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NUMERICAL METHODS IN FRACTURE MECHANICS

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Strain-softening is characterized by lack of positive definiteness of the matrix of tangential moduli, a feature which was considered first probably by Hadamard [1] who argued that this is an inadmissible property for a continuum model since the wave speed ceases to be real and wave propagation becomes impossible. This argument was later expanded by Hill, Thomas, Truesdell and others [2], but it did not become clear from experiments until the 1970's that Hadamard's argument does not quite correspond to reality in that real materials in a strain-softening state possess not only a nonpositive definite moduli matrix for further loading, but also a positive definite moduli matrix for unloading. Thus, with regard to Hadamard's argument about imaginary wave speed it should be noted that it applies only to loading waves. Materials in a strain-softening state can still propagate unloading waves. The fact that the unloading stiffness is positive definite even for strain-softening makes a crucial difference and renders strain-softening problems mathematically meaningful, even for a local continuum.

It was shown that solutions to certain wave propagation problems for a local strain-softening continuum do exist, and some are unique, even though the problem belongs to the class of ill-posed initial-boundary value problems. Moreover, explicit step-by-step finite element solutions converge to these exact solutions, and appear to do so almost quadratically [3,4,5]. Thus, the problem with strain-softening is not mathematical but physical.

Noting the need to consider a positive stiffness for unloading, Bažant showed in his analysis of strain-softening in 1974 [6,7,8] that according to a local continuum model strain-softening must localize into a zone of vanishing volume. The consequence is that the structure is predicted to fail with zero energy dissipation, which is physically unrealistic and unacceptable. The same type of behavior was confirmed for dynamic loading of structures [3,4,5,9,10]. To prevent this to happen, one must introduce into the models mathematical methods called localization limiters, which force the strain-softening zone to have a certain minimum finite size and thus assure a finite energy dissipation at failure.

The simplest localization limiter, proposed in 1974 [6] and used in the crack band model [11,12], is to limit the size of the finite element to a certain minimum. While this approach appears to give good results for fracture mechanics type problems, it might be nevertheless too crude, as it makes it impossible to resolve the distribution of damage density throughout the failure zone and thus determine the energy dissipation accurately. A general form of a localization limiter may be based on a nonlocal continuum, as proposed in 1984 [9,13]. Numerous possibilities of nonlocal formulations appear to exist, and a new one which appears to be particularly simple and effective was recently proposed by Pijaudier-Cabot and Bažant [14], and is further developed in the present lecture.

Other types of localization limiters may be based on Taylor series approximations of the averaging integral in the nonlocal model, which leads to higher order gradients in the definition of strains and in the continuum equations of motion. Alternatively, the spatial gradients may be applied to the strength or yield limit or to the yield function. Such an idea was apparently first proposed in 1952 by L'Hermite in the context of a study of shrinkage cracking, and recently this idea was developed for strain-softening in general by Schreyer [16,43] and Mang [17].

As a substitute for localization limiters, strain-softening can be replaced by a damage or cracking model based on a stress-displacement relation, as introduced into fracture mechanics by Dugdale, Barrenblatt, Knauss, Rice and Kfoury, etc., in the realm of plasticity, and by Hillerborg et al. in the realm of concrete cracking. It should be recognized, however, that this approach is not a general one and is applicable only to single cracks or cracks which do not interact with other cracks, which means that one can solve fracture specimens designed to fail with a single crack but cannot use this approach in a general finite element code. The reason is that for the situations in which damage remains distributed, being stabilized, e.g., by reinforcement or by a compression zone close ahead of the cracking front. For distributed damage one would need to know the spacing of cracks, which must be a material property if the predictions of the model should be objective and if the energy dissipation should converge on mesh refinement. The existing line crack models lack the crack spacing as a material parameter, and even if one would introduce the spacing into these models one would run into conceptual difficulties in the case of nonparallel cracks.

An alternative to the interelement line-crack models with stress displacement relation, as well as to the crack band model, is to embed a strain-softening band or line inside a finite element. Models of this type were proposed by Pietrusczak and Mróz [20] and by Willam, Sture et al. [21,22]. These approaches have the same limitation as the crack band model, i.e., they cannot resolve the distribution of damage and energy dissipation throughout the strain-softening zone, and they also lack in their present form the crack or band spacing limitation, same as the line crack models. Nevertheless, good comparisons with various experimental data were achieved with these models as well as the crack band model.

In a recent extensive review, Read and Hegemier [23] essentially claimed that strain-softening does not exist. They emphasized that the observed strain-softening is due to the decrease of the resisting area fraction of the material, caused by an increase in the cross-section area of cracks or voids. This would mean that strain-softening should be modeled by a transition from total stress $\underset{\sim}{\sigma}$ to the true stress $\underset{\sim}{\sigma}_t = \underset{\sim}{\sigma}/(1 - \omega)$ where ω is a parameter characterizing the damaged cross section of the material, while at the same time the constitutive law for the true stress $\underset{\sim}{\sigma}_t$ involves no strain-softening and is based, e.g., on hardening plasticity. This would mean that the continuum damage mechanics models [24-34] would be the only acceptable models for strain-softening, and so would Gurson's model for the failure of ductile metals [35-37], in which the hardening plastic stress-strain relation is written for the metal between the voids and the transition to the total stress is based again on the parameter ω representing the void volume fraction. Recently, however, these approaches were shown to be subject to the same difficulty as the constitutive relations which describe strain-softening directly [38,39]. Same as he models which describe strain-softening directly, the models of continuum dmage mechanics exhibit strain localization to a volume of vanishing size, as well as the inherent spurious mesh sensitivity of finite element calculations [38,39]. Thus, introduction of localization limiters is required not only for the classical strain-softening models, but also for the models of continuum damage mechanics or plasticity with void growth.

The type of localization considered here is fundamentally different from that studied by Rudnicki and Rice (1985), Rice (1986), and Prevost (1984) [44,45,46]. Those studies were concerned with plastic-hardening behavior and localization caused by geometrical nonlinear effects of finite strain which become important only just before the peak of the stress-strain diagram where the magnitudes of the tangential modulus and the stresses become of the same order. The localization due to strain-softening, whose study was initiated by Bažant in 1974, is a rather different problem, in which the geometrically nonlinear aspects are unimportant for the onset of localization because both the post-peak tangential moduli for further loading and those for unloading are orders of magnitude larger than the stresses. The source of this localization is not nonlinear geometry but constitutive properties. Moreover, material unloading properties played no role in the solutions of Rice and Rudnicki, but they are crucial for our type of localization.

There is a question whether introduction of rate-sensitivity or viscosity, whether real or artificial, can eliminate the spurious mesh sensitivity and localization to a vanishing volume. In certain cases such an approach met with success (e.g., Sandler, Needleman), but in general this is unlikely to be the remedy. In fact, Belytschko et al. [4] found that in the case of converging spherical waves the introduction of viscosity does not help to avoid chaotic response.

In the following we now describe in more detail an extension of a new model recently developed at Northwestern University [14] which employs the nonlocal approach but has several important advantages over the original nonlocal model for damage presented in 1984 [9,13].

Nonlocal Damage Theory with Local Strain

Nonlocal continuum is a continuum in which some state variables or material parameters are defined by spatial averaging. The spatial averaging operator may be defined by the equation:

$$\Omega(\underset{\sim}{x}) = \bar{\omega}(\underset{\sim}{x}) = \frac{1}{V_r(\underset{\sim}{x})} \int_{V(\underset{\sim}{x})} \alpha(\underset{\sim}{\xi} - \underset{\sim}{x})\, \omega(\underset{\sim}{\xi})dV \tag{1}$$

in which

$$V_r(\underset{\sim}{x}) = \int_{V(\underset{\sim}{x})} \alpha(\underset{\sim}{\xi} - \underset{\sim}{x})\, dV \tag{2}$$

in which ω and Ω may be considered as the local and nonlocal damage, superimposed bar denotes the spatial averaging operator, $\underset{\sim}{x}$ and $\underset{\sim}{\xi}$ are the coodinate vectors, V = volume, $V_r(\underset{\sim}{x})$ = representative volume of the material centered at point $\underset{\sim}{x}$, and α = given weighting function which is a material property. V_r has approximately but not exactly the same meaning as the representative volume in the statistical theory of heterogeneous materials [40,41]. For a uniform weighting function, $\alpha = 1$. The integration domain $V(\underset{\sim}{x})$ centered at point $\underset{\sim}{x}$ can be made to coincide with $V_r(\underset{\sim}{x})$, but a function α which decays smoothly with the distance from the center is probably more realistic. It also leads to better convergence of numerical calculations. A suitable form is the error density function:

$$\alpha(\underset{\sim}{x}) = e^{-(k|\underset{\sim}{x}|/\ell)^2} \tag{3}$$

in which we have, for one, two and three dimensions:

$$\begin{aligned} &\text{1D:} \quad |\underset{\sim}{x}|^2 = x^2, && k = \sqrt{\pi} = 1.772 \\ &\text{2D:} \quad |\underset{\sim}{x}|^2 = x^2 + y^2, && k = 2 \\ &\text{3D:} \quad |\underset{\sim}{x}|^2 = x^2 + y^2 + z^2 && k = (6\sqrt{\pi})^{1/3} = 2.149 \end{aligned} \tag{4}$$

ℓ is the characteristic length, a material property which defines the length or diameter of the representative volume (a line segment, circle, or sphere) which has the same volume as the error density function extending to infinity (x, y, z = cartesian coordinates).

For a finite body the error function extends beyond the boundary of the body. In that case the region outside the body is deleted from the integration domain $V(\underset{\sim}{x})$, both for the calculation of the average (Eq. 1) and the calculation of the representative volume V_r (Eq. 2). This fact causes V_r to depend on location $\underset{\sim}{x}$. For numerical finite element computations, the integrals in Eqs. 1 and 2 are approximated by finite sums. Only the finite elements whose integration points are closer to point $\underset{\sim}{x}$ than distance 2ℓ needs to be included in the sum, since for a greater distance the value of α is negligible. For numerical calculations, Eq. 1 is better written as

$$\Omega(\underset{\sim}{x}) = \int_{V(\underset{\sim}{x})} \alpha'(\underset{\sim}{\xi}, \underset{\sim}{x})\, \omega(\underset{\sim}{\xi})\, dV, \quad \alpha'(\underset{\sim}{\xi}, \underset{\sim}{x}) = \frac{\alpha(\underset{\sim}{\xi} - \underset{\sim}{x})}{V_r(\underset{\sim}{x})} \tag{5}$$

and the values of α' for all combinations of discrete values $\underset{\sim}{x}$ and $\underset{\sim}{\xi}$ may be evaluated and stored in the computer memory in advance for the finite element analysis.

When the nonlocal continuum idea was first applied as a localization limiter for strain-softening [13,9], it was assumed that the strain was nonlocal, i.e., the strain to be used in the constitutive equation was $\bar{\underset{\sim}{\varepsilon}}$ instead of the actual strain $\underset{\sim}{\varepsilon}$. Under that hypothesis it was shown [13] that, in contrast to the previous works on nonlocal elastic materials, the continuum equations of equilibrium or motion cannot be considered to have the standard form but must be derived from the expression for virtual work, which reads:

$$\delta W = \int_{V_b} \sigma_{ij}\, \delta\bar{\varepsilon}_{ij}\, \delta V - \int_{V_b} f_i \delta u_i\, dV - \int_{S_b} p_i\, \delta u_i\, dS \tag{6}$$

V_b and S_b are the volume and surface of the entire body, u_i = displacement components in cartesian coordinate x_i (i = 1,2,3), f_i and p_i are the distributed volume and surface forces, ε_{ij}; σ_{ij} are the nonlocal strain components and stress components used in the constitutive relation, and dS = element of body surface.

Since Eq. 6 involves the averaging operator of Eq. 1 (or its differential or finite difference approximation), the derivation of the continuum equation of equilibrium or motion and boundary conditions is rather complicated and a nonstandard form of these equations is obtained [13]. This nonstandard form yields either averaging integrals or derivatives (or finite differences) in the continuum equation of motion or equilibrium written in terms of σ_{ij}, and it also leads to extra boundary conditions. Although finite element analysis for such a theory is tractable by means of the imbricate finite element concept [9,10], the solution is, nevertheless, quite cumbersome.

This observation leads to the key idea advanced in this lecture, whose special case was already annunciated in previous work [14]. The nonlocal formulation used as a localization limiter should be of such a form that the strains are <u>local</u>.

Indeed, if the strains are local while the stresses σ_{ij} may be expressed by the constitutive equation in a form which involves some other nonlocal quantities, the standard variational derivation of the continuum equations of equilibrium or motion and the boundary conditions is the same as for the local continuum, i.e.,

$$\begin{aligned} \delta W &= \int_V \sigma_{ij}\, \delta\varepsilon_{ij}\, dV - \int_V f_i\, \delta u_i\, dV - \int_S p_i\, \delta u_i\, dS \\ &= \int_V \sigma_{ij}\, \delta u_{i,j}\, dV - \int_V f_i\, \delta u_i\, dV - \int_S p_i\, \delta u_i\, dS \\ &= \int_S (\sigma_{ij}\, n_j - p_i)\, \delta u_i\, dS - \int_V (\sigma_{ij+j} + f_i)\, \delta u_i\, dV = 0 \end{aligned} \tag{7}$$

from which the standard boundary conditions and differential equations of equilibrium follow by requiring that this equation must hold for any kinematically admissible variation δu_i. This derivation is valid whether or not the constitutive relation between σ_{ij} and ε_{ij} involves any spatial averaging or not, provided that $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ = local small strain.

In a preceding study [14] it was proposed that the nonlocal formulation for strain-softening should be such that for the special case of elastic behavior it reduces to a local form. Obviously, the present idea includes this approach, since the elastic behavior cannot be nonlocal if the strains are local, for the strain is the only variable which determines the stress in the case of elastic behavior. The present idea, however, is more restrictive since all inelastic formulations which would involve nonlocal strain are rejected.

It is easy to prove that the energy dissipation cannot localize to a zone of zero volume. To this end consider the order of continuity of various state variables. Displacements u_i are functions of at least C_1 -continuity, and strains are functions of at least C_0-continuity. The local damage rate ω is a continuous function of strains, and, therefore, ω has at least C_0-continuity. Since the nonlocal damage rate Ω is given by the integral in Eq. 1, Ω must have at least C_1 continuity, and since the energy dissipation rate due to damage is proportional to Ω, it must have also at least C_1 continuity. This means that the energy dissipation due to damage cannot localize.

To be more specific, an example of the lowest order of continuity of strains is the function $\underset{\sim}{\varepsilon} \sim \delta(\underset{\sim}{x} - \underset{\sim}{x}_A)$, and this implies that $\omega \sim \delta(\underset{\sim}{x} - \underset{\sim}{x}_A)$, in which δ denotes Dirac delta function. According to Eq. 1, the nonlocal damage rate is calculated as

$$\dot{\Omega} = \frac{1}{V_r} \int_V \alpha(\underset{\sim}{\xi} - \underset{\sim}{x})\ \delta(\underset{\sim}{\xi} - \underset{\sim}{x}_A)\ dV(\underset{\sim}{\xi}) = \frac{1}{V_r}\ \alpha(\underset{\sim}{x}_A - \underset{\sim}{x}) \tag{8}$$

which shows that Ω, and, therefore, also the energy dissipation density rate, must be a continuous function, i.e., cannot localize. This argument, however, does not prove that the strains cannot localize. This can be proven only by solving the problem on the basis of a given constitutive law.

One constitutive model which is suited for the present purpose is the continuum damage theory. In the simplest prototype of this theory in which the damage is considered as a scalar, the generalization to nonlocal damage is obtained by replacing ω by Ω. This leads to the following relations:

$$\sigma_{ij} = (1 - \Omega)\ \sigma^t_{ij}, \qquad \sigma^t_{ij} = C_{ijkm}\ \varepsilon_{km} \tag{9}$$

in which σ^t_{ij} = true stress, and C_{ijkm} = elastic moduli of undamaged material. Using the free energy density ψ, defined by $\rho\psi = \sigma_{ij}\ \varepsilon_{ij}/2$ where ρ = mass density, the stresses are obtained as $\sigma_{ij} = \partial(\rho\ \psi)/\partial\ \varepsilon_{ij}$. In the continuum damage theory, the usual expression with local damage ω may be generalized as

$$\rho\psi = \frac{1 - \Omega}{2}\ C_{ijkm}\ \varepsilon_{ij}\ \varepsilon_{km} \tag{10}$$

The energy dissipation rate density may then be expressed as

$$\dot{\phi} = -\frac{\partial(\rho\psi)}{\partial t} = -\frac{\partial(\rho\psi)}{\partial\Omega}\ \frac{\partial\Omega}{\partial t} = Y\dot{\Omega} \tag{11}$$

in which Y, called the damage energy release rate, is

$$Y = -\frac{\partial(\rho\psi)}{\partial\Omega} = \frac{1}{2}\ C_{ijkm}\ \varepsilon_{ij}\ \varepsilon_{km} \tag{12}$$

The evolution of local damage ω may be specified in the usual manner by the damage evolution equation of the general form $\dot{\omega} = F(\omega, Y, \sigma_{ij}, \varepsilon_{ij})$. A special integrable form of this equation has been considered in all the numerical computations. This form, along with the loading criterion, is expressed as follows:

If $F(\bar{\omega}) = 0$ and $\dot{F}(\bar{\omega}) = 0$, (loading) then $\dot{\Omega} = \dot{\bar{\omega}}$

If $F(\bar{\omega}) < 0$, or if $F(\bar{\omega}) = 0$ and $\dot{F}(\bar{\omega}) < 0$, (unloading or reloading) then $\dot{\Omega} = 0$ (13)

$$\text{with } \bar{\omega} = \frac{1}{V_r(\underset{\sim}{x})} \int_V \alpha(\underset{\sim}{\xi} - \underset{\sim}{x})\ \left[1 - \frac{1}{1 + b\ (Y - Y_0)^n}\right] dV(\underset{\sim}{\xi})$$

b, n, Y_0 = empirical positive constants, $n > 2$, Y_0 = local damage threshold, and $F(\bar{\omega})$ = empirical loading function, which is taken as

$$F(\bar{\omega}) = \bar{\omega} - \kappa(\bar{\omega}) \tag{14}$$

in which $\kappa(\bar{\omega})$ = hardening-softening parameter, whose initial value is taken as 0 and afterwards $\kappa(\bar{\omega})$ represents the largest value of Ω ever reached up to the current time.

Note that if the nonlocal damage Ω is replaced by the local damage ω in Eqs. 9-12, one obtains the classical local continuum damage formulation.

An alternative formulation may be obtained as a nonlocal generalization of the fracturing strain theory, in which the averaged variable is the fractoring strain instead of ω. Both this and the aforementioned continuum damage mechanics formulation work, i.e., are found in numerical calculations to indeed serve as a localization limiter and lead to a convergent solution without spurious mesh sensitivity.

In the previous work [14], the nonlocal damage Ω was not defined by averaging of the local damage ω, but was specified as a function of the average $\bar{Y}$ of the damage energy release rate Y. This may be regarded as an approximation to the present formulation in which the average quantity is $\bar{\omega}$ rather than $\bar{Y}$, and numerical results show that indeed the results are very close.

In a parallel study conducted at Northwestern University by Z. P. Bažant and F. B. Lin, an alternative nonlocal strain-softening formulation is considered as a generalization of plasticity, in which the yield limit is allowed to decrease as a function of the nonlocal plastic strain path length. This nonlocal path length is obtained by averaging of the local plastic strain path length. Since the path length is a nondecreasing quantity, this variable is suitable for the characterization of damage (in this case the yield limit degradation). Numerical results from two-dimensional finite element studies have already confirmed that this

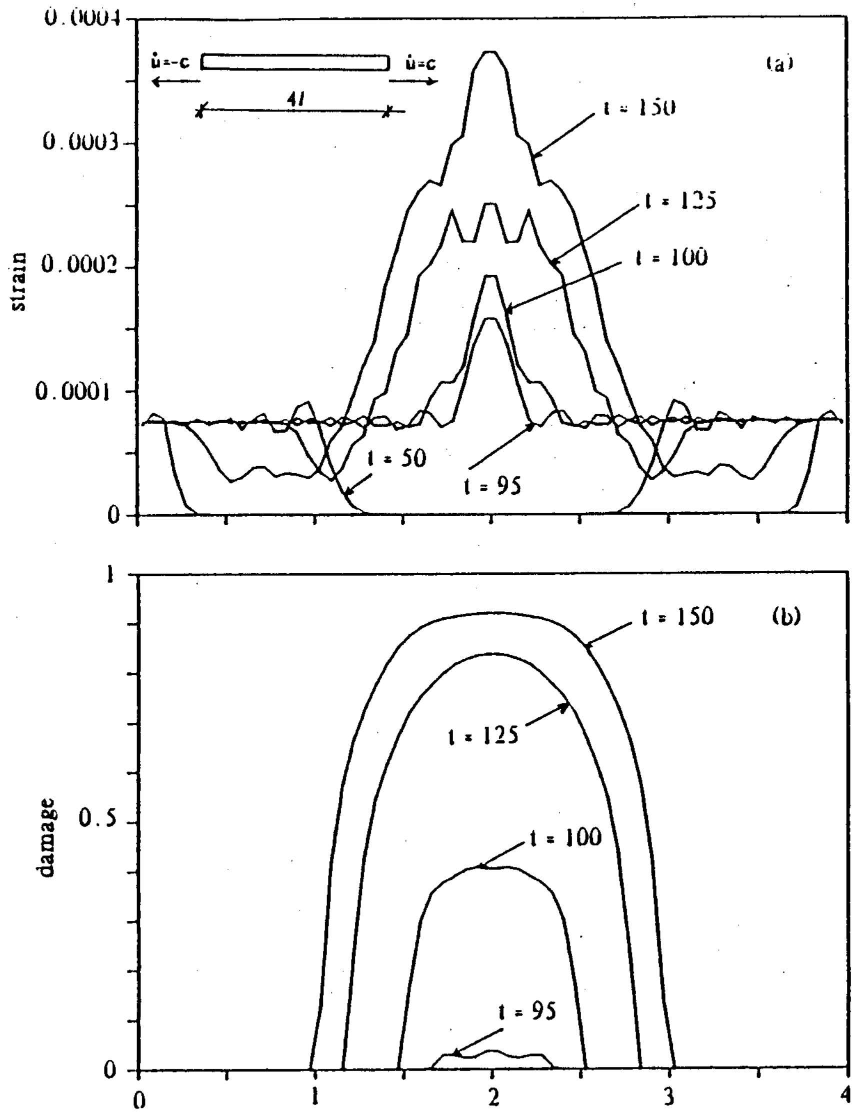

Fig. 1 Calculated profiles of strain and damage along the bar, at various times.

formulation also serves as a proper localization limiter, i.e., finite size strain-softening zones are obtained and the solution converges as the mesh is refined.

Some Typical Numerical Results

Fig. 1-3 show numerical results for wave propagation in a strain-softening rod of length 4ℓ, which is subjected beginning with time t = 0 to constant outward velocities c at the ends of the rod (Fig. 1). The problem has been solved [14] by one-dimensional finite elements using a uniform subdivision (n = number of elements). Fig. 1 shows the profiles of strain and damage at various times, which indicate that neither strain nor damage localize. Fig. 2 shows the distributions of strain, damage and stress at a fixed time, for various numbers of subdivisions. The nonlocal solution is on the left, and the corresponding local solutions are on the right. The local solutions exhibit gradual localization of the damage zone as the mesh is refined, and the local distributions converge to a Dirac delta function. On the other hand, the nonlocal solutions on the left clearly confirm that the damage remains nonlocalized and that the solution converges well as the mesh is refined. Fig. 3 shows the dependence of the energy dissipated up to this time for both the local and nonlocal solutions. For the nonlocal solution, the dissipated energy obviously converges to a finite value, and the convergence is good, while for the nonlocal solution the dissipated energy converges as the mesh is refined to a zero energy dissipation, which is, of course, physically incorrect and inadmissible. The exact solution of the local version of this problem was presented in Ref. 3 using a strain-softening stress-strain relation rather than the continuum damage theory.

Fig. 4 illustrates the solution of a static problem for a strain-softening rod. The rod is initially under uniform tensile strain, in the strain-softening range. The initial strain is incremented in small steps until an infinitely small deviation leading to nonuniform strain becomes possible. The solution is obtained by solving numerically, with high accuracy, an integral equation for the incremental strain, expressing the incremental conditions of equilibrium and respecting the unloading conditions for nonlocal damage. The figure on top of Fig. 4 represents the localization instability mode for strain, and the figure at the bottom for nonlocal damage. The symmetric curve is obtained at a smaller strain than the asymmetric curve when strain localize at the br ends. This means that the actual mode of instability is a symmetric one. This solution proves that not only the nonlocal damage, but also the strain does not localize to a point.

Fig. 5 shows the solution of the same problem for two

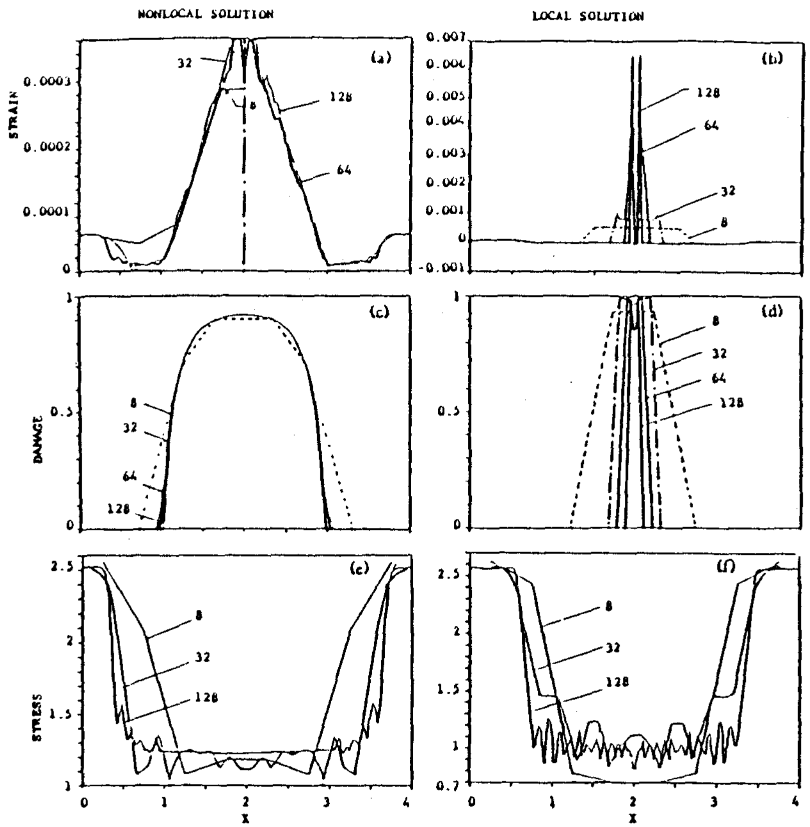

Fig. 2 Convergence of the profiles of strain, damage and stress calculated for wave propagation in a strain-softening bar (labels of the curves indicate the number of elements along the bar).

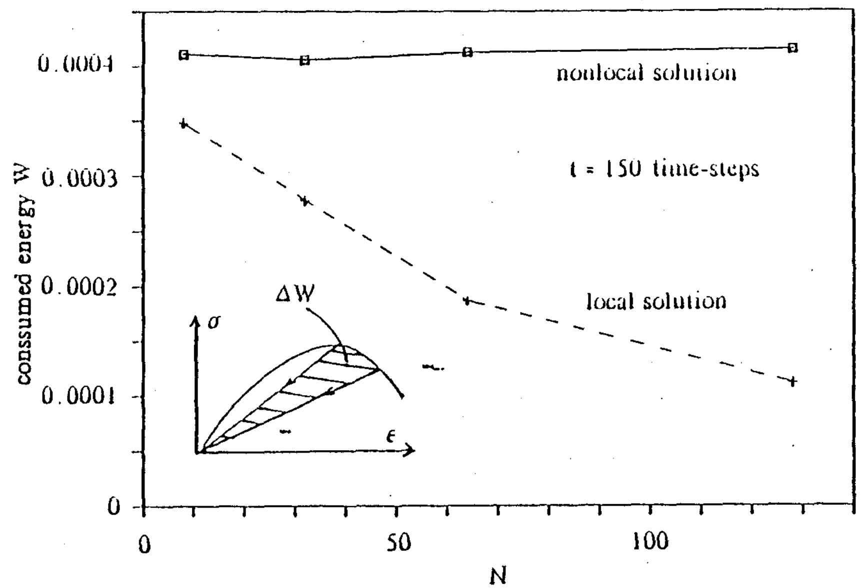

Fig. 3 Convergence of energy dissipated in the dynamically loaded strain-softening rod for both the local and nonlocal solutions.

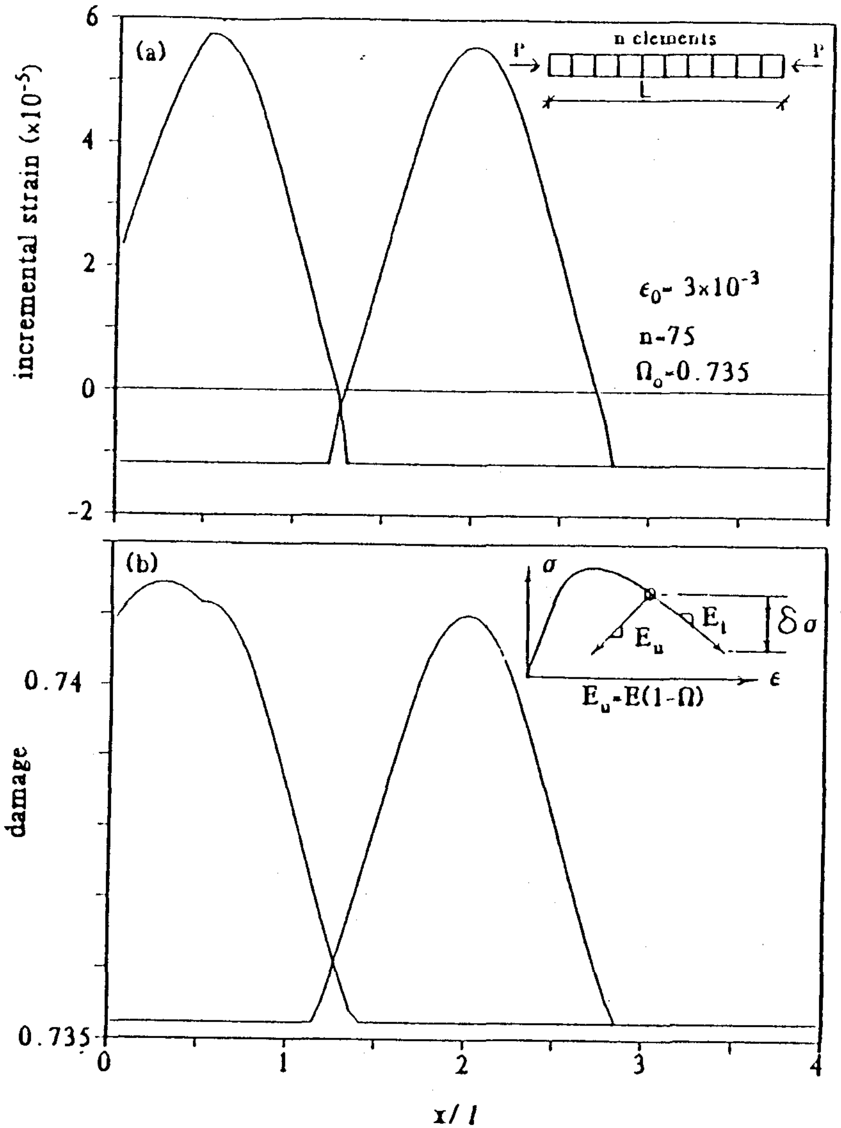

Fig. 4 Static localization stability in a bar initially at uniform strain in strain-softening range.

different versions of the nonlocal damage formulation. In the damage averaging version, the nonlocal damage is obtained by the averaging of local damage, as we already explained in the preceding equations. In the energy averaging version, the nonlocal damage is obtained as a function of the nonlocal damage energy release rate which is obtained by spatial averaging of the local damage energy release rate Y. It is seen that the difference between the two solutions is relatively small. It has been also noted that the damage averaging version converges somewhat faster as the bar subdivision into elements is refined. Recall that the energy averaging version has a certain disadvantage with regard to possible periodic distributions of strain increment, as already mentioned.

The convergence as the subdivision of the bar is refined is illustrated in Fig. 6 in which the distributions are labeled by the number of elements within the bar. The convergence is compared for averaging with a uniform weighting function, with a triangular weighting function and with an error density weighting function (Fig. 6 top, middle, bottom). We see that in the first case the convergence is the slowest, and in the last case by far the best. It is for this reason that smooth weighting functions such as the error density function should be preferred.

Conclusion

The nonlocal continuum with local strain, in which strain-softening is characterized by nonlocal damage, serves as a localization limiter and at the same time is relatively simple to implement in finite element codes. With regard to the previously proposed imbricate nonlocal finite element formulation for strain-softening, the present formulation has four distinct advantages:

1. The field equations of equilibrium and the boundary conditions or interface conditions have the standard form, and no extra boundary conditions are needed.

2. The finite element model has the same conti. requirements as the standard local finite element model.

3. The imbrication of finite elements introduced in the original nonlocal formulation is unnecessary with the present approach.

4. The continuum exhibits no periodic zero-energy instability modes, and so an overlay with the local continuum which was previously introduced to stabilize the continuum against such modes is unnecessary with the present formulation.

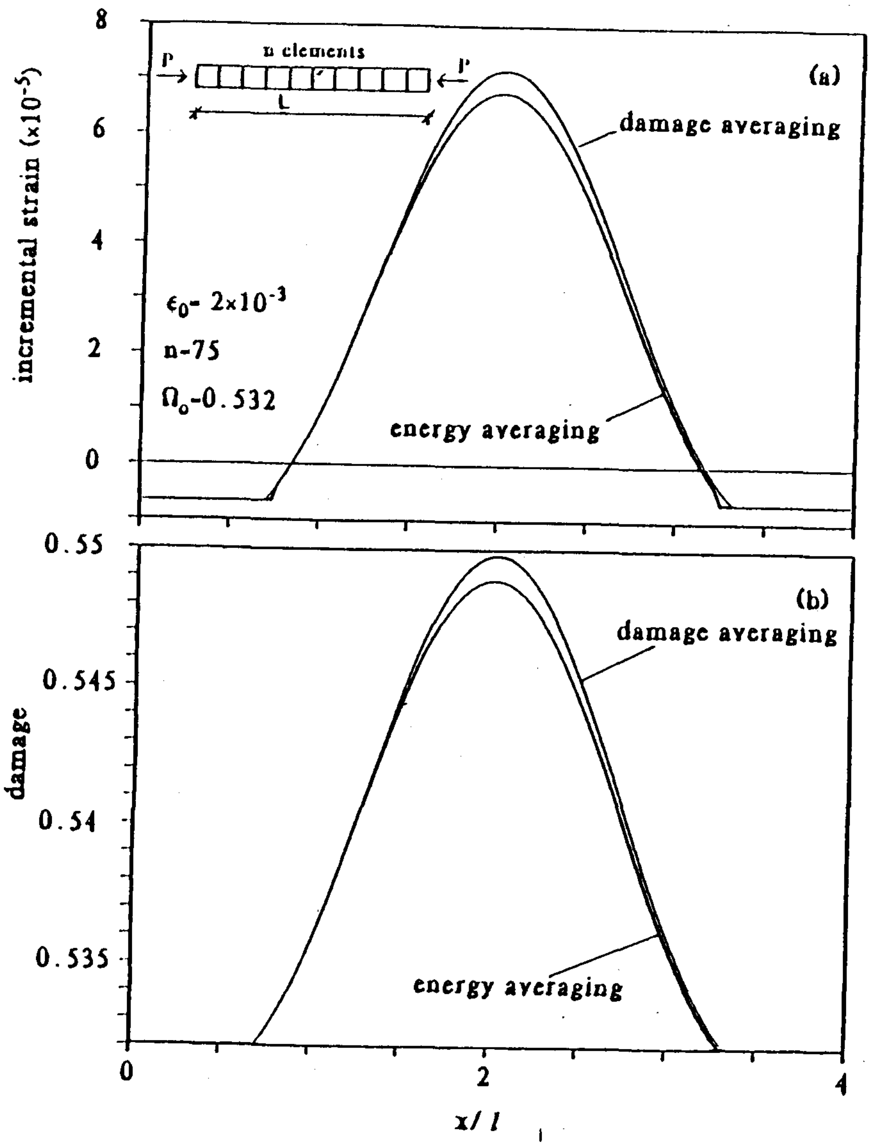

Fig. 5 Static instability in a bar initially at uniform strain, calculated for damage averaging and for damage energy release rate averaging.

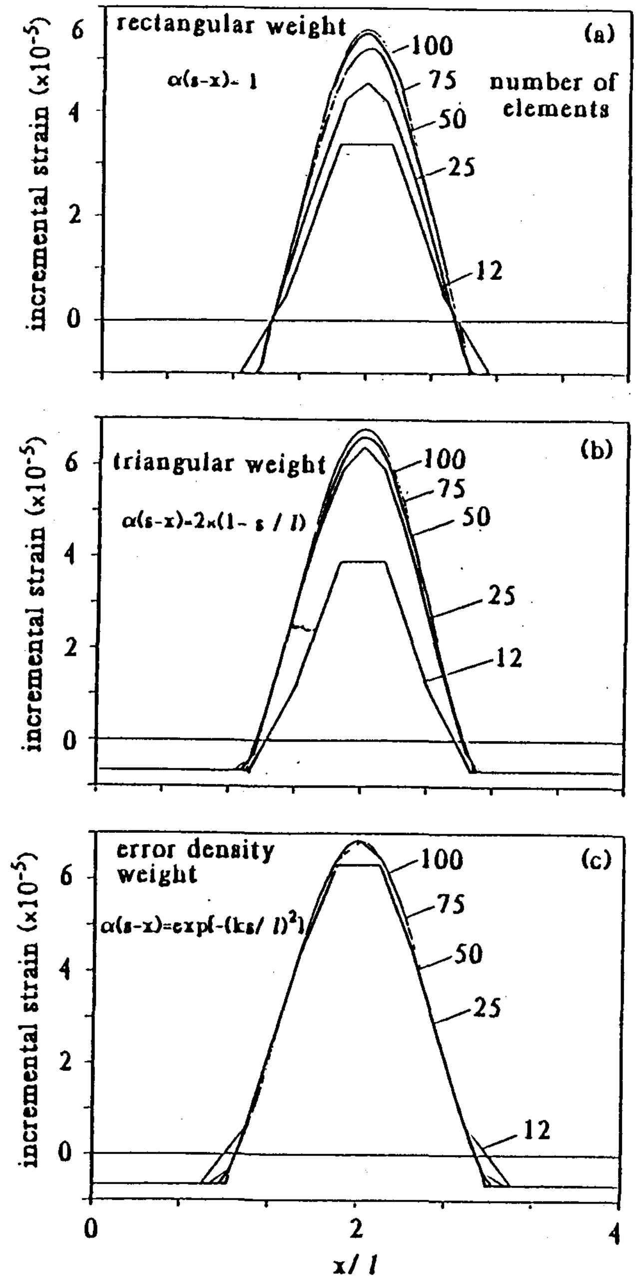

Fig. 6 Convergence of the distributions of incremental strain at the point of instability of a bar initially strained uniformly in strain-softening range, obtained from various weighting functions (uniform, triangular, and error density functions).

Smooth weighting functions give much better convergence than unsmooth ones. On mesh refinement, the energy dissipation for the present model converges to a finite value, as required.

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