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A THERMODYNAMIC CONSISTENT DAMAGE FORMULATION BASED ON A NONLOCAL DAMAGE ACTIVATION THRESHOLD

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ABSTRACT

The paper deals with a formulation for nonlocal (integral) continuum damage models where the thermodynamic principles are consistently satisfied for nonlocal media. The nonlocal field is chosen to be an internal variable which describes the activation damage threshold. The present approach possesses several analogies with a recent one proposed by Polizzotto *et al.* [1,2] for elastic-plastic softening material models. The present choice shows that, when structural strain localization starts to develop, the amplitude of the damage band tends to become narrower and narrower as the damage loading proceeds, but the solution is kept objective with respect to mesh refinements. It is a remarkable fact that the amplitude of the damage band naturally evolves without introducing any "ad-hoc" rule for the evolution of the internal length. As a drawback, a nonlocal iteration procedure is required in order to establish the damage active region.

KEYWORDS

Damage, Nonlocal formulation, Thermodynamics, Localization.

INTRODUCTION

An effective way of modelling the constitutive behaviour of quasi-brittle materials is the so-called continuum damage mechanics, which is able to represent the overall volumetric degradation of the material elastic properties and eventually the induced strain softening state [3]. On the other hand, it is known that specific difficulties arise when strain softening regime develops, mainly related to constitutive instability matters [4]. Classical local theories lead to solutions in which strain fields localize in bands with zero width measure and, consequently, the collapse occurs with zero global energy dissipation. Such a physical meaningless condition has revealed to be an intrinsic limit of the traditional formulations applied to softening regimes. These difficulties can be removed introducing regularization techniques, which basically require a proper internal length scale parameter.
Among several regularization techniques, the most effective seem to be the gradient [5,6] and the nonlocal (integral) approaches [4,7-9], which have been developed, and successfully applied, by many researchers. Modern nonlocal formulations consider as nonlocal, i.e. obtained by a spatial integral averaging, only a suitable scalar measure associated to the dissipative softening process, preserving as local all the other involved variables. In this way, traditional field relations, like equilibrium and

compatibility, remain of local type, whereas, the nonlocality complexities are confined within the dissipative part of the constitutive relations.
The present contribution starts by selecting as nonlocal field a specific internal variable which is directly related to the yield limit of the damage activation function. This choice is alternative to the most common choices which selects as nonlocal field the damage, or its thermodynamic conjugate force, which is the energy released rate. The mechanical meaning of the present choice is that when a point suffers damage flow, the neighbour points register a reduction of their damage limit strength, so that a diffusion, or a nonlocal redistribution, of the damage is possible.
The present formulation also focuses on the thermodynamic consistency of the nonlocal model and a reasoning path, recently presented for nonlocal plasticity models [1,2], is considered. In fact, as a consequence of the nonlocality, the second principle of thermodynamics is enforced in an integral form all over the spatial domain occupied by the body. Its local form is still existing but it needs an additional term, the nonlocality residual, which is related to the energy exchanges of the mutually interacting particles.

FORMULATION

In order to derive a formulation which satisfy a-priori thermodynamic restrictions, let us consider an elastic-damage material for which the Helmholtz free energy is written as

$$\psi(\boldsymbol{\varepsilon}, d, \kappa, \bar{\kappa}) = \psi_e(\boldsymbol{\varepsilon}, d) + \psi_{in}^{l}(\kappa) + \psi_{in}^{nl}(\bar{\kappa}) = \frac{1}{2}(1-d)^2 \boldsymbol{\varepsilon} : \boldsymbol{C}_0 : \boldsymbol{\varepsilon} + \frac{1}{2} h_l \kappa^2 + \frac{1}{2} h_{nl} \bar{\kappa}^2, \tag{1}$$

where $\boldsymbol{\varepsilon}$ is the (infinitesimal) strain tensor, d is the damage variable, κ and $\bar{\kappa}$ are two internal variables which describe the damage evolution and are local and nonlocal, respectively. Isotropic damage is here considered, so that the damage d is a scalar variable ranging within the interval $[0, 1]$. $\boldsymbol{C}_0$ is the elastic moduli tensor of the undamaged material. In analogy with the elastic strain energy, ψ_e, the internal energies ψ_{in}^{l} and ψ_{in}^{nl} have been assumed as quadratic forms of the local and nonlocal internal variables and, consequently, linear hardening laws follow, where $h_l > 0$ and $h_{nl} < 0$ are the hardening/softening damage moduli. The nonlocality affects only the internal variable $\bar{\kappa}$ and the physical meaning is that, when damage develops in a point, its strength to further damage developments increases by local hardening $h_l\, \kappa$, whereas the strength of the neighbour points decreases by the nonlocal damage hardening $h_{nl}\, \bar{\kappa}$. A nonlocal operator $\mathcal{R}$ transforms the local scalar field $\kappa(\boldsymbol{x})$ in the nonlocal counterpart $\bar{\kappa}(\boldsymbol{x})$ by means of the following integral relation

$$\bar{\kappa}(\boldsymbol{x}) = \mathcal{R}(\kappa)\big|_x = \frac{1}{V_r(\boldsymbol{x})} \int_V \alpha(||\boldsymbol{x} - \boldsymbol{y}||)\, \kappa(\boldsymbol{y})\, dV(\boldsymbol{y}), \tag{2}$$

where $\alpha(r)$ is a spatial influence function, which is not negative and decrease with the distance $r = ||\boldsymbol{x} - \boldsymbol{y}||$. Moreover, $V_r(\boldsymbol{x})$ is the representative volume defined as

$$V_r(\boldsymbol{x}) = \int_V \alpha(||\boldsymbol{x} - \boldsymbol{y}||)\, dV(\boldsymbol{y}). \tag{3}$$

The influence function is usually chosen as the Gaussian error function, $\alpha(r) = \exp[-(kr/\ell)^2]$, where ℓ is the material internal length scale.
To enforce the satisfaction of the second principle of thermodynamics, let us write the Clausius-Duhem inequality in global form over the entire domain V

$$\int_V (\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi})\, dV \geq 0. \tag{4}$$

Equation (4) can be written in a pointwise form after the introduction of the nonlocality residual function $P(\boldsymbol{x})$, [1,2,10], which takes in to account the energy exchanges between neighbour particles

$$\mathcal{D} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi} + P \geq 0 \qquad \text{in } V, \tag{5}$$

where $\mathcal{D}$ indicates the intrinsic local dissipation. Assuming the body a thermodynamically isolated system, the following insolation condition holds

$$\int_V P\, dV = 0. \tag{6}$$

Substitution of (1) into (5) leads to

$$\mathcal{D} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \frac{\partial \psi}{\partial d}\dot{d} - \frac{\partial \psi}{\partial \kappa}\dot{\kappa} - \frac{\partial \psi}{\partial \bar{\kappa}}\dot{\bar{\kappa}} + P \geq 0 \qquad \text{in } V, \tag{7}$$

which holds for any, reversible or irreversible, deformation mechanism. Following standard procedures, it is possible to recognize the following state laws:

$$\boldsymbol{\sigma} = \frac{\partial \phi}{\partial \boldsymbol{\varepsilon}} = (1-d)^2\, \boldsymbol{C}_0 : \boldsymbol{\varepsilon}, \qquad\qquad Y := -\frac{\partial \psi}{\partial d} = (1-d)\boldsymbol{\varepsilon} : \boldsymbol{C}_0 : \boldsymbol{\varepsilon} \tag{8a,b}$$

$$\chi := \frac{\partial \psi}{\partial \kappa} = h_l\, \kappa, \qquad\qquad \chi_{nl} := \frac{\partial \psi}{\partial \bar{\kappa}} = h_{nl}\, \bar{\kappa} = h_{nl}\, \mathcal{R}(\kappa), \tag{8c,d}$$

so that the explicit form of the dissipation function reads

$$\mathcal{D} = Y\dot{d} - \chi\, \dot{\kappa} - \chi_{nl}\, \dot{\bar{\kappa}} + P \geq 0 \qquad \text{in } V. \tag{9}$$

The thermodynamic force Y, conjugated to the damage d, represents the energy release for unitary increment of damage. χ and χ_{nl} are the thermodynamic forces associated to the local κ and nonlocal $\bar{\kappa}$ internal variables, respectively. The dissipative irreversible mechanism associated to the damage is governed by the local fluxes $\dot{d}$, $\dot{\kappa}$. The dissipation $\mathcal{D}$ can therefore alternatively be written as the bilinear form

$$\mathcal{D} = Y\, \dot{d} - X\, \dot{\kappa} \geq 0 \qquad \text{in } V, \tag{10}$$

where X represents the equivalent nonlocal force that is associated to the increment of the local variable κ. By comparing eqs. (9) and (10), we can specify P as

$$P = \chi\, \dot{\kappa} + \chi_{nl}\, \dot{\bar{\kappa}} - X\, \dot{\kappa} \qquad \text{in } V. \tag{11}$$

The imposition of the insulation condition (6) leads to

$$\int_V \left(\chi\, \dot{\kappa} + \chi_{nl}\, \dot{\bar{\kappa}} - X\, \dot{\kappa}\right) dV = 0 \tag{12}$$

for each dissipative mechanism and then for each $\dot{\kappa}$. It can be shown that the following (Green) identity holds for the operator $\mathcal{R}$

$$\int_V \chi_{nl}\, \mathcal{R}(\dot{\kappa})\, dV = \int_V \mathcal{R}^*(\chi_{nl})\, (\dot{\kappa})\, dV, \tag{13}$$

where $\mathcal{R}^*$ is the adjoint operator of $\mathcal{R}$ defined by

$$\mathcal{R}^*(\chi_{nl})\big|_x = \int_V \frac{1}{V_r(\boldsymbol{y})} \alpha(||\boldsymbol{x} - \boldsymbol{y}||)\, \chi_{nl}(\boldsymbol{y})\, dV(\boldsymbol{y}). \tag{14}$$

By considering identity (13), eq. (12) turns out to be

$$\int_V \left[\mathcal{R}^*(\chi_{nl}) + \chi - X\right] \dot{\kappa}\, dV = 0. \tag{15}$$

Since (15) has to hold for any possible damage mechanism, and thus for any choice of $\dot{\kappa}$, it follows

$$X = \mathcal{R}^*(\chi_{nl}) + \chi \qquad \text{in } V. \tag{16}$$

After substitution of (16) in (10), the dissipation can be written in explicit form

$$\mathcal{D} = Y\,\dot{d} - [\chi + \mathcal{R}^*(\chi_{nl})]\,\dot{\kappa} \geq 0. \tag{17}$$

The structure of the dissipation in eq. (17) justifies the assumption of a damage activation function $\phi(Y, X)$, which, in the hypothesis of associative damage behaviour, gives the following flow rules:

$$\dot{d} = \frac{\partial \phi}{\partial Y}\dot{\lambda}, \qquad \dot{\kappa} = -\frac{\partial \phi}{\partial X}\dot{\lambda}, \qquad \text{in V.} \tag{18a}$$

Finally, the usual loading/unloading conditions complete the constitutive damage nonlocal relations

$$\phi(Y, X) \leq 0, \qquad \dot{\lambda} \geq 0, \qquad \phi\dot{\lambda} = 0 \qquad \text{in } V. \tag{18b}$$

Relations (18) are analogous to the correspondent relations characterizing local formulations for generalized standard materials [3]. At difference with the local case here, an extra term appears in the damage activation function, that is $\bar{\chi}^*_{nl} = \mathcal{R}^*(\chi_{nl})$ and, therefore, eqs. (18) is a system of spatially coupled relations. In the present paper, for sake of simplicity, the nonlocal damage activation function

$$\phi(Y, \chi, \bar{\chi}^*_{nl}) \equiv Y - \chi - \bar{\chi}^*_{nl} - Y_0 \leq 0 \tag{19}$$

has been assumed.

FINITE ELEMENT DISCRETIZATION

A nonlinear finite element structural analysis requires an iterative incremental solution procedure, in which the equilibrium, and the constitutive relations, are satisfied implicitly in a stepwise form, i.e.

$$\sum_{e=1}^{Ne} \int_{V_e} \boldsymbol{B}_e^T(\boldsymbol{x})\,\boldsymbol{\sigma}_{k+1}(\boldsymbol{x})\,dV = \boldsymbol{F}_{k+1}, \tag{20}$$

where Ne is the total number of elements, $\boldsymbol{B}_e$ is the compatibility matrix and $\boldsymbol{F}$ is the equivalent nodal load vector. Equation (20) is the equilibrium condition to be enforced using an iterative scheme of Newton type. Inside the equilibrium loop, the integration of the constitutive relations, between the previous equilibrium state, k, and the new one, $k+1$, has to be carried out. Indicating with Δ the increment of a quantity in the step, the discrete form of the constitutive relations (18) reads

$$\Delta d = \left.\frac{\partial \phi}{\partial Y}\right|_{k+1} \Delta\lambda = \Delta\lambda, \qquad \Delta\kappa = -\left.\frac{\partial \phi}{\partial X}\right|_{k+1} \Delta\lambda = \Delta\lambda, \tag{21a}$$

$$\phi_{k+1} \leq 0, \qquad \Delta\lambda \geq 0, \qquad \Delta\lambda\,\phi_{k+1} = 0. \tag{21b}$$

Due to the nonlocality nature of X_{k+1}, equations (21b) represent an integral complementarity problem that cannot be solved localwise, but it rather requires an inner iterative loop inside the equilibrium equations.

Iterative scheme

The iterative equilibrium procedure gives the increment displacement vector $\Delta\boldsymbol{u}$ and, consequently, the increment of total strains $\Delta\boldsymbol{\varepsilon}$.

The procedure that leads to the satisfaction of the nonlocal spatially coupled constitutive relations (21) is based on:

- a *predictor* phase: at each integration point the trial value of the damage activation function is evaluated as
$$\phi_{k+1}^{tr} = Y_{k+1}^{tr} - X_k - Y_0, \tag{22}$$
where $Y_{k+1}^{tr} = (1-d_k)(\boldsymbol{\varepsilon}+\Delta\boldsymbol{\varepsilon}) : \boldsymbol{C}_0 : (\boldsymbol{\varepsilon}+\Delta\boldsymbol{\varepsilon})$ and X_k is the nonlocal internal variable obtained at the previous equilibrium iteration. If, at some points $\phi_{k+1}^{tr} > 0$, then a corrector phase is necessary, otherwise a new equilibrium loop begins;
- a *corrector* phase: a further iterative inner loop is devoted to the identification of the damage active points as well as the damage increments. The procedure used closely follows the scheme originally proposed by Strömberg and Ristinmaa [11] for nonlocal plasticity.

The solution of the consistency condition $\phi_{k+1} = 0$ is then obtained iteratively. In fact, the solution requires at each point the knowledge of the unknown damage increments of the neighbour points. If a trial damage increment distribution is assumed, the set of equations $\phi_{k+1} = 0$ can be solved at each integration point and a new set of active damage points emerges, i.e. some new points can now be involved and some other can cease to be active. The new values are then assumed for a subsequent iteration until fulfillment of eqs. (21b)
The numerical strategy to solve the nonlinear equations $\phi_{k+1} = Y_{k+1} - X_{k+1} - Y_0 = 0$, where

$$X_{k+1}(\boldsymbol{x}) = h_l(d_k(\boldsymbol{x}) + \Delta d(\boldsymbol{x})) + h_{nl} \int_V \frac{\alpha(||\boldsymbol{x}-\boldsymbol{y}||)}{V_r^2(\boldsymbol{y})} \int_V \alpha(||\boldsymbol{y}-\boldsymbol{z}||)[d_k(\boldsymbol{z}) + \Delta d(\boldsymbol{z})]\, dV(\boldsymbol{z})\, dV(\boldsymbol{y}) \tag{23}$$

is based on a modified Newton-Raphson technique. The linearization of the consistency condition leads to

$$\phi_{k+1}(d + \Delta d + \delta d) = \phi_{k+1}(d + \Delta d) + \left.\frac{\partial \phi}{\partial\, \Delta d}\right|_{d+\Delta d} \delta d = 0, \tag{24}$$

which gives the correction increment

$$\delta d = -\left[\frac{\partial \phi}{\partial\, \Delta d}\right]^{-1}_{d+\Delta d} \phi_{k+1}(d + \Delta d). \tag{25}$$

Finally, instead of evaluating the Hessian, the following (local) approximation is adopted

$$\frac{\partial \phi}{\partial\, \Delta d} \approx [h_l + h_{nl} + (\boldsymbol{\varepsilon}+\Delta\boldsymbol{\varepsilon}) : \boldsymbol{C}_0(\boldsymbol{\varepsilon}+\Delta\boldsymbol{\varepsilon})] \tag{26}$$

so that eq. (25), which is spatially coupled, can be evaluated localwise.
Numerical tests have shown that this approach is quite effective, even if the nonlocal iteration loop inside the equilibrium iterations increases the overall computational cost of the analysis.

NUMERICAL APPLICATIONS

In order to investigate the capability of the proposed method, a simple application has been carried out. The analysis has been performed for a 1-D bar in a uniform state of stress. The length of the bar is 100 mm. In the middle part there is a zone, 10 mm long, where an initial damage has been imposed in order to trigger the damage localization. The material is characterized by the Young's modulus $E = 20000$ N/mm^2, the hardening parameters are assumed as $h_l = 0.0008$ N/mm^2 and $h_{nl} = -0.0004$ N/mm^2. Finally, the initial damage threshold is $Y_0 = 0.0001$ N/mm^2 and the internal length is $\ell = 5$ mm. The bar has been discretized by simple constant strain elements and the analysis has been performed with 20, 40, 80 and 160 elements. Figure 1a shows the load-displacement curves for the four different discretizations. It appears that the response is objective with respect to mesh refinement, at least until the very last part of the analysis. In Figure 1b, the damage distributions, at different levels of the loading process, are reported with reference to the analysis performed with

160 elements. It can be observed that the strain localization phenomenon is well regularized and, moreover, the damage band tends to shrink as the damage loading proceed. This aspect is quite remarkable, since it has been obtained without enforcing any special evolution law for the internal length parameter, which is kept constant in the analysis.
To conclude, numerical tests of 2-D structures are at the moment under study. It is expected that such analysis will confirm the above discussed properties of the presented thermodynamically consistent damage model.

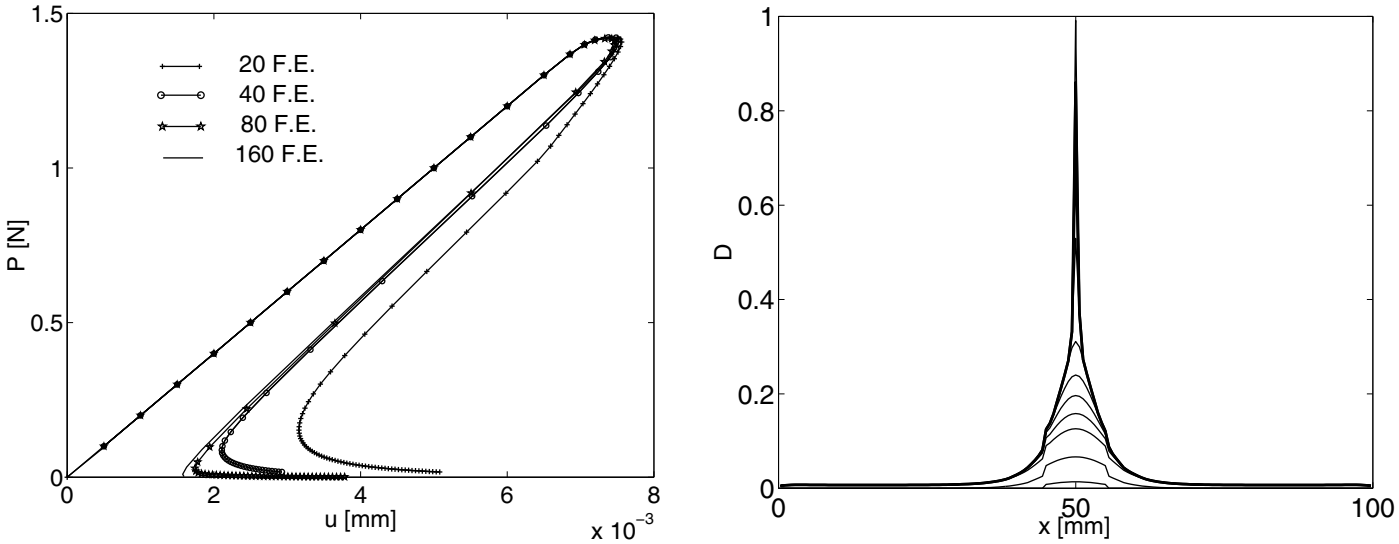

Fig. 1 (a) Load-displacement curves obtained with 20, 40, 80 and 160 elements. (b) Evolution of the damage profile at increasing damage loading steps. Results obtained with 160 elements.

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