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ON IMPLICIT GRADIENT MODELS FOR QUASI-BRITTLE MATERIALS

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Abstract
In the context of the Continuum Damage Mechanics, different types of non-local formulations are discussed, i.e., non local integral models, and gradient models both of explicit and implicit type. A unifying approach is described, based on the introduction of the nonlocality constraint into the energy expression through a lagrangian multiplier. Therefore, the solving equations of the problems follow as stationarity conditions of the lagrangian functional. Finally, some numerical results for a 2D example are presented.

Sommario
Vengono discussi alcuni modelli non locali di tipo integrale, gradiente esplicito ed implicito nell'ambito della Meccanica del Danneggiamento. Si mostra che le equazioni risolventi possono anche essere ricavate dal calcolo delle condizioni di stazionarietá del funzionale lagrangiano ottenuto introducendo, tramite un moltiplicatore di Lagrange, il vincolo di nonlocalitá nell'espressione dell'energia. Infine, si riportano alcuni risultati numerici relativi ad un esempio 2D.

1. Introduction

Quasi-brittle materials generally exhibit a load-carrying capacity which decreases for increasing values of the strain after a (strain) threshold has been overcome. The equilibrium is governed by partial differential equations, which, in case of softening behavior, lose ellipticity in quasi static analysis or hyperbolicity in dynamics [1]. Correspondingly, the tendency of the calculated strain field to localize into a volume with zero width measure can be observed, so that the bulk deformation energy dissipated into the process zone tends to vanish. As a numerical counterpart, the response of standard finite elements models pathologically depends on the size and the orientation of the adopted mesh: different meshes lead to different solutions.

What is lacking, is the presence of a finite bound on the dissipation of energy, and this can be obtained by assuming at the constitutive level some internal lengths characteristic of the material [2]. For instance, thus justifying the evident recent interest in nonlocal models, the existence of a finite characteristic length is guaranteed if the principle of local action is abandoned [3].

However, some mechanical and numerical aspects of the nonlocal formulations should be clarified. For example, the choice regarding which of the involved variables should be written as non local is really a crucial point. No agreement has been reached in literature about the mechanical consistency of averaging a state variable as the strain, rather than some internal variable, like the damage or the equivalent strain. [2, 4].

In the context of the Damage Continuum Mechanics, here, different types of nonlocal formulations will be considered, i.e., non local integral models, and gradient models both of explicit and implicit type. In Sections 4 and 5, a unifying approach will be described, based on the introduction of the nonlocality constraint into the energy expression through a lagrangian multiplier. The solving equations of the problems follow as stationarity conditions of the lagrangian formulation.

2. Isotropic damage: basic relationships

The constitutive relation for a damaging material can be written in the usual form

$$\boldsymbol{\sigma} = (1 - D)\,\mathbb{E}\boldsymbol{\varepsilon}\,, \tag{1}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ represent, respectively, the stress and the infinitesimal strain tensor, $\mathbb{E}$ is the constitutive tensor of the sound material, D is the damage parameter, more precisely scalar in the case of isotropic damage, and such that $D = 0$ when the material is sound, whereas $D = 1$ for a complete state of damage. According to [2] and [4], it is assumed that the damage depends on a suitable scalar function of the strain tensor, the equivalent strain ε_{eq}, $D = D(\varepsilon_{eq})$. For instance, in [5]

$$\varepsilon_{eq}(\boldsymbol{\varepsilon}) = \sqrt{\sum_{i=1}^{3} \langle \varepsilon_i \rangle^2}, \tag{2}$$

with ε_i, $i = 1, 2, 3$, the principal strains and $\langle\cdot\rangle = \frac{|\cdot|+\cdot}{2}$. Alternatively, the following form of the equivalent strain can be considered [6]

$$\varepsilon_{eq}(\boldsymbol{\varepsilon}) = \frac{r-1}{2r(1-2\nu)} I_1 + \frac{1}{2r}\sqrt{\frac{(r-1)^2}{(1-2\nu)^2} I_1^2 + \frac{2r}{(1+\nu)^2} J_2}\,, \tag{3}$$

where ν is the Poisson coefficient, and the strain tensor invariants I_1 and J_2 are defined as

$$I_1 = tr(\boldsymbol{\varepsilon}) = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \tag{4a}$$

$$J_2 = 3tr(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}) - tr^2(\boldsymbol{\varepsilon}) = (\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_2 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_1)^2\,, \tag{4b}$$

and $r = \sigma_{fc}/\sigma_{ft}$ denotes the ratio between the compressive and the tensile strengths, so that if r tends to infinite no failure due to compression can occur. Because the evolution of the damage depends on the deformation history, a threshold parameter κ has to be introduced to indicate the most severe deformation the material has experienced, or, in other words, the threshold of the equivalent strain over which the damage increments. Following [2, 6], the damage D and κ are related by

$$D(\kappa) = \begin{cases} 0 & \text{if } \kappa < \kappa_0 \\ 1 - \frac{\kappa_0}{\kappa}[1 - \alpha + \alpha \exp(-\beta(\kappa - \kappa_0))] & \text{otherwise} \end{cases}, \tag{5}$$

where α and β are parameters to be determined experimentally, and κ_0 is an initial damage threshold. The resulting stress strain relation for a homogeneous (local) material in the one-dimensional case is described by Figure 1.

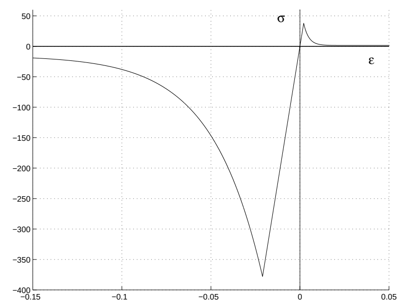

Figure 1: One-dimensional stress strain relation (E=18000 N/mm^2, $r = 10$).

3. Nonlocal formulations

It has been showed that it is not necessary to consider as nonlocal all the involved state variables in order to regularize the solution [2]. Because the softening behavior is a consequence of the damage phenomena, it seems reasonable, other than sufficient, to take into account the nonlocal form of the variable which governs the damage itself, i.e., in the present contribution, the equivalent strain ε_{eq}. Practically, from the local variable ε_{eq} the correspondent non local variable

$$\bar{\varepsilon}_{eq} = L(\varepsilon_{eq}), \tag{6}$$

is derived, where the operator L is the averaging operator

$$L(\varepsilon_{eq})(x) = \int_{V(x)} \psi(x - s)\, \varepsilon_{eq}(s)\, ds, \tag{7}$$

ψ being a suitable weight function defined over the whole body with volume $V(x)$. For instance, Ψ can be taken as the Gauss function $e^{-k^2 r^2/l^2}$, where r denotes the distance between the point at hand and the surrounding points, k is a constant, and l introduces an interaction length. Alternatively, provided the Taylor expansion of ε_{eq} exists, $L(\varepsilon_{eq})$ can be approximated through a gradient in the explicit form

$$L(\varepsilon_{eq})(x) = \varepsilon_{eq}\,(x) + c\nabla^2\varepsilon_{eq}\,(x) \qquad \text{on } \Omega \tag{8a}$$
$$\nabla\varepsilon_{eq}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega, \tag{8b}$$

where c is a positive scalar, which influences the width of the computed process volume. In the two-dimensional case, and for the choice $k = 2$, the gradient constant c and the parameter of the gaussian l are related by $c = l^2/16$. As shown above, a boundary condition has to be imposed in case of gradient formulations for providing a solution to the differential equation (8.a). Here, the widely used boundary condition (8.b) has been adopted, where $\mathbf{n}$ and ∇ are, respectively, the normal to the boundary of the body and the gradient operator, and ∇^2, multiplied by the constant c, represents the laplacian, which can be written

$$\nabla^2\varepsilon_{eq} = div(\nabla\varepsilon_{eq}). \tag{9}$$

It should be underlined, that the choice (8.b) has been not mechanically motivated. It partially recalls [7], where, for elasto-plastic non local material, $\nabla\boldsymbol{\varepsilon}^P\cdot\mathbf{n} = 0$ on the boundary of the process zone, $\boldsymbol{\varepsilon}^P$ being the plastic strain component. However, the problem of the definition of suitable boundary conditions arises also in the case of nonlocal integral models, because of the modification of the averaging operator at the boundary [8].

Gradient formulations in the implicit form

$$\bar{\varepsilon}_{eq}(x) = \varepsilon_{eq}(x) + c\nabla^2\bar{\varepsilon}_{eq}(x) \qquad \text{on } \Omega, \tag{10a}$$
$$\nabla\bar{\varepsilon}_{eq}\cdot\mathbf{n} = 0 \qquad \text{on } \partial\Omega, \tag{10b}$$

have been proposed as alternative to the explicit form (8), also[4, 6]. It is worth noting, that the advantage of using implicit formulation with respect to the explicit one, lies in the fact that, in this case, the laplacian operator applies to $\bar{\varepsilon}_{eq}$, which is treated as an independent unknown, and not to the local field, which can be not smooth. Let us also observe that, from the numerical point of view, the two cases of integral and gradient models should be distinguished. In the latter case, indeed, the necessity of calculating the second derivative of the local field can be alleviated by application of the Gauss-Green formula, but the price to pay is that the additional boundary condition (8.b), or (10.b), has to be specified.

In [9], a comparison between explicit and implicit type gradient formulations (for plasticity) reveals that the amount of spurious stress oscillations is reduced in the latter case with respect to the former one. For the sake of an example of implicit gradient model, let us consider that formulated in [4, 6] for quasi-brittle damaging materials, where the displacement and the averaged equivalent strain fields are unknown. Let us consider the case of a body with volume Ω, subject to body forces $\mathbf{b}$, to tractions $\mathbf{p}$ on the portion Γ_p of the boundary Γ, with prescribed displacements $\bar{\mathbf{u}}$ on Γ_u. The incremental equilibrium problem

$$
\begin{aligned}
div\,\dot{\boldsymbol{\sigma}} + \dot{\mathbf{b}} =& 0 && \text{on } \Omega, && \text{(11a)}\\
\dot{\boldsymbol{\sigma}} \cdot \mathbf{n} =& \dot{\mathbf{p}} && \text{on } \Gamma_p, && \text{(11b)}\\
\dot{\mathbf{u}} =& \dot{\bar{\mathbf{u}}} && \text{on } \Gamma_u, && \text{(11c)}\\
\bar{\varepsilon}_{eq}(x) =& \varepsilon_{eq}(x) + c\nabla^2\bar{\varepsilon}_{eq}(x) && \text{on } \Omega, && \text{(11d)}
\end{aligned}
$$

has been solved by considering the weak form of each equation in (11) (weighted residual method) through standard finite element method, and applying the Gauss Green formula to the term with the laplacian. The damage parameter D, which appears in the definition of the stress (1), is considered to be a function of the averaged equivalent strain $\bar{\varepsilon}_{eq}$, $D = D(\bar{\varepsilon}_{eq})$. The loading function $f = \bar{\varepsilon}_{eq} - \kappa$ governs the damage evolution according to the Kuhn Tucker conditions

$$
\dot{\kappa} \geq 0, \quad f \leq 0, \quad f\,\dot{\kappa} = 0\,. \tag{12}
$$

4. A Lagrangian formulation for an implicit gradient model

In alternative to the above presented formulation, it is possible to introduce the constraint of nonlocality, in its most general expression (6), by means of a lagrangian multiplier into the principle of virtual power, which does not require the existence of a potential energy and can be written also for non-conservative problems (for instance, for the explicit gradient case, in [10], a kinematic constraint is incorporated in this way in the virtual power functional). Whenever the problem is selfadjoint, the latter approach is equivalent to minimize the total potential energy. In the following, we will focus our attention on the minimum of a functional, which is analogous to the potential energy written in terms of velocity, subject to the constraint of non locality (6). It can be showed that this procedure is general and contains as particular cases some of the formulations previously proposed in the literature.

From here on, for simplicity, the overwritten dots indicating incremental quantities will be omitted and zero body forces will be considered. The problem of finding the minimum points of the functional

$$
\mathcal{F}(\mathbf{u}, \bar{\varepsilon}_{eq}) = \int_\Omega \frac{1}{2}\boldsymbol{\varepsilon} : (1 - D(\bar{\varepsilon}_{eq}))\mathbb{E} : \boldsymbol{\varepsilon}\; d\Omega - \int_\Gamma \mathbf{p}\mathbf{u}\; dS\;, \tag{13}
$$

subject to (gradient relation of implicit type)

$$
\mathcal{G}(\mathbf{u}, \bar{\varepsilon}_{eq}) = \bar{\varepsilon}_{eq} - c\nabla^2\bar{\varepsilon}_{eq} - \varepsilon_{eq} = 0\;, \tag{14}
$$

is studied. In analogy with [7], the boundary condition

$$
\nabla\bar{\varepsilon}_{eq} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \tag{15}
$$

is imposed a priori. The above problem is equivalent to that of finding the saddle points of

$$
\mathcal{L}(\mathbf{u}, \bar{\varepsilon}_{eq}, \lambda) = \mathcal{F}(\mathbf{u}, \bar{\varepsilon}_{eq}) + \int_\Omega \lambda\,(\bar{\varepsilon}_{eq} - c\nabla^2\bar{\varepsilon}_{eq} - \varepsilon_{eq})\; d\Omega, \tag{16}
$$

where λ denotes the lagrangian multiplier. If we remember (9), the term on which the laplacian operator applies to the averaged equivalent strain can be transformed by application of Gauss-Green formula. Therefore, after imposition of the boundary condition (15), the functional (16) can be written as

$$\mathcal{L}(\mathbf{u}, \bar{\varepsilon}_{eq}, \lambda) = \int_\Omega \frac{1}{2} \boldsymbol{\varepsilon} : (1 - D(\bar{\varepsilon}_{eq}))\mathbb{E} : \boldsymbol{\varepsilon} \, d\Omega + \int_\Omega [\lambda(\bar{\varepsilon}_{eq} - \varepsilon_{eq}) + c\nabla\lambda \cdot \nabla\bar{\varepsilon}_{eq}] \, d\Omega - \int_\Gamma \mathbf{p} \cdot \mathbf{u} \, dS. \tag{17}$$

The boundary condition (14) is weakened to

$$\int_{\partial\Omega} \lambda(\nabla\bar{\varepsilon}_{eq} \cdot \mathbf{n}) \, dS = 0, \tag{18}$$

which is obviously satisfied if equation (15) is assumed, and this probably is the actual justification of this choice. It is worth remarking, that the condition (15) seems to be more reasonable when the non local field is derived from an internal variable, like the equivalent strain ε_{eq}, and not from a state variable, like, for instance, the strain; in the latter case, in fact, the flux of the strain field across the boundary can not be arbitrarily set equal to zero. As it will be showed in the following section, such a problem does not arise if the integral formulation is considered, because no higher order derivatives are implied.

Now, discretization of the continuous unknown fields ($\mathbf{u}$, $\bar{\varepsilon}_{eq}$, λ) is performed by setting

$$\mathbf{u}(x) = \mathbf{N}(x)\underset{\sim}{\mathbf{u}}; \quad \bar{\varepsilon}_{eq}(x) = \tilde{\mathbf{N}}(x)\underset{\sim}{\bar{\varepsilon}_{eq}} \quad \lambda(x) = \tilde{\mathbf{N}}(x)\underset{\sim}{\lambda}$$
$$\boldsymbol{\varepsilon}(x) = \mathbf{B}(x)\underset{\sim}{\mathbf{u}}; \quad \nabla\bar{\varepsilon}_{eq}(x) = \tilde{\mathbf{B}}(x)\underset{\sim}{\bar{\varepsilon}_{eq}} \quad \nabla\lambda(x) = \tilde{\mathbf{B}}(x)\underset{\sim}{\lambda}\,, \tag{19}$$

where the same interpolation functions are chosen for approximation of $\bar{\varepsilon}_{eq}$ and of the lagrangian multiplier λ.

Requiring the stationarity conditions of the discretized functional leads to a non linear system of equations, to be solved through an iterative process. The same set of equations can be obtained starting from the virtual work principle and assuming the same basis function for virtual and real displacements.

We may point out, that three unknown fields have been considered, because the lagrangian multiplier is an additional unknown, while, in the implicit gradient formulation [4], two unknown fields are computed. On the other hand, here, the tangent stiffness matrix is symmetric and not asymmetric at variance with the one in [4].

5. Lagrangian formulation for an integral model

Let us consider the stationarity of the following functional

$$\mathcal{L}(\mathbf{u}, \bar{\varepsilon}_{eq}, \lambda) = \mathcal{F}(\mathbf{u}, \bar{\varepsilon}_{eq}) + \int_\Omega \lambda \left(\bar{\varepsilon}_{eq} - \int_V \psi(x - s)\varepsilon_{eq} \, ds\right) d\Omega,$$

where $\mathcal{F}(\cdot,\cdot)$ is defined as in (7). Again, we reduce ourselves to calculate the stationarity condition of the corresponding discretized form.

let us observe, that a Penalty method could be employed at the place of the Lagrangian method. In this case, the saddle points of the functional

$$\mathcal{L}(u, \bar{\varepsilon}_{eq}, \lambda) = \mathcal{F}(u, \bar{\varepsilon}_{eq}) + \frac{\gamma}{2} \int_{\Omega} (\bar{\varepsilon}_{eq} - \int_{V} \psi(x-s) \varepsilon_{eq} \, ds)^2 \, d\Omega. \qquad (20)$$

have to be found, where γ is a the penalty parameter, and no additional unknowns are introduced into the variational formulation.

6. Numerical examples

As an example, the concrete specimen studied by Hassanzadeh [11] is ana-

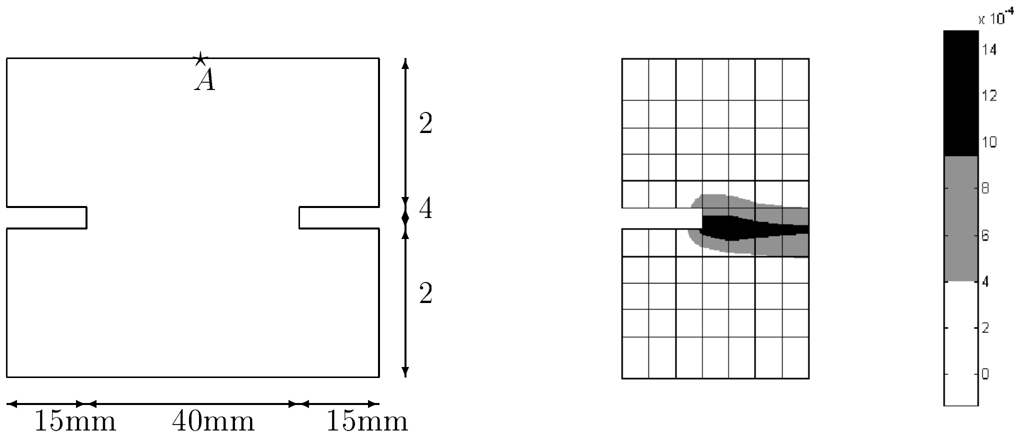

Figure 2: 2.1) Concrete specimen: geometrical features 2.2) Contour plot of $\bar{\varepsilon}_{eq}$ for $P = 58$ N

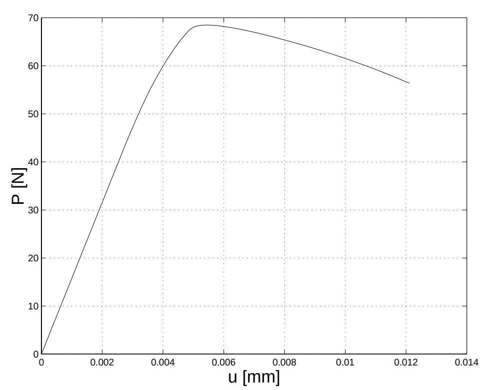

Figure 3: Total load versus vertical displacement of the point A.

lyzed through the implicit gradient model [4], where the gradient parameter c has been set equal to 1 mm^2. However, in this numerical example, a uniform distribution of traction loads is considered applied at the top of the specimen, whereas the nodes at the bottom are fixed. The loading procedure has been controlled by means of an arc length technique. The equivalent strain definition (4), and the damage relation (5) have been used, where the ratio between compressive and tensile strength $r = 10$, the parameters $\alpha = 0.96$, $\beta = 350$, and the damage threshold $\kappa_0 = 10^{-4}$ have been assumed. The material has a Young modulus E= 32900N/mm^2, and a Poisson ratio $\nu = 0.2$. A plane stress state has been considered.

Because of the symmetry of the specimen, only one half of it has been studied. The mesh of Figure 2.2 has been adopted, constituted by 74 eight-noded serendipity elements for the displacement field and four-noded bilinear elements for the averaged equivalent strain field. Moreover, both fields have been integrated with a four-point integration scheme.

The damage zone, strictly related to the value of the averaged equivalent strain, tends to localize at the notch (see Figure 2). The resultant total load has been plotted (Figure 3) versus the vertical displacement of the point A placed on the symmetry axis (see Figure 2.1).

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