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Nonlinear Elastic Brittle Problems: Operator Split Methods in Numerical Solution

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ABSTRACT: In order to avoid the loss of well-posedness in the post-localization range, some continuum damage theories for elastic materials introduce higher order gradients of the damage variable in the constitutive model. Although such theories allow a mathematically correct modelling of the strain localization phenomena, they are usually considered very complex to handle from the numerical point of view. The present work is concerned with the numerical implementation of a gradient-enhanced damage theory for elastic materials. A simple numerical technique, based on the finite element method, is proposed to approximate the solution of the resulting nonlinear mathematical problems. The coupling between damage and strain variables is circumvented by means of a splitting technique.

Introduction

In the last few years, many different continuum damage theories have been proposed. Since the increase of damage generally leads to a local softening behaviour, the models based on a local approach, see (1) and (2), may lead to a physically unrealistic description of strain localization phenomena when the hypothesis of quasi-static and isothermal processes are considered. In general, due to the loss of ellipticity of the governing equations in the post-localization range, the resulting mathematical problems may present an infinity number of solutions with discontinuous fields of displacement gradients what leads to numerical difficulties of mesh-dependence, see (3) - (7).

Some alternative approaches to the local damage theories have been proposed in the last years, see **(8) - (11)** for example. The present paper deals with an alternative theory in which the continuum is supposed to possess a microstructure. Since damage results from microscopic movements, it is proposed a reformation of the kinematics and of some basic governing principles of the classical Continuum Mechanics in order to account for such "micromovements". The constitutive equations are developed within a thermodynamic framework - the free energy is supposed to depend not only on the strain and the damage variable but on the damage gradient as well. Besides, to account for microscopic effects, the power of the internal forces depends not only on the velocity and its gradient, but also on the damage velocity and its gradient

The main goal of the present paper is to present a numerical technique for approximating the resulting nonlinear mathematical problems. The coupling between damage and strain is circumvented by means of a splitting technique which allows to study the nonlinear problem through a sequence of simpler linear problems. This technique requires, at each time step, the solution of two problems: one similar to an equilibrium problem in linear elasticity and the other similar to a heat transfer problem in a rigid body. In order to assess the main features of the numerical method, a number of examples is presented showing that the numerical computations are not mesh dependent.

Modelling

A body is defined as a set of material points B which occupies a region Ω of the Euclidean space at the reference configuration. In this theory, besides the classical variables that characterize the kinematics of a continuum medium (displacements and velocities of material points), an additional scalar variable $\beta \in [0,1]$, is introduced. This variable is related with the links between material points and can be interpreted as a measure of the local cohesion state of the material. If $\beta = 1$, all the links are preserved and the initial material properties are preserved. If $\beta = 0$ a local rupture is considered since all the links between material points have been broken. The variable β is associated to the damage variable D by the following relation: $\beta = 1 - D$. Since the degradation is an irreversible phenomena, the rate $\dot{\beta}$ must be negative or equal to zero.

A detailed presentation of the basic principles that govern the evolution of such kind of continuum can be found in **(12)**, **(13)** and **(14)**. A summary of the basic principles are presented in this section. For the sake of simplicity the hypothesis of quasi-static and isothermal processes is adopted throughout this work. Besides it is also assumed the hypothesis of small deformation and consequently the conservation of mass principle is automatically satisfied.

The Principle of Virtual Power

Let a body B that occupies a region $\Omega \subset R^3$ with a sufficiently regular boundary Γ be subjected at each time instant t to external forces $g(t) : \Gamma_2 \subset \Gamma \to R^3$, $b(t) : \Omega \to R^3$ to external microscopic forces $p(t) : \Omega \to R$, $q(t) : \Gamma_2 \subset \Gamma \to R$ and to prescribed displacements $u(t) = 0$ em $\Gamma_1 \subset \Gamma$, where $\Gamma = \Gamma_1 \cup \Gamma_2$ and $\Gamma_1 \cap \Gamma_2 = \varnothing$.

Under the hypothesis of slow deformations, the inertial effects can be neglected and the principle of Virtual Power can be expressed as:

$$\pi_{int} + \pi_{ext} = 0 \tag{1}$$

for any admissible variations of the fields (u and β) that characterize the kinematics of the medium.

The power π_{int} of the internal generalized forces σ , F and H can be written as:

$$\pi_{int} = -\int_{\Omega} (\sigma \cdot \nabla \hat{u}) dV - \int_{\Omega} (F\hat{\beta} + H \cdot \nabla \hat{\beta}) dV \tag{2}$$

Here $\hat{u} : \Omega \to R^3$ is an element of the set V_v of the virtual velocities $\hat{u}$ such that $\hat{u} \,|\, \Gamma_1 = 0$ and $\hat{\beta} : \Omega \to R$ is an element of the set V_β of the virtual variations of β .

The corresponding power π_{ext} of the external generalized forces b, g, p and q assumes the representation:

$$\pi_{ext} = \int_{\Omega} (b \cdot \hat{u}) dV + \int_{\Gamma_2} (g \cdot \hat{u}) dA + \int_{\Omega} (p\hat{\beta}) dV + \int_{\Gamma} (q\hat{\beta}) dA \tag{3}$$

Where $p : \Omega \to R$ is defined as a microscopic distance force while $q : \Gamma \to R$ is a microscopic contact force, both in duality with β . The microscopic forces are related to non

mechanical actions (chemical and electromagnetic, for instance), that can cause an evolution of the damage.

Under assumptions of π_{int} and π_{ext} and the hypothesis of slow deformations, the inertial effects can be neglected and the principle of virtual power can be expressed as:

$$\int_{\Omega} [\sigma \cdot (\nabla \hat{u}) - b \cdot \hat{u}] dV - \int_{\Gamma_2} (g \cdot \hat{u}) dA + \int_{\Omega} [H \cdot (\nabla \hat{\beta}) + F\hat{\beta} - p\hat{\beta}] dV -$$

$$- \int_{\Gamma} (q\hat{\beta}) dA = 0, \quad \forall \hat{u} \in V_v, \ \forall \hat{\beta} \in V_\beta \tag{4}$$

Constitutive Equations

Under the hypothesis of small deformations and isothermal processes, the free energy is supposed to be a function of the deformation ε, the temperature θ, the damage variable β and its gradient $\nabla\beta$. In order to resume the presentation, the thermodynamic framework used to obtain the constitutive equations is not presented in this paper, for further details see **(12)**. The final relations are the following:

$$\sigma = (\frac{\beta E}{1+\nu})[\frac{\nu}{1-2\nu} tr(\varepsilon) I + \varepsilon] = \beta[\lambda (tr\ \varepsilon) I + 2\mu\ \varepsilon] \tag{5}$$

$$F = (\frac{E}{2(1+\nu)})[\frac{\nu}{(1-2\nu)} (tr(\varepsilon))^2 + \varepsilon . \varepsilon] - w + \lambda_\beta + C\dot{\beta} + \lambda_{\dot{\beta}} =$$

$$= [\frac{1}{2}\lambda (tr\ \varepsilon)^2 + \mu\ \varepsilon . \varepsilon] - w + \lambda_\beta + C\dot{\beta} + \lambda_{\dot{\beta}} \tag{6}$$

$$H = k(\nabla\beta) \tag{7}$$

Where E is the Young modulus, ν is the Poisson's ratio and λ and μ are the Lamé constants. The therms λ_β and $\lambda_{\dot{\beta}}$ are lagrange multipliers associated, respectively, to the constraints $\beta \geq 0$ and $\dot{\beta} \leq 0$, they are such that: $\lambda_\beta \leq 0$, $\beta\lambda_\beta = 0$ and $\lambda_{\dot{\beta}} \leq 0$, $\dot{\beta}\lambda_\beta = 0$.

The Mechanical Problem

Introducing the constitutive equations (5), (6) in (4), neglecting the external microscopic forces (which are related to chemical or electromagnetic actions) and considering the initial conditions: $\beta(x, t=0)=1,\ \forall x \in \Omega$, the following mathematical problem is obtained:

Find $(u(x,t), \beta(x,t))$, respectively the displacement field $u(t): \Omega \rightarrow R^3$ such that $u(t)|_{\Gamma_1} = \bar{u}(t)$ and the field $\beta(t): \Omega \rightarrow R$ such that, for all time instant $t \in [0, \tau]$:

$$\int_{\Omega} \beta(t)[\lambda\, \mathrm{divu}\, \mathrm{div}\, \hat{u} + 2\mu\ \varepsilon(u).\varepsilon(\hat{u})]dV - \int_{\Omega} b(t).\hat{u}dV - \int_{\Gamma_2} g.\hat{u}dA = 0 \quad \forall \hat{u} \in V_v \tag{8}$$

$$\int_{\Omega} (k\nabla\beta).\nabla\hat{\beta}\, dV + \int_{\Omega} [\frac{1}{2}\lambda\, (\mathrm{divu})^2 + \mu\ \varepsilon.\varepsilon - w]\, \hat{\beta} dV + \int_{\Omega} C\dot{\beta}\hat{\beta}\, dV = 0 \quad \forall \hat{\beta} \in V_{\beta} \tag{9}$$

Subjected to the following constraints:

$$0 \leq \beta \ \text{ e } \ \dot{\beta} \leq 0$$

And with the following initial condition:

$$\beta(t=0) \equiv 1$$

Numerical Aproximation

The nonlinear mathematic damage evolution problem resulting from the model, accounting for the coupling between damage and displacement fields, can be solved through a staggered algorithm, in which the coupled system is partitioned, often according to the different coupled fields, and each partition can be treated by a different time-stepping algorithm.

The approach proposed in this work is motivated by the realization that a partition of the coupled system only defines an operator split of the evolution problem. In this context, a staggered scheme is viewed as a product formula algorithm dictated by the specific operator split, exactly as in the classical method of fractional steps, see (15). This point of view is

also adopted in (16), where standard staggered algorithms for coupled thermomechanical problems, consisting of an isothermal phase followed by a heart conduction phase at fixed configuration, are cast into the format of a fractional step method.

Semi-Discrete Problem: Finite Element Methods

The solution of the damage evolution problem is based on a spatial discretization using the Finite Element Methods (FEM) leading in a semi-discrete version constituted of a nonlinear system of Ordinary Differential Equations (EDO). This system is accomplished by means of a splitting strategy resulting in a sequence of simpler evolution problems, which are in turn solved by standard techniques like backward and forward Euler and the trapezoidal rule, see (17).

Let the base function (or interpolation function) traditionally provided by the MEF, see (18), $N_i \in V_v^h$, where V_v^h is a finite sub-space of the space V_β, and $\varphi_i \in V_\beta^h$, where V_β^h is a finite sub-space of the space V_β. These base functions allow the construction of the following approximations:

$$u_h(x,t) = \sum_{i=1}^{m_h} u_i(t) N_i(x), \; i = 1,\ldots, m_h$$

$$\beta_h(x,t) = \sum_{i=1}^{m_h} \beta_i(t) \varphi_i(x), \; i = 1,\ldots, m_h \qquad (10)$$

Where m_h is the nodal point number of the finite element mesh and h is the mesh parameter, a scalar that is associated with the mesh refinement.

The semi-discrete problem is obtained by replacing u by u_h and β by β_h, defined by equation (10), in equations (8) and (9). The semi-discrete problem is a nonlinear system of ordinary differencial equations with the following form:

$$\mathbf{K}[(\beta_h)]\underline{u} = \mathbf{R} \tag{11}$$

$$\mathbf{C}\dot{\underline{\beta}} + \mathbf{A}\underline{\beta} + \mathbf{F}(\underline{u}) = 0 \tag{12}$$

With the following initial condition:

$$\beta_h(x,0) = 1 \quad \text{e} \quad u_h(x,0) = 0$$

And the following constraints:

$$0 \le \beta_h(x,t) \le 1 \quad \text{e} \quad \dot{\beta}_h(x,t) \le 0.$$

Where,

$$[\mathbf{K}(\beta_h)]_{ij} = \int_\Omega \beta_h \, [\mathbf{B}^T\mathbf{D}\mathbf{B}]_{ij} dV, \quad i,j = 1,\ldots 3*m_h \tag{13}$$

$$[\mathbf{R}]_i = \int_\Omega b_k N_l \, dV - \int_\Gamma g_k N_l \, dA \; ; \tag{14}$$

$$[\mathbf{C}]_{ij} = \int_\Omega C\varphi_i\varphi_j \, dV, \quad i,j = 1,\ldots m_h \tag{15}$$

$$[\mathbf{A}]_{ij} = \int_\Omega (k\nabla\varphi_i \nabla\varphi_j) dV, \quad i,j = 1,\ldots m_h \; ; \tag{16}$$

$$[\mathbf{F}(\underline{u})]_i = \int_\Omega [\frac{1}{2}(\overline{\mathbf{B}}^T\mathbf{D}\mathbf{B}\ \underline{u}\cdot\underline{u}) - w]\varphi_i \, dV, \quad i,j = 1,\ldots m_h \tag{17}$$

and **B** denotes the standard discretized differential operator and **D** is the matrix of the elastic constitutive coefficients, defined according (**18**).

The Operator Split Technique Applied to the Semi-Discrete Problem

The Operator Split Technique is used to approximate the nonlinear semi-discrete problem through a sequence of simpler linear problems. Two partitions of operator were considered, one related to u_h ("equilibrium problem") and the other to β_h ("damage evolution problem"). The proposed scheme can result in two different algorithms depending on the order of the sequence of the operators. These algorithms, resumed below, will be named DANO_1 and DANO_2.

The DANO_1 algorithm first solves the "damage evolution problem", remaining the displacement field unaltered. At this first stage, the associated ordinary differential equation is solved using a time integration method, that can be described as:

$$\mathbf{C}[\theta\beta^{n+1}+(1-\theta)\hat{\beta}^{n}]+\Delta t[\theta\,\mathbf{A}\,\beta^{n+1}+(1-\theta)\,\mathbf{A}\,\beta^{n}]+\Delta t\,{}^{n}[\theta\,\tilde{\mathbf{F}}^{\,n+1}+(1-\theta)\,\mathbf{F}^{\,n}]=0 \quad (18)$$

Where, θ define the integration method: $\theta=0$, forward Euler; $\theta=1$, backward Euler and $\theta=1/2$, trapezoidal rule, see (17). The subscript h was omitted and the superscript n means that the function is approximated at the instant t_n. Besides, $\tilde{F}^{n+1}$ does not represent the function F evaluated at t_{n+1}, since u_{n+1} is not known. At the first phase ($\dot{u}=0$) $\tilde{F}^{n+1}$ is calculated using u_n.

The second phase of DANO_1 solves the "equilibrium problem":

$$\mathbf{K}[(\underline{\beta}_{n+1})]\underline{\mathbf{u}}_{n+1}=\mathbf{R}_{n+1} \quad (19)$$

Where,

$$[\mathbf{R}_{n+1}]_i=\int_{\Omega}(b_k)_{n+1}N_i\,dV-\int_{\Gamma}(g_k)_{n+1}N_i\,dA \quad (20)$$

The DANO_2 algorithm consists in the order inversion of the stages of DANO_1.

The computational implementation of the two algorithms can be considered simple, since both algorithms can be obtained from a standard finite element scheme. It can be observed that "damage evolution problem" phase is similar to a heat conduction problem, while the other phase, the "equilibrium problem", is similar to a classical elasticity problem.

Analysis of Numerical Examples

In order to assess the features of the modelling in a multiaxial stress state, a problem of a square plate with a central circular hole is analyzed. The square plate (200 mm x 200 mm x 1 mm) with a central circular hole, which radius is 50 mm, is supported at the left side and loaded with a prescribed displacement u(t) at the opposite side, figure 1. Because of the existent symmetry the analysis is performed for the upper right quarter of the plate.

In this study was considered a plate of concrete, which has the following mechanical characteristics: E = 27.0 GPa, w = 5.0×10^{-5} MPa, C = 1.0×10^{-3} MPa.s e

$k = 0.2 MPa.mm^2$, see (19). The prescribed displacement and the adopted time step are respectively given by $u(L,t) = \alpha t$, ($\alpha = 5.0x10^{-3} mm/s$) and $\Delta t = 1.0 \times 10^{-4} s$.

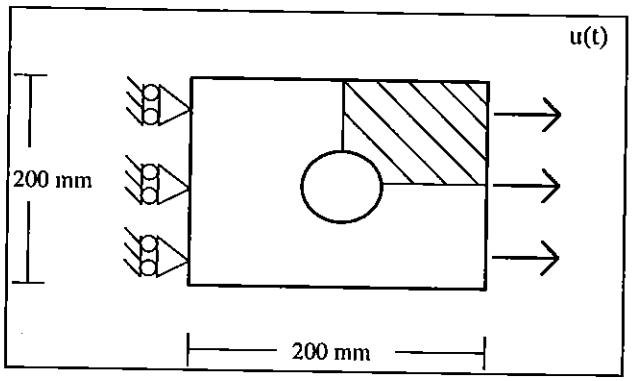


Figure 1: Plate with a central circular hole.

The usual bi-linear quadrilateral finite element is used.

Damage Propagation

The evolution of the damage variable $D = (1-\beta)$ on the plate is depicted in figures 2 up to 5. These figures demonstrate that the damage initially appear at a local near the hole, see figures 2 and 3, what is expected for a body with this kind of geometry and submitted to a tension load. Then the damage propagates in the direction of the free end of the plate, perpendicular to the load direction, until the plate is broken completely.

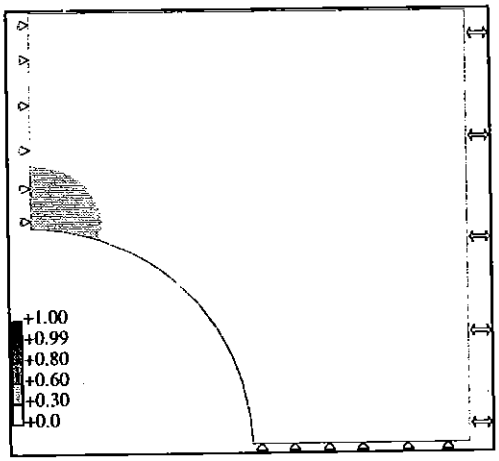


Figure 2: Damage levels, t = 2.5 s.

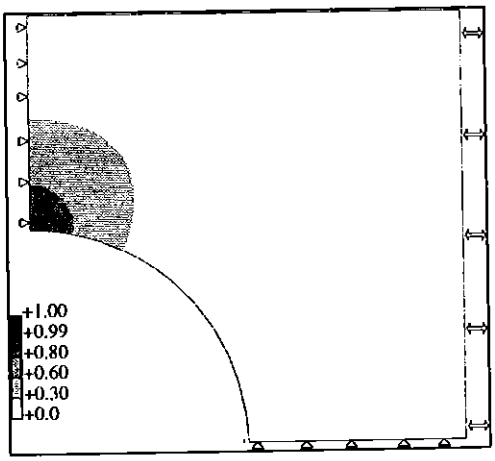


Figure 3: Damage levels, t = 2.8 s.

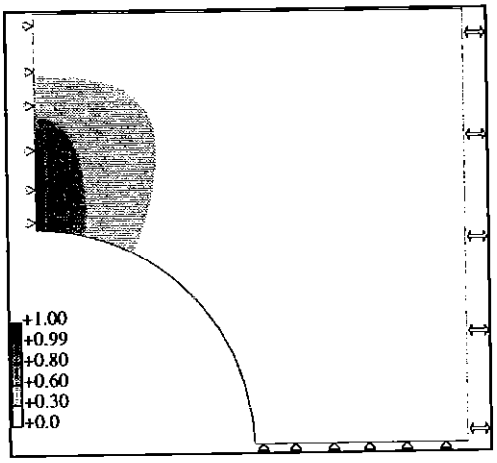


Figure 4: Damage levels, t = 3.0s.

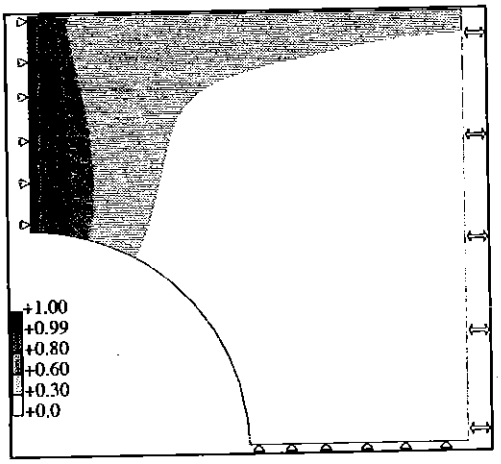


Figure 5: Damage levels, t = 3.35s.

Mesh Dependence

To demonstrate that the problem solution is not mesh-dependent two different spatial discretization meshes, that are presented in the figures 6 and 7, were used. The difference between these meshes is the degree of the discretization in the region where the highest levels of damage occur. Besides, the different levels of damage at the instant t = 3.0s,

obtained using these meshes are also presented. The figures permit to observe that the damage distribution are similar.

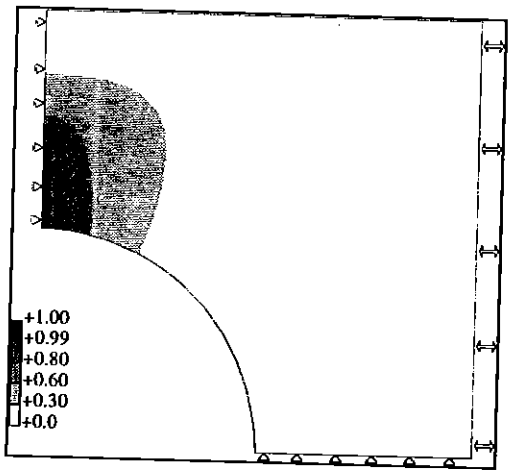
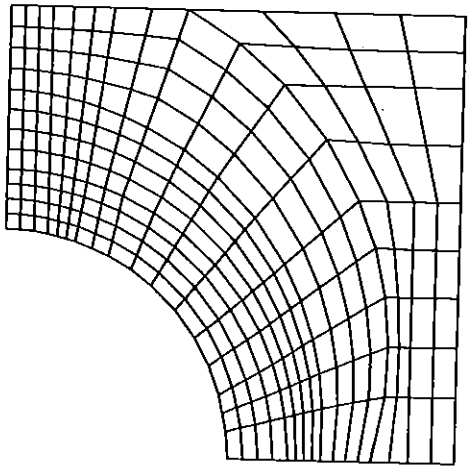


Figure 6: Damage levels, instant t = 3.0s.



Mesh-1: 274 nodes and 240 elements.

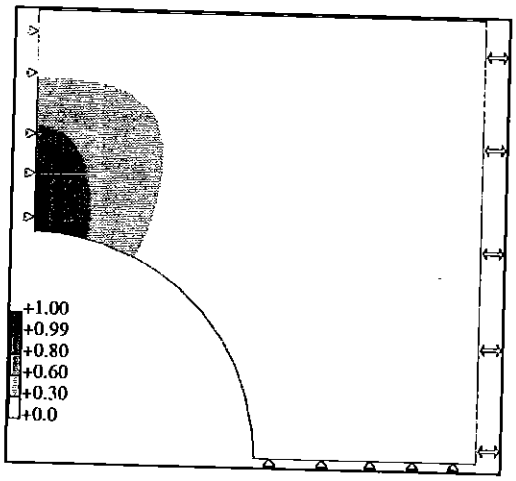
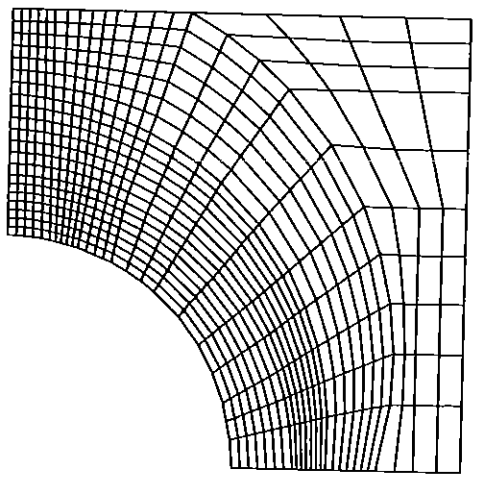


Figure 7: Damage levels, instant t = 3.0s.



Mesh-2: 594 nodes e 544 elements.

The figures 8 permit to observe the behaviour of the damage along the longitudinal lines A (x,y ≈ 53.0 mm) and B (x, y ≈ 60.0 mm). The shape of the curves and the values of the damage at different points along the lines are almost the same.

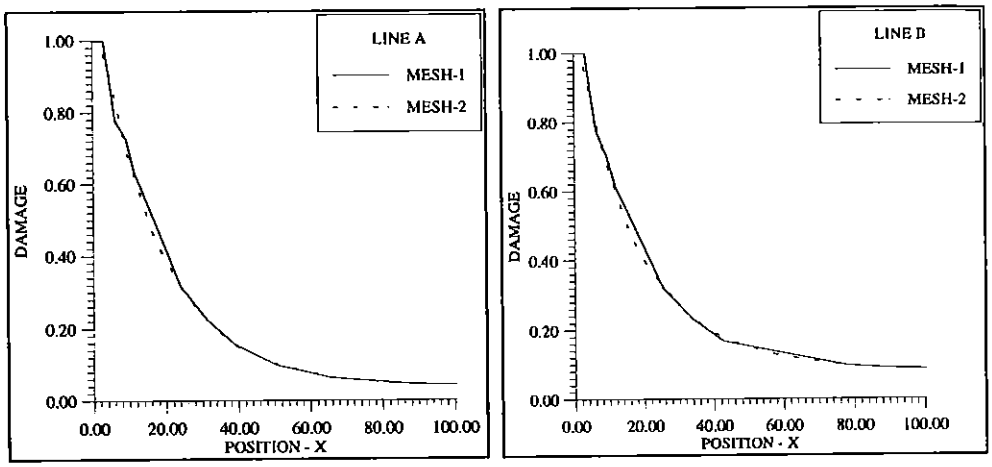


Figure 8: Damage along the lines A and B for different meshes.

The curves of the applied force x displacement obtained using these different meshes are presented to complety the mesh-dependence verification, see figure 9. The result represents the behaviour of the global structure. Once more, it is possible to note that the shape of the solution is not affected by the different spatial discretization. Figure 9 also permits to observe the softening behaviour. The same kind of no mesh-dependence was found in several examples, see **(14)**. So, although no theoretical result is presented, the presented formulation is believed not to suffer of any numerical pathology due to mesh-dependence.

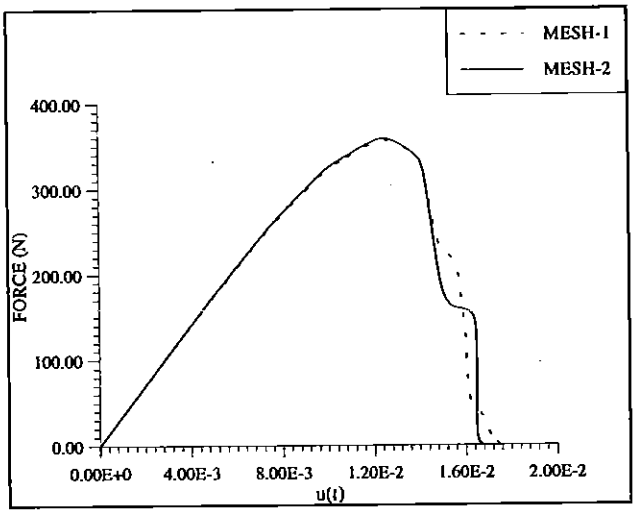


Figure 9: Force x Displacement curves for different meshes.

Precision and Stability of the Proposed Algorithm

The performance of the proposed algorithm is explored in a problem of a rectangular clamped plate, see figure 10, with a prescribed displacement $\bar{u}(t) = \alpha t$ ($u_x(x = L, y) = \alpha t$ e $u_y(x = L, y) = 0$) at the end x = L, plane strain state and the following boundary conditions: $\beta: \frac{\partial \beta}{\partial x} = 0$ in x = 0 e x = L.

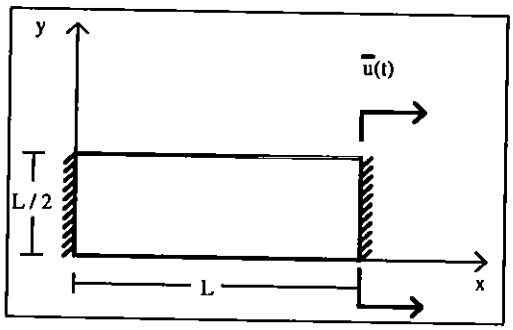


Figure 10: Rectangular plate with prescribed displacement, $\bar{u}(t)$.

The following values were considered: $\alpha = 5.0 \times 10^{-3}$mm/s, L = 20.0mm, E = 50.0GPa, $\nu = 0.2$, w = 0.025MPa, D_{Cr} =1.0, C = 0.1MPa.s and k = 0.1MPa.mm^2.

A mesh of 289 nodal points and 256 elements was used to solve the problem, see figure 11. The dashed line defines the longitudinal line at the central region of the plane, where are the analyzed nodal points (137 up to 153).

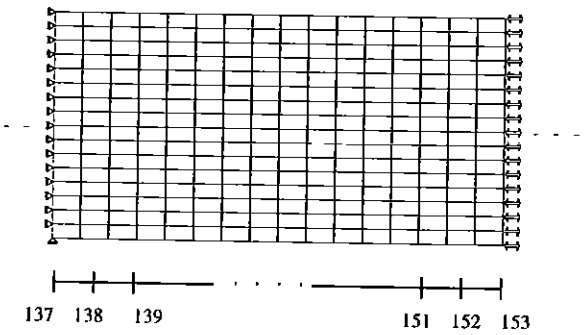


Figure 11: Finite element mesh.

The backward Euler method was adopted to solve the damage evolution problem. The analysis shows that a reasonable time step is 0.001s for this kind of mesh.

The precision analysis of the proposed algorithm consists of comparing the results obtained using the operator split methods with different numerical integration methods (forward and backward Euler and trapezoidal rule) and the results of a coupled solution strategy, where the Euler and Newton Methods are used together.

The figure 12 presents the results obtained using the different numerical methods at the instant t = 5.5 s.

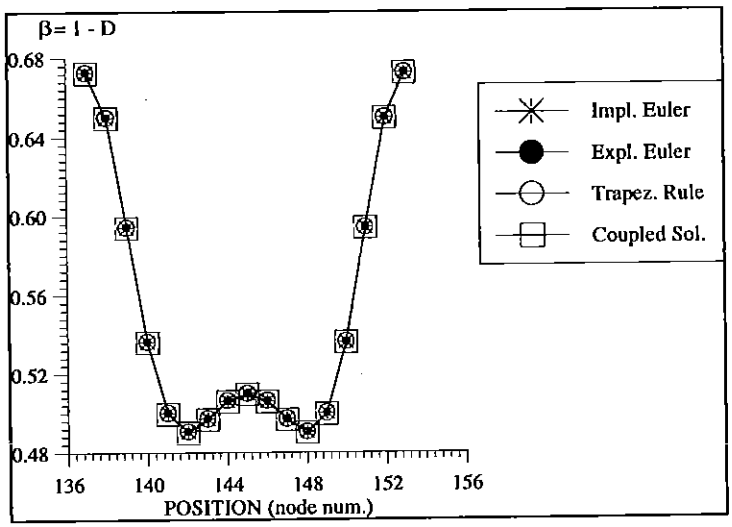


Figure 12: Different numerical methods, t = 5.5 s.

It is possible to observe that the results are quite similar using the different algorithms. Then, the results presented in this section denote that the Operator Split Method was able to give results with the same precision order than the other methods that solve the coupled problem. It is worthwhile to emphasize that the last one have a more expensive computational cost.

Conclusion

A simple numerical method was used to approximate the solution of the resulting nonlinear mathematical problem without the necessity of a radical modification of a ordinary finite element code. This simple numerical method is formed by the combination of MEF and operator split technique, that transform the global nonlinear problem in a sequence of linear problems. Besides, the proposed numerical method have good stability and precision.

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