A REGULARIZATION METHOD APPLIED IN ELASTOPLASTICITY PROBLEMS

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Abstract. The numeric simulation of the mechanical behaviour of industrial materials is widely used in the companies for viability verification, improvement and optimization of designs. This work presents the main ideas of Tikhonov Regularization Method applied to dynamic elastoplasticity problems (J2 model with damage and isotropic-kinetic hardening), besides some mathematical formalities associated to the formulation (well-posed/existence and uniqueness) of the dynamic elastoplasticity problem. The numeric problems of this approach are discussed and some strategies are suggested to solve these misfortunes satisfactorily. The numerical technique for the physical problem is by classical Gelerkin method.

Keywords: Elastoplasticity, regularization method, Galerkin method.

1. INTRODUCTION

Some matrials has a rate independent (in deformation sense) mechanical behaviour, in this case the eslastoplastic models have been widely used for forecast of these materials behaviour (see Desai (2001)). The numerical approch from this models come across ill-conditioning matrix problems, as for the case to finite or infinitesimal deformations (see Owen (1980)) due to the tangent operator to be sufficiently near of the identicaly null fourth order tensor operator on critical/limit points neighbourhood.

A complete investigation of the non linear behaviour of structures it follows from the equilibrium path of the body, in which come the singular (limit) points and/or bifurcation points. Several techniques to solve the numerical problems associated to these points have been disposed in the specialized literature, as for instance the call Load controlled Newton-Raphson method and displacement controlled techniques. Although most of these methods fail (due to problems convergence for ill-conditioning) in the neighbour of the limit points, mainly in the structures analysis that possess a (λ load factor, *u*-displacement) snap-through or snap-back equilibrium path shape (see Bashir-Ahmed and Xiao-zu (2004)).

Aiming at to transpose these difficulties this work proposes the use of the L-curve Tikhonov regularization method (see Calvettia *et al.* (2000), Bloom (1991), Hansen (1998) and Viloche Bazán (2008)) for the treatment of these limit points. The main objective are a first investigate of the potential of this approach under the mathematical formalism inherent to the formulation of the elastoplastic problem for inifinitesimal strain measurement. In the next section, it is presented the weak form and correpondig strong form for elastic problem. An overview of elastoplastic contitutive model is shown in section 3. Details about incremental approach are presented in sections 4 and 5. In section 6, it is presented the L-curve Thikhonov regularization method and main properties are shown. In section 7, a numerical problem case are presented to verify the efficacy of this proposed approch and concluding remarks are made in section 8.

2. THE ELASTIC PROBLEM

Under kinematic motion of deformable continuum body hypothesis, one has $u(\mathbf{x}, t) = u(\varphi_t(\mathbf{x}_o), t) = \bar{u}(\mathbf{x}_o, t)$ on $\mathbf{x}_o \in \Gamma_o^u$, where for each $t \in S$, $\varphi_t : \Omega_o \to \Omega$ is a sufficiently regular motion function. The relationship between normal vectors to surfaces in reference configuration (._o) and actual configuration can be expressed by

$$\mathbf{n}dA = \det\left(\mathbf{F}\right)\mathbf{F}^{-T}\mathbf{n}_{o}dA_{o},\tag{1}$$

where n_o is the external normal unit vector to surface in reference configuration. In this way, it follows the strong and weak formulation.

2.1 The Strong Formulation: Reference Configuration

The problem is given by:

Problem 1. Determine $\mathbf{u}_o(\mathbf{x}_o, t)$, for each $t \in S$, such that

$$div \mathbf{P}(\mathbf{x}_{o}, t) + \rho_{o}(\mathbf{x}_{o}) \,\bar{\mathbf{b}}(\mathbf{x}_{o}, t) = \rho_{o}(\mathbf{x}_{o}) \,\ddot{u}_{o}, \qquad in \quad \mathbf{x}_{o} \in \Omega_{o};$$
⁽²⁾

$$\mathbf{P}(\mathbf{x}_{o},t)\mathbf{n}_{o}(\mathbf{x}_{o},t) = \overline{\mathbf{t}}_{o}(\mathbf{x}_{o},t), \quad in \quad \mathbf{x}_{o} \in \Gamma_{o}^{t};$$
(3)

$$\mathbf{u}_{o}\left(\mathbf{x}_{o},t\right) = \bar{\mathbf{u}}_{o}\left(\mathbf{x}_{o},t\right), \quad in \qquad \mathbf{x}_{o} \in \Gamma_{o}^{u} \tag{4}$$

with $\bar{t}_{oi} \in H^{\frac{1}{2}}(\Gamma_o^t)$ and $\bar{b}_i \in L^2(\Omega_o)$, where **P** is the first Piola-Kirschhoff stress tensor.

2.2 The Weak Formulation: Reference Configuration

Defining in this moment the following sets for each $t \in S$

$$Kin_{u}(\Omega_{o}) = \left\{ u_{oi}: \Omega_{o} \to \mathbb{R} \mid u_{oi} \in H^{1}(\Omega_{o}), u_{oi}\left(\mathbf{x}_{o}, t\right) = \bar{u}_{oi}\left(\mathbf{x}_{o}, t\right) \text{ em } \mathbf{x}_{o} \in \Gamma_{o}^{u} \right\};$$

$$Var_{u}(\Omega_{o}) = \left\{ \hat{v}_{i}: \Omega_{o} \to \mathbb{R} \mid \hat{v}_{i} \in H^{1}(\Omega_{o}), \hat{v}_{i}\left(\mathbf{x}_{o}\right) = 0 \text{ em } \mathbf{x}_{o} \in \Gamma_{o}^{u} \right\},$$
(5)

denoting, for each $t \in S$,

$$F(u_o; \mathbf{\hat{v}}) = \int_{\Omega_o} \mathbf{P} : \nabla \mathbf{\hat{v}} d\Omega_o - \int_{\Omega_o} \rho_o \left(\mathbf{\bar{b}} - \ddot{u}_o \right) \cdot \mathbf{\hat{v}} d\Omega_o - \int_{\Gamma_o^t} \mathbf{t}_o \cdot \mathbf{\hat{v}} dA_o$$
(6)

the problem may be written in following way

Problem 2. Determine $u_o(\mathbf{x}_o, t) \in Kin_u(\Omega_o)$, for each $t \in S$, such that

$$F(u_o; \hat{\mathbf{v}}) = 0, \forall \ \hat{\mathbf{v}} \in Var_u(\Omega_o).$$
(7)

3. YIELDING AND HARDENING LAWS (THE ELASTOPLASTIC CONSTITUTIVE MODEL)

The complete characterization of a general elastoplastic model request the definition of evolutionary laws of internal variables, i. e., variables associated to dissipative phenomena (ε^p and α_k - associated with the kinematic hardening mechanism).

The departure point is the determination of the plastic multiplier $\dot{\lambda}$, that follows from consistence condition ($\mathcal{F} = 0$ and $\dot{\lambda} > 0$). Let remembering the definition of α_k in terms of free energy potential and evolutionary law, one has

$$\dot{\lambda} = \frac{\frac{\partial \mathcal{F}}{\partial \sigma} : \mathbb{D}\dot{\varepsilon}}{\left\{\frac{\partial \mathcal{F}}{\partial \sigma} : \mathbb{D}\mathbf{N} - \rho \frac{\partial \mathcal{F}}{\partial \alpha_k} \cdot \left[\frac{\partial^2 \Psi^p}{\partial \beta_k^2}\right] \mathbf{H}\right\}}$$
(8)

More details about constitutive Lemaitre's elastoplastic-damage simplified model with isotropic hardening see Lubliner (1990), Lemaitre (1996), Lemaitre and Chaboche (1990) and Owen (1980). It observes the following procedure

Elastoplastic Constitutive Model

1. Strain Tensor Additive Decomposition

 $\varepsilon = \varepsilon^{e} + \varepsilon^{p}.$ 2. Free Energy Potential Definition $\Psi \left(\varepsilon^{e}, r, \alpha^{D}, D \right) = \Psi^{e} \left(\varepsilon^{e}, D \right) + \Psi^{p} \left(r, \alpha^{D} \right)$ where α^{D} is the deviator part of backstrain tensor, r is the accumulated plastic strain, D is the isotropic damage variable. 3. Constitutive equation for σ and thermodynamics forces β_{k} $\sigma = \rho \frac{\partial \Psi^{e}}{\partial \varepsilon^{e}}$ and $\beta_{k} = \rho \frac{\partial \Psi^{p}}{\partial \alpha_{k}}.$ 4. Elastic-damage Coupling $\sigma = (1 - D)\mathbb{D}\varepsilon^{e}.$ 5. Yield Function/Dissipation Potential(Associative Approach) $\mathcal{F}_{p} = \|\tilde{\sigma}^{D} - \chi^{D}\| - (R + \sigma_{y})$ where $\tilde{\sigma}_{eq}^{D} = \left\{ \frac{3}{2} \tilde{\sigma}^{D} : \tilde{\sigma}^{D} \right\}^{\frac{1}{2}},$ $\tilde{\sigma}^{D} = \frac{1}{(1-D)} \left\{ \sigma - \sigma_{H}I \right\}$ and $\sigma_{H} = \frac{1}{3}tr(\sigma).$ 6. Hardening and Evolutionary Plastic Laws $\dot{\varepsilon}^{p} = \dot{\lambda} \frac{\partial \mathcal{F}_{p}}{\partial \sigma}, \dot{r} = -\dot{\lambda} \frac{\partial \mathcal{F}_{p}}{\partial R}$ and $\dot{D} = \dot{\lambda} \frac{\partial \mathcal{F}_{D}}{\partial Y}$ where $\mathcal{F} = \mathcal{F}_{p} + \mathcal{F}_{D}$ with $\mathcal{F}_{p} = \|\tilde{\sigma}^{D} - \chi^{D}\| - (R + \sigma_{y})$ and $\mathcal{F}_{D} = \frac{Y^{2}}{2S(1-D)}H(p - p_{d}).$ From these potentials it follows that

$$\dot{\varepsilon}^{p} = \frac{3}{2} \frac{\dot{\lambda}}{(1-D)} \frac{\sigma^{D}}{\sigma^{D}_{eq}}, \ \dot{\chi} = \gamma(\chi_{\infty} \dot{\varepsilon}^{p} - \chi \dot{\lambda}), \ \dot{R} = b(R_{\infty} - R)\dot{\lambda} \ \text{and} \ \dot{D} = \frac{Y}{S} \dot{p} H(p - p_{d}).$$
Then
$$\dot{p} = \frac{\dot{\lambda}}{(1-D)} \ \text{and} \ Y = \frac{\left(\tilde{\sigma}^{D}\right)^{2}}{2E} \left\{ \frac{2}{3} \left(1 + \nu\right) + 3 \left(1 - 2\nu\right) \left(\frac{\sigma_{H}}{\sigma^{D}_{eq}}\right)^{2} \right\}.$$
7. Consistence Condition under Plastic Yielding $\left(\dot{\lambda} \neq 0\right)$

$$\mathcal{F}(\sigma, \alpha_{k}) \leq 0, \quad \dot{\lambda} \geq 0, \quad \mathcal{F}(\sigma, \alpha_{k}) \dot{\lambda} = 0$$

and $\dot{\lambda} \dot{\mathcal{F}}(\sigma, \alpha_k) = 0.$

4. OPERATOR-SPLITTING ALGORITHM

The general algorithm for elastoplasticity-damage with isotropic/kinematic hardening can be described in following way:

Trial Elastic Problem

Given the strain history $\varepsilon(t)$, $t \in [t_n, t_{n+1}]$, determine $\varepsilon_{n+1}^{e\ trial}$ and α_{n+1}^{trial} , with $\alpha_{n+1}^{trial} \equiv (\varepsilon_{n+1}^{p\ trial}, R_{n+1}^{trial}, \chi_{n+1}^{trial}, D_{n+1}^{trial})$, so that

$$\dot{\varepsilon}^{e\ trial} = \dot{\varepsilon} \text{ and } \dot{\alpha}^{trial} = 0$$
(9)

in which $\dot{\alpha}^{trial} = (\dot{\varepsilon}^{p \ trial}, \dot{R}^{trial}, \chi^{trial}, \dot{D}^{trial}) = 0$.

The initial conditions for t_{n+1} are the conditions of elastoplastic state determined on t_n , i. e.

$$\varepsilon^{e\ trial}(t_n) = \varepsilon_n^e \text{ and } \alpha^{trial}(t_n) = \alpha_n^{trial}$$
 (10)

The trial elastic problem solution on t_{n+1} , denoted for $\varepsilon_{n+1}^{e\ trial}$ and α_{n+1}^{trial} defining the elastic trial state.

• Plastic Damage Correction Problem

The problem is formulated in following way: Determine $\alpha = (\varepsilon^p, R, \chi, D)$ and ε^e that satisfy the following equations:

$$\dot{\varepsilon}^{p} = \frac{3}{2} \frac{\dot{\lambda}}{(1-D)} \frac{\sigma^{D}}{\sigma^{D}_{eq}}, \ \dot{\chi} = \gamma (\chi_{\infty} \dot{\varepsilon}^{p} - \chi \dot{\lambda}), \ \dot{R} = b(R_{\infty} - R)\dot{\lambda}$$

and $\dot{D} = \frac{Y}{S} \frac{\dot{\lambda}}{(1-D)} H(p - p_{d})$ (11)

with

$$\dot{\lambda} \ge 0, \quad \mathcal{F} \le 0 \quad \text{and} \quad \dot{\lambda}\mathcal{F} = 0.$$
 (12)

For $\mathcal{F} = 0$ the consistence condition used to $\dot{\lambda}$ computation is:

$$\dot{\lambda}\,\dot{\mathcal{F}}=0.\tag{13}$$

In the plastic damage correction problem the initial conditions are:

$$\varepsilon^e(t_n) = \varepsilon^e_{n+1} \text{ and } \alpha(t_n) = \alpha^{trial}_{n+1}.$$
 (14)

The solution obtained for the problem on t_{n+1} , denoted by

$$\left\{\sigma_{n+1},\varepsilon_{n+1}^{e},\varepsilon_{n+1}^{p}R_{n+1},D_{n+1}\right\},\tag{15}$$

is the final solution of this initial value problem.

5. INCREMENTAL FORMULATION

The incremental formulation between t_n and t_{n+1} instants consider that all state variables are known on Ω_n and the equilibrium equations are imposed in Ω_{n+1} . In this way, on t_{n+1} , the weak formulation of this problem can be formulated as:

$$u_o(\mathbf{x}_o, t_n) = \mathbf{x}_n - \mathbf{x}_o \qquad \therefore \qquad u_n = u_o(\mathbf{x}_o, t_n); \tag{16}$$

$$u_o(\mathbf{x}_o, t_{n+1}) = \mathbf{x}_{n+1} - \mathbf{x}_o \qquad \therefore \qquad u_{n+1} = u_o(\mathbf{x}_o, t_{n+1}).$$
(17)

Problem 3. Determine $u_{n+1} \in Kin_o^u$ such that

$$F(u_{n+1}; \hat{\mathbf{v}}) = 0, \qquad \forall \ \hat{v} \in Var_o^u, \tag{18}$$

where

$$F\left(u_{n+1}; \hat{\mathbf{v}}\right) = \int_{\Omega_o} \mathbf{P}\left(u_{n+1}\right) : \nabla \hat{\mathbf{v}} d\Omega_o - \int_{\Omega_o} \rho_o \left(\bar{\mathbf{b}} - \ddot{u}_n\right) \cdot \hat{\mathbf{v}} d\Omega_o - \int_{\Gamma_o^t} \mathbf{t} \cdot \hat{\mathbf{v}} dA_o.$$
(19)

To solve the above non linear problem in terms of u_{n+1} is used the Newton method.

5.1 The Newton Method

Let

$$u_{n+1}^0 = u_n, \qquad k = 0 \tag{20}$$

where k denotes the iteration step in Newton method process started on k = 0 and supposing that the initial condition is given by the last increment step converged solution, i. e., u_n , then on k-th iteration one has

$$u_{n+1}^{k+1} = u_{n+1}^k + \Delta u_{n+1}^k.$$
(21)

To determine $\Delta \mathbf{u}_{n+1}^k$ is imposed the condition

$$F\left(u_{n+1}^{k+1}; \hat{\mathbf{v}}\right) = 0, \qquad \forall \ \hat{\mathbf{v}} \in Var_o^u.$$
(22)

i. e.,

$$F\left(u_{n+1}^{k+1}; \hat{\mathbf{v}}\right) = F\left(u_{n+1}^{k} + \Delta u_{n+1}^{k}; \hat{\mathbf{v}}\right) = 0 \qquad \forall \ \hat{\mathbf{v}} \in Var_{o}^{u}.$$
(23)

Let $F(\cdot, \cdot)$ sufficiently regular and expanding $F(u_{n+1}^k + \Delta u_{n+1}^k; \hat{\mathbf{v}})$ in a Taylor series on \mathbf{u}_{n+1}^k , one has for a first order approximation,

$$F\left(u_{n+1}^{k} + \Delta u_{n+1}^{k}; \hat{\mathbf{v}}\right) \simeq F\left(u_{n+1}^{k}; \hat{\mathbf{v}}\right) + DF\left(u_{n+1}^{k}; \hat{\mathbf{v}}\right) \left[\Delta u_{n+1}^{k}\right].$$

$$(24)$$

From above comments one has

$$DF\left(u_{n+1}^{k};\hat{\mathbf{v}}\right)\left[\Delta u_{n+1}^{k}\right] = -F\left(u_{n+1}^{k};\hat{\mathbf{v}}\right).$$
(25)

5.1.1 Computation of $D \not\models \left(u_{n+1}^k; \hat{\mathbf{v}} \right) \left[\Delta u_{n+1}^k \right]$

From definition, it follows

$$DF\left(u_{n+1}^{k};\hat{\mathbf{v}}\right)\left[\Delta u_{n+1}^{k}\right] = \int_{\Omega_{o}} \frac{d}{d\epsilon} \left[\mathbf{P}\left(u_{n+1}^{k} + \epsilon \Delta u_{n+1}^{k}\right)\right]_{\epsilon=0} : \nabla \hat{\mathbf{v}} \, d\Omega_{o},\tag{26}$$

where Ω_o is fixed in space and it is supposing that $\mathbf{t}_{o_{n+1}}$ and \mathbf{b}_{n+1} are non depended of u. After some algebraic calculations, one is concluded that

$$DF\left(u_{n+1}^{k}; \hat{\mathbf{v}}\right) \left[\Delta u_{n+1}^{k}\right] = \int_{\Omega_{o}} \left[\mathbb{A}\left(u_{n+1}^{k}\right)\right] \nabla \left(\Delta u_{n+1}^{k}\right) : \nabla \hat{\mathbf{v}} \, d\Omega_{o}, \tag{27}$$

where \mathbb{A} (fourth order tensor) is the global tangent modulus, that is given bellow

$$\left[\mathbb{A}\left(\mathbf{u}_{n+1}^{k}\right)\right]_{ijkl} = \left.\frac{\partial P_{ij}}{\partial F_{kl}}\right|_{\mathbf{u}_{n+1}^{k}}.$$
(28)

Remark 1. Observing the problem from an Eulerian point of view, it is defined a couple of sets for each $t \in S$

$$Kin_{u}(\Omega) = \left\{ u_{i}: \Omega \to \mathbb{R} \mid u_{i} \in H^{1}(\Omega) \text{, } u\left(\mathbf{x}, t\right) = \bar{u}\left(\mathbf{x}, t\right) \text{ where } \mathbf{x} \in \Gamma^{u} \right\};$$

$$(29)$$

$$Var_{u}(\Omega) = \left\{ \hat{v}_{i} : \Omega \to \mathbb{R} \mid \hat{v}_{i} \in H^{1}(\Omega_{t}), \, \hat{v}_{i}\left(\mathbf{x}\right) = 0 \text{ where } \mathbf{x} \in \Gamma^{u} \right\},\tag{30}$$

the weak formulation of the problem can be written in the following way:

Problem 4. Determine $u(\mathbf{x}, t) \in Kin_u(\Omega)$, for each $t \in S$, such that

$$\int_{\Omega} \sigma \colon \nabla \hat{\mathbf{v}} d\Omega = \int_{\Omega} \rho \left(\mathbf{b} - \ddot{u} \right) \cdot \hat{\mathbf{v}} d\Omega + \int_{\Gamma^t} \mathbf{t} \cdot \hat{\mathbf{v}} dA, \qquad \forall \ \hat{\mathbf{v}} \in Var_u(\Omega).$$
(31)

In this case the tangent operator can be described as:

$$\left[\mathbb{A}\left(u_{n+1}^{k}\right)\right]_{ijkl} = \left.\frac{\partial\sigma_{ij}}{\partial\epsilon_{kl}}\right|_{\mathbf{u}_{n+1}^{k}}.$$
(32)

6. THE TIKHONOV REGULARIZATION METHOD

After the Galerkin method discretization the problem described above numerically belongs

$$\min_{\mathbf{f}\in\mathbb{R}^n} \|\mathbf{A}\mathbf{f} - \mathbf{g}\|_2, \quad \mathbf{A}\in\mathbb{R}^{n\times n} \quad \mathbf{g}\in\mathbb{R}^n,$$
(33)

where the matrix **A** (it refer to matrix representation for discretized tangent operator $\left[\mathbb{A}\left(\mathbf{u}_{n+1}^{k}\right)\right]_{ijkl}$) has high condition number (ill-conditioned and singular values decreasing to zero without a gap on spectrum) on limit points neighbour $(\partial \sigma_{ij} / \partial \epsilon_{kl} \approx$ null fourth order tensor) due to the shape of the equilibrium path response. The **g** consists to vectorial numerical representation of $-\mathcal{F}\left(\mathbf{u}_{n+1}^{k}; \hat{\mathbf{v}}\right)$. Unfortunately for the standard least square (LS) the solution can be presented as $\mathbf{f}_{ls} = \mathbf{A}^{\dagger}\mathbf{g}$ (where \mathbf{A}^{\dagger} denotes the pseudoinverse of **A**) has serious numerical spurious error. In this the regularization method is a natural way to is a mod of aiding for a less susceptible to numeric error stable computation of solution. The classical Tikhonov method (see Tikhonov (1963) and Hansen (1998)) consists in a solution of the problem

$$\min_{\mathbf{f}\in\mathbf{B}^n} \exists \left(\mathbf{f}\right) = \|\mathbf{A}\mathbf{f} - \mathbf{g}\|^2 + \tilde{\lambda}\|\mathbf{f}\|^2$$
(34)

where $\hat{\lambda} > 0$ is the regularization parameter. Solve (34) is equivalent to research the solution of the regularized normal equation

$$(\mathbf{A}^T \mathbf{A} + \tilde{\lambda} \mathbf{I}_n) \mathbf{f} = \mathbf{A}^T \mathbf{g},\tag{35}$$

whose solution is $\mathbf{f}_{\tilde{\lambda}} = (\mathbf{A}^T \mathbf{A} + \tilde{\lambda} \mathbf{I}_n)^{-1} \mathbf{A}^T \mathbf{g}$, and \mathbf{I}_n is the identity matrix $n \times n$. Now the problem is how to determine $\tilde{\lambda}$ parameter such that $\mathbf{f}_{\tilde{\lambda}}$ be the nearest solution of the solution without numeric errors. A lot of techniques for the regularization parameter choice were developed and they are presented in the specialized literature. These techniques can be organized in two classes: techniques that involves the pre-known (or estimative) of the norm error *e* behaviour, as discrepancy principle (DP) evidenced in Morozov Morozov (1984), and techniques that do not explore this information. In this second class it can be cited the L-curved method (see Hansen and O'Leary (1993)), generalized cross-validation (GCV) (see Golub *et al.* (1979)), weighted-GCV (W-GCV) (see Chung *et al.* (2008)), and a fixed point method (FP-method) (see Viloche Bazán (2008)). For an overview of parameter-choice techniques for Tikhonov regularization method see Hansen (1998) and recently Belge *et al.* (2002); Hämarik and Raus (2006); Hämarik *et al.* (2007); Johnston and Gulrajani (2002); Krawczy-Stando and Rudnicki (2007); Kilmer and O'Leary (2001); Rust and O'Leary (2008); Zibetti *et al.* (2008).

Note that the Thikhonov problem (34) and considering SVD of \mathbf{A} , $\mathbf{A} = \hat{\mathbf{S}}_1 \hat{\mathbf{S}}_2 \hat{\mathbf{S}}_3^T$, where $\hat{\mathbf{S}}_2 \in \mathbb{R}^{n \times n}$ is a singular value diagonal matrix, and $\hat{\mathbf{S}}_1, \hat{\mathbf{S}}_3 \in \mathbb{R}^{n \times n}$ are unitary matrixes, with $\hat{\mathbf{S}}_3$ non sigular matrix.

$$(\mathbf{A}^T \mathbf{A} + \tilde{\lambda} \mathbf{I}_n) \mathbf{f}_{\tilde{\lambda}} = \mathbf{A}^T \mathbf{g} \therefore \mathbf{f}_{\tilde{\lambda}} = \hat{\mathbf{S}}_3 (\hat{\mathbf{S}}_2^2 + \tilde{\lambda} \mathbf{I}_n)^{-1} \hat{\mathbf{S}}_2 \hat{\mathbf{S}}_1^T \mathbf{g},$$
(36)

or $\mathbf{f}_{\tilde{\lambda}} = \sum_{i=1}^{n} \frac{\hat{S}_{2_{i}}^{2}}{\hat{S}_{2_{i}}^{2} + \tilde{\lambda}^{2}} \frac{\hat{\mathbf{S}}_{1_{i}}^{T} \mathbf{g}}{\hat{S}_{2_{i}}} \hat{\mathbf{S}}_{3_{i}}$ with $\hat{S}_{2_{i}}^{2}$ representing the *i*-th singular value, $\hat{\mathbf{S}}_{1_{i}}$ is the *i*-th colum vector of $\hat{\mathbf{S}}_{1}$ and $\hat{\mathbf{S}}_{3_{i}}$ is the *i*-th colum vector of $\hat{\mathbf{S}}_{3}$.

Observing the problem (34) it is expected that the solution of this optimization problem converges to the solution of the equation $\mathbf{Af} = \mathbf{g}$ as $\tilde{\lambda}$ tends to zero. Some of the main properties of Tikhonov regularization method are collected in the following theorem

Theorem 1. Let $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$ be bounded. For every $\tilde{\lambda} > 0$ there exists a unique minimum $\mathbf{f}_{\tilde{\lambda}}$ of (34). Furthermore, $\mathbf{f}_{\tilde{\lambda}}$ satisfies the normal equation

$$\tilde{\lambda} \left\langle \mathbf{f}_{\tilde{\lambda}}, \omega \right\rangle + \left\langle \mathbf{A} \mathbf{f}_{\tilde{\lambda}} - \mathbf{g}, \mathbf{A} \omega \right\rangle = 0, \forall \omega \in \mathbb{R}^{n}, \tag{37}$$

or, using the adjoint $\mathbf{A}^* = \mathbf{A}^T : \mathbb{R}^n \to \mathbb{R}^n$ of \mathbf{A} ,

$$(\mathbf{A}^T \mathbf{A} + \tilde{\lambda} \mathbf{I}_n) \mathbf{f}_{\tilde{\lambda}} = \mathbf{A}^T \mathbf{g}.$$
(38)

If, in addition, **A** is one-to-one and $\mathbf{f} \in \mathbb{R}^n$ is the (unique) solution of the equation $\mathbf{A}\mathbf{f} = \mathbf{g}$ then $\mathbf{f}_{\tilde{\lambda}} \to \mathbf{f}$ as $\tilde{\lambda}$ tends to zero. Finally, if $\mathbf{f} \in \mathbf{A}^T(\mathbb{R}^n)$ or $\mathbf{f} \in \mathbf{A}^T(\mathbb{R}^n)$, then $\exists c > 0$ with $\|\mathbf{f}_{\tilde{\lambda}} - \mathbf{f}\| = c\sqrt{\tilde{\lambda}}$ or $\|\mathbf{f}_{\tilde{\lambda}} - \mathbf{f}\| = c\tilde{\lambda}$, respectively.

6.1 The L-curve Technique

Let $f_{\tilde{\lambda}}$ for be the family of solutions of the method of Tikhonov and set

$$\vartheta_{1\tilde{\lambda}} := \|\mathbf{A}\mathbf{f}_{\tilde{\lambda}} - \mathbf{g}\|^2 \text{ and } \vartheta_{2\tilde{\lambda}} := \|\mathbf{f}_{\tilde{\lambda}}\|^2 \tag{39}$$

, it can be verified that $\mathbf{f}_{\tilde{\lambda}}$ is a solution of the method of residuals $(e_1 := \sqrt{\vartheta_{1\tilde{\lambda}}})$ and quasisolutions $(e_2 := \sqrt{\vartheta_{2\tilde{\lambda}}})$. Defining the bounded set

$$C := \left\{ (c_1, c_2) \in \mathbb{R}^2 | \exists \mathbf{f} \in \mathbb{R}^n \text{ with } \| \mathbf{A}\mathbf{f} - \mathbf{g} \| \le c_1 \text{ and } \| \mathbf{f} \| \le c_2 \right\},\tag{40}$$

it can be shown that the function $\tilde{\lambda} \mapsto e_{1\tilde{\lambda}}$ is increasing, $\tilde{\lambda} \mapsto e_{2\tilde{\lambda}}$ is decreasing and *C* is a convex set with boundary given from the curve $\tilde{\lambda} \mapsto (e_{1\tilde{\lambda}}, e_{2\tilde{\lambda}})$. Although if it cannot determine the rate $\frac{e_1}{e_2}$, it must be have to specify a method/technique to determine $\tilde{\lambda}$ in an optimal sense with using $\vartheta_{1\tilde{\lambda}}$ and $\vartheta_{2\tilde{\lambda}}$. In this way the L-curve criterion consists in determine $\tilde{\lambda}$ which maximizes the curvature in the typical L-shaped plot of the curve $\ell : \tilde{\lambda} \in (0, \infty) \mapsto (\ln(e_1), \ln(e_2)) \in \mathbb{R}^2$. The main motivation comes from the observation that in almost vertical portion of the graph for very small changes of $\tilde{\lambda}$ values corresponds to rapidly varying to regularized solutions norm with very little change in $\vartheta_{1\tilde{\lambda}}$, while on horizontal part of the graphic for larger values of $\tilde{\lambda}$ corresponds to regularized solutions norm where the plot is flat or slowly decreasing for more detail see Hansen and O'Leary (1993). From this arguments the L-curve corner is located in a natural transition point that links these two regions, for more details and substantial results see Hansen (1998).

Now consider the L-curve $(\vartheta_{1\tilde{\lambda}}, \vartheta_{2\tilde{\lambda}})$ for Tikhonov regularization, taking \mathbf{r}_{\perp} as the least squares residual (i. e. the component of g orthogonal to $\hat{\mathbf{S}}_{1_1}, \ldots, \hat{\mathbf{S}}_{1_n}$), one has

$$\vartheta_{1\tilde{\lambda}} = \sum_{i=1}^{n} \frac{\tilde{\lambda}^{4} \left(\hat{\mathbf{S}}_{1_{i}}^{T} \mathbf{g}\right)^{2}}{\left(\hat{S}_{2_{i}}^{2} + \tilde{\lambda}^{2}\right)^{2}} + \|\mathbf{r}_{\perp}\|^{2} \therefore \frac{d\vartheta_{1\tilde{\lambda}}}{d\tilde{\lambda}} = 4\tilde{\lambda}^{3} \sum_{i=1}^{n} \frac{\hat{S}_{2_{i}}^{2} \left(\hat{\mathbf{S}}_{1_{i}}^{T} \mathbf{g}\right)^{2}}{\left(\hat{S}_{2_{i}}^{2} + \tilde{\lambda}^{2}\right)^{3}}; \tag{41}$$

$$\vartheta_{2\tilde{\lambda}} = \sum_{i=1}^{n} \frac{\hat{S}_{2_{i}}^{2} \left(\hat{\mathbf{S}}_{1_{i}}^{T} \mathbf{g}\right)^{2}}{\left(\hat{S}_{2_{i}}^{2} + \tilde{\lambda}^{2}\right)^{2}} \therefore \frac{d\vartheta_{2\tilde{\lambda}}}{d\tilde{\lambda}} = -4\tilde{\lambda} \sum_{i=1}^{n} \frac{\hat{S}_{2_{i}}^{2} \left(\hat{\mathbf{S}}_{1_{i}}^{T} \mathbf{g}\right)^{2}}{\left(\hat{S}_{2_{i}}^{2} + \tilde{\lambda}^{2}\right)^{3}},\tag{42}$$

therefore $\frac{d\vartheta_{2\bar{\lambda}}}{d\vartheta_{1\bar{\lambda}}} = -\tilde{\lambda}^{-2}$, the avaliation of second derivatives shows that the curve is convex and steeper as $\tilde{\lambda}$ approaches to the smallest sigular value. The L-curve consists of a vertical part where e_2 is near of the maximum value and adjacent part with smaller slope and the more horizontal part corresponds to solutions dominated by regularization errors where the regularization parameter is too large. In this sense the problem is to seek the L-curve point where the maximum curvature is reached.

Noting that if the L-curve is sufficiently smooth (twice continously differentiable with $\tilde{\lambda}$ -parameter), then it can be computed the curvature $\kappa \left(\tilde{\lambda} \right)$ as

$$\kappa\left(\tilde{\lambda}\right) = \frac{e_1^{'}e_2^{''} - e_1^{''}e_2^{'}}{\left(\left(e_1^{'}\right)^2 + \left(e_2^{'}\right)^2\right)^{\frac{3}{2}}},\tag{43}$$

where ' denotes a derivative with respect to $\tilde{\lambda}$ regularization parameter and any one dimetional optimization method can be used to solve $\tilde{\lambda}$ for the maximum curvature problem. It must be to point out that the numerical effort involved in minimization is smaller than that SVD computation. Although in many cases it is limited a finite set of points on L-curve, then the curvature $\kappa(\tilde{\lambda})$ cannot be computed. In a numerical sense the L-curve consists of a number of discrete points correponding to differents regularization parameter values $\tilde{\lambda}$ at which it has evaluated e_1 and e_2 . Thus it must be defined a sufficiently smooth curve associated to discret points in such way that the overall shape of L-curve is maintained. This procedure consists in determine an aproximating smooth curve and the reasonable approach for this is a cubic spline pair fitting for e_1 and e_2 . Such a curve has some interesting properties as twice differentiable, numerically differentiable in stable way and local shape preserving features. In this sense one has a two-step algorithm to the cubic spline fitting due to the non local smooth desired property.

L-curve Fitting

- 1. Perform a local low-degree polynomial fitting to a few neighbouring point in which each point is replaced by a new smoothed point;
- 2. Use the new smoothed points as control points for the cubic spline curve with N + 4 knots, where N is the number L-curve points.

Then assuming that one knows a few points on each side of the corener, a sketch of the algorithm it follows below

Regularization Solutions Associated to L-curve Approach

- 1. Start with a few points $(\ln (e_{1i}), \ln (e_{2i}))$ on each side of the corner;
- 2. Compute an approximating three-dimensional cubic spline curve S by L-curve Fitting algorithm for the points $(\ln(e_{1i}), \ln(e_{2i}), \tilde{\lambda}_i)$ where $\tilde{\lambda}_i$ is the regularization parameter that corresponds to $(\ln(e_{1i}), \ln(e_{2i}))$;
- 3. Let S_2 denote the first two coordinates of S, such that S_2 approximates the L-curve;
- 4. Compute the point on S_2 with maximum curvature, and find the corresponding regularization parameter λ_0 from the third coordinate of S;
- 5. Solve the regularization problem for $\tilde{\lambda} = \tilde{\lambda}_0$ and add the new point $(\ln(e_{10}), \ln(e_{20}))$ to the L-curve;
- 6. Repeat from step 2 until convergence.

Note that in step 2, it is necessary to introduce $\tilde{\lambda}_i$ as the third coordinate of S because one need to associate a regularization parameter with each point on S (a two-dimensional spline curve with $\tilde{\lambda}_i$ as knots does not provide this feature). Initial points for step 1 can be generated by choosing a number of regularization parameters ranging from very "large" values to very "small" values. It's important to point iut that the computational implementation of Tikhonov L–curve regularization tecnhique is based on criteria described in Hansen (1994) and Hansen and O'Leary (1993).

7. NUMERICAL EXAMPLE

The objective of this example is to attest the efficiency of the regularization technique for the time evolutionary numerical analysis in elastoplasticity problems. The evolutionary numerical approach analysis is given by a comparative response between a regularized (Tikhonov L-curve parameter choice) numerical solution and a non-regularized numerical solution. The numerical example presented here consist of a 1-D low cycle fatigue requests. The body has 100 mm initial length, the elasticity modulus $E = 2 \times 10^5 MPa$, Poisson ratio $\nu = 0.3$, yield stress $\sigma_y = 260 MPa$, kinematic hardening constants $\chi_{\infty} = 200 MPa$ (kinematic hardening amplitude) and $\gamma = 2.0$ (controls the kinematic hardening increase rate), isotropic hardening constants $R_{\infty} = 300 MPa$ (isotropic hardening amplitude) and b = 1 (controls the isotropic hardening increase rate), and damage constants $P_d = 0.0005$ and $D_c = 0.2$ (critical value of damage). This last value depends upon the material and the loading conditions and represents the final decohesion of atoms is characterized by a critical value of the effective stress acting on the resisting area. It is important to cite that D_c gives the critical value of the damage at a mesocrack initiation occuring for the unidimensional stress, usually $D_c \in [0.2, 0.5]$. A sketch of the problem cases may be seen in the figure below (see Fig.1).



Figure 1. Problem Case Domain Sketch

The load, in this example, is given by $\bar{u}(x,t) = 0.8t$ where t is in load cycles. For this application it was construct a fictitious exact solution (fes) and under 10^{-4} tolerance they were computed a regularized numerical solution (rns) and a non-regularized numerical solution (nrns) for analysis over $t \in [0, 10]$. A important fact that must be noted is any numerical solution cannot be realize the entire analysis over $t \in [0, 10]$. However without the use of Tikhonov regularization technique the "nrns" was capable to continue with the analysis to t = 7.547 cycles. The "rns-analysis", that use the Tikhonov regularization technique, can be cover the range of $t \in [0, 9.291]$ cycles with a excellent agreement with the "fes" as it can be seen in the figure (Fig. 2) below.

The nrns-analysis failed due to ill-condition problems, at point t = 7.547 cycles the condition number associated to the linearised system on Newton method iteration is 1.4×10^8 .

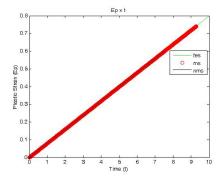


Figure 2. Plastic Strain vs. Time

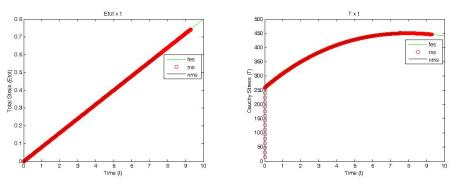


Figure 3. Total Strain vs. Time / Cauchy Stress vs. Time

For this case the number of iteration extrapolated a lot the allowed limit (500 iterations) with residual norm value oscillating in one belittles strip around 10^{-3} , growing up the allowed limit of iteration the same pattern is the reached until 661110 iterations. At the figure (3) it can be seen a good agreement between "fes" and "rns". Note that the rns-response was capable to reproduce the softening behaviour beginning. At figure (4) it can see the hardening behaviour during analyzed time. Note that for this instance there is a good agreements again among the results reached by "fes" and "rns" strategy.

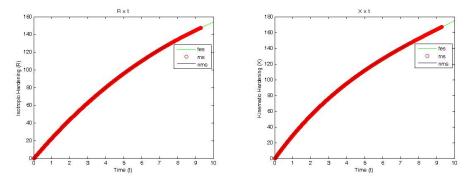


Figure 4. Isotropic Hardening vs. Time / Kinematic Hardening vs. Time

Now it is presented the responses about damage variable and storage plastic strain (see Fig. 5). Noting that in the storage plastic strain behaviour one has "fes-rns" perfect agreement, although for the damage variable evolutionary profile it is detected a little bit discrepancy between "fes" and "rns" that research maximum at t = 7.546 cycles with 2.5% as relative error. It is important to stand out although that in this case there is a tendency to both graphs ("fes" and "rns") coincides. The Tikhonov regularization process is setting to act when the condition number is equal or greater than 1.4×10^8 . Other settings are tested but the same unexpected pattern on rns-response was observed and non significant changes are noted.

The Tikhonov regularization method allowed that the numerical analysis continues until to reach t = 9.291 cycles. Note that at this point the the condition number value from the linearised system on Newton method iteration is 1.1×10^8 .

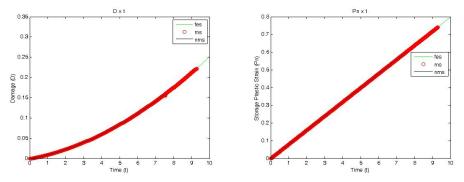


Figure 5. Damage vs. Time / Storage Plastic Strain vs. Time

The numerical analysis can run through the critical and move more torward the limit of the adopted model (see Figs. 5 and 6). The regularization parameter computed for the last Newton's iteration is $\tilde{\lambda} \approx 0.0271$.

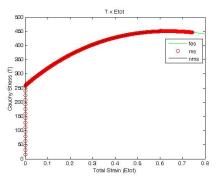


Figure 6. Cauchy Stress vs. Total Strain

8. CONCLUSION

In this work, it has discussed/analyzed the computational implementation of elastoplsticity problem. As mentioned above to treat the critical points on equilibrium-path it was proposed a Thikhonov L-cruve regularization approach over Newton method. In this sense it has prsented some theoretical results from Thikonov regularization method and your application over numerical dynamic elastoplastic problem as an efficient form of transposing the numerical problems associated to ill-conditioning happened in neighbourhoods of critical points.

It is important to comment that the Thikonov L-curve regularization method approach in elastoplasticity numerical analysis showed robustness, efficiency and potential as it can be seen in the comparative numerical examples here presented. The used tolerance convergence criterion (10^{-4}) was obtained after tests with larger and smaller tolerance values, in that none differences in the pattern of the responses was noticed. In this numerical example it was verified the consistency, performance and computational accuracy of the approach proposed. In fact, there was an excellent agreement between the regularized numerical response and fictitious exact solution, adding numerical stability and possibiliting advances in the time of analysis over permanent deformation computational modelling. Although, it is clear that new numerical experiments in terms of applications to explore as problems involving time rate dependences (viscoplasticity) over permanent/plastic deformations.

Additionally it is important to point out that besides new applications, other choosing parameters techniques (see Zibetti *et al.* (2008) and Viloche Bazán (2008)) must be investigated in terms of computational efforts, accuracy and performance in relation to L-curve approach. In particular, some experience is needed with large problems from distinct application requiring the use of general-form Tikhonov regularization. These are the subject of a research that should be continued.

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