode I at any location **x** and time *t* can be defined to be

$$d(\mathbf{x},t) = \lambda_1 \frac{\varepsilon_{\nu f} - \varepsilon_{\nu}}{\varepsilon_{\nu f}}$$
(12)

in which ε_{vf} represents the value of ε_v at the final state before rupture. As can be seen, the diffusion process will diminish with the evolution of failure and the model parameter λ_1 controls the rate of diffusion.

To initiate the diffusion of damage, an internal damage evolution per unit time must be given here, which takes the form of

$$Q(\mathbf{x},t) = \frac{5k}{2t_d} \left(\frac{K_{IC}}{\rho c \varepsilon_{max}}\right)^2 \varepsilon_v^m$$
(13)

when $\varepsilon_v - \varepsilon_{vl} \ge 0$. In Eq. 13, t_d and ε_{vl} denote the characteristic time of the concentration diffusion of microcracks and the critical state strain, respectively. The concentration of microcracks *C* is related to the crack-density parameter, C_d , that represents the volume fraction of material made up of microcracks, namely,

$$C_d = \lambda_2 C \tag{14}$$

where λ_2 is the characteristic volume of a microcrack. The equation governing the tensile damage diffusion can then be written as, in a standard form,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial \mathbf{n}} \cdot \left(d \frac{\partial C}{\partial \mathbf{n}} \right) + Q \tag{15}$$

The above diffusion equation can be solved in parallel with the wave equation to simulate the evolution of dynamic localization.

For the sample problems considered in the next section, central-difference in space and forward integration in time will be used to solve the diffusion equation, while constant stress elements in space and forward integration in time will be employed to solve the wave equation. When the diffusion equation and wave equation are solved in a parallel (staggered) setting, the time step satisfying both stability conditions is used to solve the whole problem at the same time.



Figure 1 : Damage histories for three strain rates



Figure 2 : Pressure-volumetric strain for three strain rates

4 Demonstrations

To demonstrate the proposed procedure, the model parameters are assigned the following values:

$$\begin{array}{ll} E = 50 \, Gpa, & \nu = 0.3, & \rho = 2500 \, kg/m^3 \\ K_{IC} = 1.0 \, Mpa \sqrt{m}, & m = 7, & k = 5 \times 10^2 2 \, l/m^3 \\ \varepsilon_{\nu l} = 0.002, & \varepsilon_{\nu f} = 0.01, \\ \lambda_1 = 500, & \lambda_2 = 0.01, & t_d = 0.01. \end{array}$$

With the time increment being 10^{-7} second for the damage model solver, Fig. 1 shows the strain rate effect on the damage histories under a constant uniaxial tensile strain rate condition. Fig. 2 illustrates the corresponding pressure versus volumetric strain curves for three constant strain rates. As can be obersved, the strain rate effect on the limit state can be predicted by this tensile damage model.

The geometry and notation for the plane problem are shown in



Figure 3 : The problem geometry and boundary conditions for 2-D simulation

Fig. 3. The dimensions used for the analysis are $L_x = 1.0 m$ and $L_y = 1.5 m$. The initial condition consists of zero displacement and zero velocity throughout the problem domain, while the boundary condition is shown in Fig. 3. A constant load is applied suddenly through a mechanism that provides no lateral constraint and ensures that the displacement in the y-direction is the same for all points on the upper surface. Element mesh I and II are defined to be 20×30 and 10×15 quadrilateral cells with each cell consisting of 4 triangle elements, respectively. The location of the imperfection point is at the origin, at which the failure is initiated when $\varepsilon_v > \varepsilon_{vl}$ and $\dot{\varepsilon} > 0$.

With the time step satisfying the stability criteria, Figs. 4-7. demonstrate the evolution of the effective strain field and corresponding effective stress field in the post-limit regime with element mesh I. The numerical test indicates that the strain within the localization zone is increasing with the decrease of the corresponding stress. Fig. 8 illustrates the effective strain field, obtained by using mesh II. Fig. 9 and 10 show the damage contour in the deep post-limit regime with mesh I and II, respectively. As can be seen, the numerical solutions are not mesh-sensitive although mesh I is double-refined from mesh II.

5 Conclusions

Based on the dynamic failure mechanisms of brittle solids, an effective numerical procedure is proposed to simulate the evolution of localization due to microcracking. A threedimensional diffusion equation is formulated with a ratedependent tensile damage model. As a result, a single higher



Figure 4 : The strain profile in the middle post-limit regime with mesh I



Figure 5 : The stress profile corresponding to Fig. 4



Figure 6 : The strain profile in the deep post-limit regime with mesh I



Figure 7 : The stress profile corresponding to Fig. 6



Figure 9 : The damage contour corresponding to Fig. 6



Figure 8 : The strain profile in the deep post-limit regime with mesh II



Figure 10 : The damage contour corresponding to Fig. 8

order governing equation can be replaced with two lower order governing equations in a single computational domain for localization problems. Two-dimensional sample problems are considered to illustrate how the dynamic evolution of localization can be simulated without using nonlocal models in the strain-stress space. As can be found from the numerical solutions, the essential features of the evolution of localization, and a localization zone of finite width can be predicted with the proposed procedure.

Future research is required to better understand the convergent behavior, to perform the bifurcation analysis for the diffusion equation, and to apply the proposed procedure to general cases. Acknowledgement: This work was sponsored in part by DOE/SNL and NSF.

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