

COMPARISON OF IMPLICIT-GRADIENT DAMAGE-PLASTIC MODELS

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Abstract: Damage mechanics coupled with the theory of plasticity is a suitable framework for description of the complex behavior of materials such as concrete [Grassl and Jirásek (2006)], steel [Engelen, Geers and Baaijens (2003)], or bone [Charlebois, Jirásek and Zysset (2010)]. However, the classical theory fails after the loss of ellipticity of the governing differential equation. From the numerical point of view, loss of ellipticity is manifested by the patholocical dependence of the results on the size and orientation of the finite elements. This paper describes two different formulations of coupled damage-plastic models, and their nonlocal enhancements based on the implicit gradient approach. The difference between the formulations is discussed and illustrated by a numerical example.

Keywords: damage, plasticity, nonlocal continuum, implicit-gradient formulation

1. Introduction

This paper presents coupled damage-plasticity models. Continuum damage mechanics is suitable for the description of stiffness degradation due to the growth of defects such as micro-voids and micro-cracks, while plasticity theory describes permanent deformations of a material induced e.g. by slip mechanisms. However, standard damage-plasticity models with softening would lead to a pathological sensitivity of the numerical solution, converging to physically meaningless results. In this contribution, two different ways of coupling damage with plasticity are considered, and a method that can provide an objective description of localized inelastic processes is described.

2. Plasticity

The main feature of plasticity models is irreversibility of plastic strain. We restrict our attention to the associative plasticity with isotropic hardening or softening under small strain. The basic equations include an additive decomposition of the total strain into an elastic (reversible) part and a plastic (irreversible) part,

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p,\tag{1}$$

the stress-strain law,

$$\boldsymbol{\sigma} = \mathbb{D}_e : \boldsymbol{\varepsilon}_e, \tag{2}$$

the definition of the yield function

$$f(\boldsymbol{\sigma}, \kappa) = \tilde{\sigma}(\boldsymbol{\sigma}) - \sigma_Y(\kappa) \tag{3}$$

loading-unloading conditions in the Kuhn-Tucker form,

$$f(\boldsymbol{\sigma},\kappa) \le 0 \qquad \dot{\lambda} \ge 0 \qquad \dot{\lambda}f(\boldsymbol{\sigma},\kappa) = 0,$$
 (4)

flow rule as the evolution law for plastic strain

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial f}{\partial \boldsymbol{\sigma}},\tag{5}$$

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evolution law for cumulated plastic strain,

$$\dot{\kappa} = \sqrt{\dot{\varepsilon_p} : \dot{\varepsilon}_p},\tag{6}$$

and the isotropic hardening (softening) law, described by the function $\sigma_Y(\kappa)$ that is embedded in the definition of the yield function (3). In the equations above, σ is the stress tensor, \mathbb{D}_e is the elastic stiffness tensor, $\tilde{\sigma}$ is a seminorm of the stress tensor, λ is the plastic multiplier, κ is the cumulated plastic strain and σ_Y is the current yield stress. An overdot marks the derivative with respect to time. To describe the behavior of a specific material, a concrete form of the stress seminorm has to be introduced. In the subsequent chapters, we will use the Mises yield condition, which belongs to the most used yield criteria and defines the stress seminorm as

$$\tilde{\sigma}(\boldsymbol{\sigma}) = \sqrt{\frac{3}{2}\boldsymbol{s}} \cdot \boldsymbol{s}$$
(7)

where s is the deviatoric part of the stress. Note that for Mises plasticity, yielding has a purely deviatoric character.

2.1. Implementation

To implement the constitutive model into a displacement-driven finite element code, an algorithm for the evaluation of the stress increment from a given strain increment must be developed. This procedure is usually called the stress-return algorithm. The stress return algorithm is based on the elastic-plastic operator split, which consists of a trial elastic predictor followed by the return mapping algorithm. In the first step, the trial stress

$$s^{tr} = 2G\left(e^{n+1} - e_p^n\right) \tag{8}$$

is computed. Here, G is the shear modulus of elasticity and e is the deviatoric part of the strain. If the trial stress satisfies the condition of plastic admissibility, $F(\sigma^{tr}, \kappa^n) \leq 0$, the step is elastic and the trial stress σ^{tr} is accepted as the actual stress σ^{n+1} . If the trial stress violates the yield condition, the step is plastic and the return mapping algorithm has to be used. Here we describe the so-called radial-return algorithm [Krieg and Key (1976)], which represents a radial projection of the trial stress onto the yield surface. The formula for s^{n+1} has the following form:

$$s^{n+1} = s^{tr} - 2G\Delta e_p \tag{9}$$

After using the discrete version of equation (5) in combination with equation (9), we arrive at

$$s^{n+1} = s^{tr} - \sqrt{6}G\Delta\kappa \frac{s^{n+1}}{\|s^{n+1}\|}$$
(10)

Clearly, s^{n+1} and s^{tr} are colinear, thus

$$\frac{s^{n+1}}{\|s^{n+1}\|} = \frac{s^{tr}}{\|s^{tr}\|} \tag{11}$$

Substituting (11) into (10), the radial mapping of the trial stress onto the yield surface is obtained:

$$s^{n+1} = \left(1 - \frac{\sqrt{6}G\Delta\kappa}{s^{n+1}}\right)s^{n+1} \tag{12}$$

Moreover, the yield criterion must be fullfiled at the end of the step:

$$f(s^{n+1}, \kappa^n + \Delta \kappa) = 0 \tag{13}$$

Substitution equation (12) into (13) leads to one nonlinear scalar equation for $\Delta \kappa$. For linear hardening plasticity, in the form $\sigma_Y(\kappa) = \sigma_0 + H\kappa$, this equation is reduced to a linear equation, and $\Delta \kappa$ can be obtained directly as

$$\Delta \kappa = \frac{f^{tr}}{3G + H} \tag{14}$$

where $f^{tr} = f(s^{tr}, \kappa^n)$, H is the plastic modulus, and σ_0 is the initial yield stress.

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3. Coupling of damage and plasticity

In this section, a brief description of the continuum damage mechanics and its coupling with the plasticity theory is discussed, see [Maugin (1992)] for more details. The isotropic damage mechanics is considered, which means that one single scalar damage variable is introduced. The damage variable describes the reduction of stiffness and strength of material due to the creation, coalescence and growth of voids and microcracks. There exists at least two ways of coupling the plasticity theory to the damage mechanics. The first approach is based on the formulation of the plasticity problem in the effective (i.e. undamaged) stress space. The second approach relies on the plasticity formulated in the nominal (i.e. damaged) stress space. For both approaches, the stress-strain law has the form

$$\boldsymbol{\sigma} = (1 - \omega)\bar{\boldsymbol{\sigma}} = (1 - \omega)\mathbb{D}_e : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) \tag{15}$$

where $\bar{\sigma}$ is the effective stress and ω is the damage variable that ranges from zero (virgin material) to one (completely damaged material).

For the model based on effective stress, equations (2)–(5) are reformulated in the effective stress space

$$\bar{\boldsymbol{\sigma}} = \mathbb{D}_e : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p), \tag{16}$$

$$f(\bar{\boldsymbol{\sigma}},\kappa) = \tilde{\sigma}(\bar{\boldsymbol{\sigma}}) - \bar{\sigma}_Y(\kappa), \tag{17}$$

$$f(\bar{\sigma},\kappa) \le 0 \qquad \dot{\lambda} \ge 0 \qquad \dot{\lambda}f(\bar{\sigma},\kappa) = 0,$$
 (18)

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial f}{\partial \bar{\boldsymbol{\sigma}}},\tag{19}$$

Moreover, the damage law is needed. Usually it is postulated as

$$\omega = g(\kappa) \tag{20}$$

For the second group of models, all equations are formulated in terms of nominal stress. However, this formulation can be rewritten in terms of the effective stress, and the hardening (softening) function would by given by

$$\bar{\sigma}_Y = \frac{\sigma_Y}{(1 - g(\kappa))} \tag{21}$$

In the first case, the evolution of damage and the effective yield stress is prescribed, while in the second case the evolution of the nominal yield stress and damage is prescribed. Since the nominal stress is directly available from the stress-strain diagram, it may be simpler to describe it directly and then consider the effective yield stress as a derived quantity. The models are fully equivalent; however, it is neccesary to pay attention when constructing the nonlocal extension. Nonlocal extension of both classes of models will be described in the next chapter.

3.1. Implementation

Implementation of the formulation based on the effective stress is very similar to the implementation of pure plasticity and consist of the return mapping algorithm followed by the explicit evaluation of damage. To implement a damage plastic model based on the nominal stress, the formula for the trial stress has to be changed to

$$\boldsymbol{s}^{tr} = (1 - \omega^n) 2G \left(\boldsymbol{e}^{n+1} - \boldsymbol{e}_p^n \right)$$
(22)

Again, if the trial stress satisfies the yield condition, the step is elastic and the trial stress is accepted as the actual stress. If the trial stress violates the yield condition, the step is plastic and the return mapping algorithm has to be used. The formula for s^{n+1} reads

$$s^{n+1} = s^{tr} - 2G\Delta\omega \left(e^{n+1} - e_p^n \right) - (1 - \omega^{n+1}) 2G\Delta e_p^n$$
(23)

After substitution of (5) into (23), multiplication of the second term by $\frac{1-\omega^n}{1-\omega^n}$, and some algebra, we get

$$s^{n+1} = \frac{1 - \omega^{n+1}}{1 - \omega^n} s^{tr} - (1 - \omega^{n+1}) \sqrt{6} G \Delta \kappa \frac{s^{n+1}}{\|s^{n+1}\|}$$
(24)

Obviously, s^{n+1} and s^{tr} are colinear; therefore, we arrive at the radial return mapping of the trial stress onto the yield surface:

$$s^{n+1} = \left(\frac{1 - \omega^{n+1}}{1 - \omega^n} - \frac{(1 - \omega^{n+1})\sqrt{6}G\Delta\kappa}{\|s^{tr}\|}\right)s^{tr}$$
(25)

Combining the yield criterion (13) with (25) leads to one scalar nonlinear equation

$$\sqrt{\frac{3}{2}} \left(\frac{1 - \omega(\kappa^n + \Delta\kappa)}{1 - \omega(\kappa^n)} \left\| \boldsymbol{s}^{tr} \right\| - (1 - \omega(\kappa^n + \Delta\kappa))\sqrt{6}G\Delta\kappa \right) - \sigma_Y(\kappa^n + \Delta\kappa) = 0$$
(26)

with $\Delta \kappa$ as the unknown. This equation can be solved iteratively, for example by the Newton method.

4. Implicit-gradient regularization

In the previous section, two formulations coupling damage mechanics to the theory of plasticity were described, and their numerical implementation was presented. Now we focus on the regularization of the coupled damage-plastic models by the implicit-gradient formulation, with nonlocal cumulated plastic strain. In the regularized implicit-gradient formulation, the constitutive equations are enhanced by the nonlocal cumulated plastic strain, which is computed from a Helmholtz-type differential equation

$$\bar{\kappa} - l^2 \nabla^2 \bar{\kappa} = \kappa \tag{27}$$

with homogeneous Neumann boundary condition

$$\frac{\partial \bar{\kappa}}{\partial n} = \mathbf{0}.$$
(28)

In the equations above, l is a length scale parameter, ∇ is the Laplace operator, and n is an outer normal.

To regularize the constitutive model properly, attention must be palf to its localization properties. For the local model, localization can occur if the tangent plastic modulus, i.e., the derivative of σ_Y with respect to κ , becomes equal to or less than the critical value H_c derived by the localization analysis based on the acoustic tensor [Ottosen and Runesson (1991)]. For a model with an associated flow rule, this critical value is never positive. Therefore, localization cannot happen before peak, but at peak or after peak it may occur. It can be shown that a nonlocal model provides a proper regularization (nonzero width of the localized process zone and nonzero dissipation) if the derivative of the nominal yield stress with respect to the local κ , denoted as H_L , remains above H_c . To be on the safe side, we would like to keep H_L positive, because $H_c \leq 0$.

For instance for a model with

$$\sigma_Y = \sigma_Y(\bar{\kappa}) \tag{29}$$

we have $H_L = 0$ and there is a danger of localization into an arbitrarily thin layer. This is the so-called basic nonlocal plastic model, which can be improved by the overnonlocal formulation, with

$$\sigma_Y = \sigma_Y(\hat{\kappa}) \tag{30}$$

where

$$\hat{\kappa} = m\bar{\kappa} + (1-m)\kappa \tag{31}$$

is the overnonlocal variable. In this case, $H_L = (1-m)\sigma'_Y$ where σ'_Y is the derivative of σ_Y with respect to its argument. If the nominal yield stress is decreasing, we have $\sigma'_Y < 0$ and then the condition $H_L > 0$ is satisfied for m > 1. However, this formulation fails if σ'_Y is changing from positive to negative values (first hardening, then softening), because the condition $H_L > 0$ cannot be satisfied in both ranges with the same constant m.

The standard nonlocal formulation of a damage-plastic model is based on

$$\sigma_Y = (1 - g(\hat{\kappa}))\bar{\sigma}_Y(\kappa) \tag{32}$$

The local plastic modulus is given by

$$H_L = -(1-m)g'\bar{\sigma}_Y + (1-g)\bar{\sigma}'_Y \tag{33}$$

and the condition $H_L > 0$ translates into

$$\bar{\sigma}_Y' > \frac{(1-m)g'\bar{\sigma}_Y}{1-g} \tag{34}$$

where $\bar{\sigma}'_Y$ is the derivative of function $\bar{\sigma}_Y$ with respect to its argument and corresponds to the plastic modulus of the elastoplastic model without damage. The condition can be satisfied at least in two ways:

- using $\bar{\sigma}'_Y > 0$ and m = 1, which is the formulation with the usual nonlocal variable and with hardening elastoplastic part, see [Grassl and Jirásek (2006)];
- using $\bar{\sigma}'_Y \ge 0$ and m > 1, which is the overnonlocal formulation with an elastoplastic part that can contain a plateau (perfect plasticity without hardening) but must not soften, see [Charlebois, Jirásek and Zysset (2010)].

Localization capabilities of different implicit-gradient formulations will be explored in the next chapters by a representative numerical example.

4.1. Implementation of implicit gradient model

The implementation of the implicit gradient formulation is based on mixed finite elements. We start from the strong form of the set of governing differential equations

$$\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{0} \tag{35}$$

$$\bar{\kappa} - l^2 \nabla^2 \bar{\kappa} = \kappa \tag{36}$$

Following the standard procedure, equations (35) and (36) are recast in the weak form,

$$\int_{V} (\nabla \cdot \boldsymbol{\sigma}) \cdot \boldsymbol{\eta} \, \mathrm{d}\boldsymbol{x} = 0 \tag{37}$$

$$\int_{V} (\bar{\kappa} - l^2 \nabla^2 \bar{\kappa}) \eta \, \mathrm{d}\boldsymbol{x} = \int_{V} \kappa \eta \, \mathrm{d}\boldsymbol{x}$$
(38)

where η and η are suitable test functions. The displacements and the nonlocal cumulative plastic strains are approximated at the element level by

$$\boldsymbol{u} = \boldsymbol{N}\boldsymbol{d} \qquad \bar{\boldsymbol{\kappa}} = \boldsymbol{N}_{\bar{\boldsymbol{\kappa}}}\boldsymbol{d}_{\bar{\boldsymbol{\kappa}}} \tag{39}$$

where N and $N_{\bar{\kappa}}$ are matrices containing the shape functions and d and $d_{\bar{\kappa}}$ are vectors with the corresponding degrees of freedom (nodal displacements and nodal values of the nonlocal cumulated plastic strain). After discretization, we obtain the set of nonlinear algebraic equations

$$\left\{ \begin{array}{c} \boldsymbol{f}_{int} \\ \boldsymbol{\phi}_{int} \end{array} \right\} = \left\{ \begin{array}{c} \boldsymbol{f}_{ext} \\ \boldsymbol{0} \end{array} \right\}$$
(40)

in which f_{int} and f_{ext} are the standard internal and external forces and $\phi_{int} = \int_{V} (N_{\bar{k}}^{T} N_{\bar{k}} d_{\bar{k}} + l^2 B_{\bar{k}}^{T} B_{\bar{k}} d_{\bar{k}} - \kappa N_{\bar{k}}^{T}) dx$ are generalized internal forces. The set of nonlinear equations is solved by the Newton-Raphson iteration scheme. This numerical method requires a tangent matrix, which is obtained by differentiating the internal force vector with respect to the nodal unknowns:

$$\boldsymbol{K} = \begin{bmatrix} \frac{\partial \boldsymbol{f}_{int}}{\partial \boldsymbol{d}} & \frac{\partial \boldsymbol{f}_{int}}{\partial \boldsymbol{d}_{\bar{\kappa}}} \\ \\ \frac{\partial \boldsymbol{\phi}_{int}}{\partial \boldsymbol{d}} & \frac{\partial \boldsymbol{\phi}_{int}}{\partial \boldsymbol{d}_{\bar{\kappa}}} \end{bmatrix}$$
(41)



Fig. 1: Uniaxial tension test: Geometry and Loading

where

$$\frac{\partial \boldsymbol{f}_{int}}{\partial \boldsymbol{d}} = \int_{V} (1-\omega) \boldsymbol{B}^{T} \frac{\partial \boldsymbol{\theta}}{\partial \varepsilon} \boldsymbol{B} \, \mathrm{d}\boldsymbol{x} \qquad \frac{\partial \boldsymbol{f}_{int}}{\partial \boldsymbol{d}_{\bar{\kappa}}} = -\int_{V} \frac{d\omega}{d\kappa} \boldsymbol{B}^{T} \bar{\boldsymbol{\sigma}} \boldsymbol{N}_{\bar{\kappa}} \, \mathrm{d}\boldsymbol{x}$$
$$\frac{\partial \boldsymbol{\phi}_{int}}{\partial \boldsymbol{d}} = -\int_{V} \boldsymbol{N}_{\bar{\kappa}}^{T} \frac{\partial \boldsymbol{\theta}_{\kappa}}{\partial \varepsilon} \boldsymbol{B} \, \mathrm{d}\boldsymbol{x} \qquad \frac{\partial \boldsymbol{\phi}_{int}}{\partial \boldsymbol{d}_{\bar{\kappa}}} = \int_{V} \left(\boldsymbol{N}_{\bar{\kappa}}^{T} \left(1 + \frac{\partial \boldsymbol{\theta}_{\kappa}}{\partial \bar{\kappa}} \right) \boldsymbol{N}_{\bar{\kappa}} + l^{2} \boldsymbol{B}_{\bar{\kappa}}^{T} \boldsymbol{B}_{\bar{\kappa}} \right) \mathrm{d}\boldsymbol{x}$$

In the equations above, B and $B_{\bar{\kappa}}$ are matrices containing derivatives of the shape functions, $\frac{\partial \theta}{\partial \varepsilon}$ corresponds to classical elasto-plasto-damage stiffness and functions θ_{κ} is supplied by the return mapping algorithm.

5. Numerical example

Simulation of a one-dimensional bar in tension is carried out to demonstrate regularization properties of different implicit-gradient formulations of plasticity coupled to isotropic damage. Geometry of the problem is plotted in Fig. 1, the material and geometrical parameters are summarized in Tab. 1. Influence of the nonlocal formulation on the profile of damage along the bar is studied. Isotropic linear hardening of the effective yield stress and exponetial evolution of damage is considered:

$$\bar{\sigma}_Y = \sigma_0 + H\kappa \tag{42}$$

$$\omega = 1 - e^{-a\kappa} \tag{43}$$

This yields to the nominal stress in the form

$$\sigma_Y = (1 - e^{-a\kappa})(\sigma_0 + H\kappa) \tag{44}$$

At first, the over-nonlocal regularization based on nonlocal damage is considered, i.e. $\omega = g(\hat{\kappa})$. In this approach, the nonlocal cumulated plastic strain affects only the damage variable, while plasticity is formulated in the effective stress space and therefore remains local. The advantage of this approach is in a simple implementation based on the local return mapping algorithm followed by an explicit evaluation of the damage variable. The second class of models considered here is based on the over-nonlocal averaging of the nominal yield stress, $\sigma_Y = \sigma_Y(\hat{\kappa})$. Fig. 2 and Fig. 3 show the distribution of damage along the bar for different stages of loading for the first approach and the second approach, respectively. Finally, Fig. 4 compares the distribution of the damage variable obtained by the formulation based on the effective stress and by the formulation based on the nominal stress.

6. Conclusions

We have presented two formulations coupling plasticity with damage, and introduced two different implicit-gradient regularization schemes which lead to an objective description of localized failure processes. We have shown that even if the local models are fully equivalent, the nonlocal formulation can lead to substantially different results; therefore it is neccessary to pay attention when constructing the nonlocal extension. Further research will focus on the comparison of the computational efficiency of both models, and on extensions of the gradient regularization to more general yield conditions.

| Length of bar | L | 100 mm |
|-------------------------------------|---------------------------------|---------|
| Length of imperfection | s | 20 mm |
| Cross-sectional area | A | 100 m |
| Young's modulus | E | 20 GPa |
| Isotropic hardening law | $\sigma_Y = \sigma_0 + H\kappa$ | |
| Initial yield stress | σ_0 | 2 MPa |
| Initial yield stress (imperfection) | σ_0 | 1.8 MPa |
| Hardening modulus | Н | 600 MPa |
| Damage law | $\omega = 1 - \exp^{-a\kappa}$ | |
| Dimensionless damage parameter | a | 300 |
| Characteristic length | l | 5 mm |

Tab. 1: Uniaxial tension test: Geometrical and material parameters



Fig. 2: Evolution of damage profile for formulation 1



Fig. 3: Evolution of damage profile for formulation 2



Fig. 4: Comparison of damage distribution

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