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Research Paper

An improved numerical integration algorithm for elastoplastic constitutive equations

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ABSTRACT

A simplified methodology is proposed for elastoplastic calculations which holds for associative models. It is based on the representation of the elastoplastic model based on a rotation of the principal stresses and the fact that, in such system of coordinates, the direction that minimizes the square of a distance between a trial stress and the plastic surface has the same direction as the plastic deformation evolution. Such an approach allows for the elastoplastic calculation of complex models to be simpler and more efficient computationally. The proposed methodology is verified by the application to the elastoplastic model of Sandler–DiMaggio.

1. Introduction

The mechanical behavior of granular materials is very complex, involving plasticity by hydrostatic pressure, differences in the resistance for triaxial compression and triaxial stress, and porosity dependency, among other factors. In order to capture these effects, advanced constitutive models are necessary.

Elastoplastic constitutive models are based on a yield criterion, a flow rule and a hardening law, giving rise to an initial value problem with restrictions. Due the complexity of realistic constitutive models, stiff non-linear systems are generated and the use of efficient numerical integration methods are required.

An approach for the computation of elastoplastic problems is described in the book [1], Chapter 7, where the numerical integration is divided into two main steps: the elastic trial step and the plastic corrector step (or return-mapping algorithm). If trial stress computed in the first step fails to verify the plastically admissible condition, it is projected onto the yield surface by the return-mapping algorithm.

In the present paper we propose a simplified implementation of the plastic corrector step procedure, which holds for associative models, reducing the number non-linear equations to be solved and improving efficiency.

Using an iterative method for solving a system of non-linear elastoplastic equations, the convergence behavior is strongly dependent on the choice of variables to represent the residual vector. In this sense, an elastoplastic model can be better represented in terms of the principal stresses. Furthermore, in plastic calculations numerical instabilities can occur, in which small variations in the representation of floating point numbers may decide the feasibility of pursuing the calculations. Therefore, in addition to modeling the problem in the space of the principal stresses, we propose a distance function that has to be minimized in order to determine the projection of the plastic deformation on the yield surface. This geometric plastic calculation is possible thanks to the representation of the yield surface within a Haigh–Westergaard cylindrical coordinates [2], and the application of a rotation to a state of intermediate pressure. This procedure avoids the work in three-dimensional space, with a reduction in the number of unknowns of the elastoplastic problem. Thus, the convergence of the iterative method can be easily obtained, stabilizing the calculation, with a consequent significant savings in computational time.

To illustrate the effect of using this new approach, we consider the elastoplastic model described in the article [3], where the closure of the cap and the surface fault model are modified to allow the adjustment of the surface so that it is possible to characterize the material in triaxial compression and triaxial traction. For the results presented here, the implementation uses the NeoPZ library

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[4,5], which is an object-oriented programming environment providing a framework for developing finite element simulations, augmented with special classes required for the integration of elastoplastic constitutive models.

2. Constitutive elastoplastic model

The total deformation tensor ε can be divided into two parts: $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$, an elastic part $\boldsymbol{\varepsilon}^e$ and a plastic part $\boldsymbol{\varepsilon}^p$. The free energy φ is also divided into portions of elastic $\varphi^e(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p)$ and plastic contributions $\varphi^p(\alpha)$, in which α is the internal damage variable. The elastic law establishes the tensor $\boldsymbol{\sigma} = \bar{\rho}\frac{\partial \varphi^e}{\partial \varepsilon^e}$, in which $\bar{\rho}$ is the specific mass in the reference configuration. The plastic portion is not related to the strain state of the material; instead, it is related to the history of irreversible dissipative processes to which the material was submitted based on three fundamental axioms: an yield criterion, a flow rule, and a hardening law.

- *Yield criterion*. Describes the transition between the elastic and plastic domains through a plasticity function $\Phi = \Phi(\boldsymbol{\sigma}, A)$, where $A = \bar{\rho}\partial\varphi^p/\partial\alpha$ is the hardening thermodynamic force. The plasticity function assumes non-positive values in an elastic basis and null values in a plastic basis.
- *Flow rule*. Assumes the existence of a plastic potential function $\Psi = \Psi(\boldsymbol{\sigma}, A)$, which specifies how the plastic deformation tensor $\boldsymbol{\varepsilon}^p$ evolves in a plasticity process $\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}\boldsymbol{N}$, in which $\boldsymbol{N}(\boldsymbol{\sigma}, A) = \partial\Psi/\partial\boldsymbol{\sigma}$ is the flow direction, and $\gamma(t)$ is a plastic multiplier.
- *Hardening law*. Specifies how the internal damage variable evolves $\dot{\boldsymbol{\alpha}} = \dot{\gamma}\boldsymbol{H}$, in which $\boldsymbol{H}(\boldsymbol{\sigma}, A) = -\partial\Psi/\partial A$ is the hardening modulus.

In summary, the elastic–plastic constitutive model is formed by the following initial value problem: given the initial values $\boldsymbol{\varepsilon}^p(t_0)$ and $\boldsymbol{\alpha}(t_0)$ and the history of the infinitesimal deformation tensor $\boldsymbol{\varepsilon}(t),\ t \in [t_0, T]$, to find the functions that define the plastic deformation tensor $\boldsymbol{\varepsilon}^p(t)$, the internal damage variable $\boldsymbol{\alpha}(t)$ and a plastic multiplier $\dot{\gamma}(t)$ that meet the constitutive elastoplastic equations

$$\begin{cases} \dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}\boldsymbol{N} \\ \dot{\boldsymbol{\alpha}} = \dot{\gamma}\boldsymbol{H} \end{cases} \tag{1}$$

with the restrictions $\dot{\gamma}(t) \geqslant 0,\ \Phi(\sigma(t), A(t)) \leq 0,\ \dot{\gamma}(t)\Phi(\sigma(t), A(t)) = 0$ in each (pseudo) instant $t \in [t_0, T]$.

2.1. Algorithm for solving the incremental elastoplastic constitutive problem

For the integration of elastoplastic non-linear systems, the use efficient numerical integration methods is required. Using the implicit Euler method at a step of (pseudo) time $[t_n, t_{n+1}]$ of a loading cycle, given a deformation state $\boldsymbol{\varepsilon}^n$ and the corresponding plastic deformation $\boldsymbol{\varepsilon}^{p,n}$ and the internal state variable $\boldsymbol{\alpha}^n$ at t_n, for a prescribed incremental strain $\Delta\boldsymbol{\varepsilon}$, then the plastic deformation $\boldsymbol{\varepsilon}^{p,n+1}$, the internal variable $\boldsymbol{\alpha}^{n+1}$ and $\Delta\gamma$ at the next step are obtained as a solution of the problem that consists of the incremental non-linear system of equations

$$\begin{aligned} \boldsymbol{\varepsilon}^{e,n+1} &= \boldsymbol{\varepsilon}^{e,n} + \Delta\boldsymbol{\varepsilon} - \Delta\gamma\boldsymbol{N}^{n+1} \\ \boldsymbol{\alpha}^{n+1} &= \boldsymbol{\alpha}^n + \Delta\gamma\boldsymbol{H}^{n+1} \end{aligned} \tag{2}$$

for the unknowns $\boldsymbol{\varepsilon}^{e,n+1},\ \boldsymbol{\alpha}^{n+1}$ and $\Delta\gamma$, subjected to the restrictions

$$\Delta\gamma \geqslant 0, \quad \Phi(\boldsymbol{\sigma}^{n+1}, A) \leq 0, \quad \Delta\gamma\Phi(\boldsymbol{\sigma}^{n+1}, A) = 0 \tag{3}$$

As shown in [1], the imposition of restrictions suggests a procedure for solving the problem in two major steps. It begins with a purely elastic predictor process (*elastic trial step*), with $\Delta\gamma = 0$. In this case, trial elastic strain $\boldsymbol{\varepsilon}^e_{trial} = \boldsymbol{\varepsilon}^{e,n} + \Delta\boldsymbol{\varepsilon}$ and internal variables $\boldsymbol{\alpha}_{trial} = \boldsymbol{\alpha}^n$ are defined. Then $\boldsymbol{\sigma}_{trial}$ is calculated according to $\boldsymbol{\varepsilon}^e_{trial}$, and the corresponding $\Phi(\boldsymbol{\sigma}_{trial}, A)$ is given. If $\Phi(\boldsymbol{\sigma}_{trial}, A) \leqslant 0$, already a valid solution to the system is reached, and the variables are updated by the trial ones. Otherwise, a *plastic corrector step* (also known as *plastic return-mapping* scheme) is performed reformulating the incremental problem searching $\boldsymbol{\varepsilon}^{e,n+1},\ \boldsymbol{\alpha}^{n+1}$ and $\Delta\gamma$ satisfying

$$\boldsymbol{\varepsilon}^{e,n+1} = \boldsymbol{\varepsilon}^e_{trial} - \Delta\gamma\boldsymbol{N}(\boldsymbol{\sigma}^{n+1}, A) \tag{4}$$

$$\boldsymbol{\alpha}^{n+1} = \boldsymbol{\alpha}_{trial} + \Delta\gamma\boldsymbol{H}(\boldsymbol{\sigma}^{n+1}, A) \tag{5}$$

$$\Delta\gamma > 0, \quad \Phi(\boldsymbol{\sigma}^{n+1}, A) = 0 \tag{6}$$

Next, the plastic strain is updated

$$\boldsymbol{\varepsilon}^{p,n+1} = \boldsymbol{\varepsilon}^{p,n} + \Delta\boldsymbol{\varepsilon} - \Delta\boldsymbol{\varepsilon}^e$$

For the specific resolution of the initial elastoplastic value problem, five main classes of tools are available at NeoPZ environment:

- *Tensorial*: implements tensor in tree dimensions.
- *Elastic response:* implements the elastic response of an isotropic material.
- *Yield criterion:* implements the plastic function Φ, the plastic flow vector $\boldsymbol{N}$, and the hardening modulus $\boldsymbol{H}$.
- *Thermodynamic hardening force:* implements the calculation of the thermodynamic force A.
- *Incremental stress calculation:* implements the solution of the elastoplastic initial value problem using the Newton's method.

3. Plastic return-mapping scheme using rotated principal stresses

In the study of plasticity, instead of using the six stress independent components for the geometric representation of a state of stress at a point, a simplified alternative is to calculate the principal stresses $\sigma = [\sigma_1, \sigma_2, \sigma_3]^T$ as coordinates. This space is called Haigh–Westergaard stress space (HW). Furthermore, the constitutive law may be simplified by the introduction of a new coordinate system of rotated principal variables, similar to the decompositions defined in [6,7].

3.1. Haigh–Westergaard stress space

According to [2], the stress tensor $\boldsymbol{\sigma}$ may be represented in terms of the principal stresses sorted in descending order $\sigma_1 > \sigma_2 > \sigma_3$, which are given by the equations

$$\sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}}\xi + \sqrt{\frac{2}{3}}\rho\cos(\beta) \\ \frac{1}{\sqrt{3}}\xi + \sqrt{\frac{2}{3}}\rho\cos\left(\beta - \frac{2\pi}{3}\right) \\ \frac{1}{\sqrt{3}}\xi + \sqrt{\frac{2}{3}}\rho\cos\left(\beta + \frac{2\pi}{3}\right) \end{bmatrix} \tag{7}$$

in terms of the hidrostatic and deviatoric components, and the Lode angle

$$\xi = \frac{I_1}{\sqrt{3}}, \quad \rho = \sqrt{2J_2}, \quad \beta = \frac{1}{3}\cos^{-1}\left(\frac{3\sqrt{2}}{2}\frac{J_3}{J_2^{3/2}}\right) \tag{8}$$

which is only valid for the $\beta \in \left[0, \frac{\pi}{3}\right]$, I_1, J_2 and J_3 being the first invariant of the stress tensor, the second and third invariants of the deviatoric stress tensor, respectively.

The stress strain relation is given by

$$\varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{bmatrix} = (\mathbf{D}_{HW})^{-1}\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_2 \end{bmatrix} \tag{9}$$