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Direct integration method for hyperplastic models

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ABSTRACT: Hyperplasticity offers a reliable framework to construct thermodynamically consistent constitutive models. It starts by the specification of a free energy potential and a dissipation function (that is enriched by kinematic constrains), followed by a degenerate Legendre transformation to reach the regular elements of the traditional elastoplasticity, e.g. yield function. The latter step is mainly conducted for implementation purposes to follow the traditional elastoplasticity approach of integration. This transformation is a quite straightforward step for simple dissipation functions. For a more sophisticated choice, conducting the transformation might be hindered by mathematical complexities. This difficulty appears to limit the application of the hyperplasticity framework. However, the degenerate Legendre transformation is not a necessary step to capture the material behaviour since the free energy and dissipation functions already contain all necessary information of the model. In this paper, an implicit integration scheme to capture the elastoplastic response of the material directly from free energy and dissipation functions, is introduced. The scheme does not depend on the establishment of expressions for the yield and plastic potential surfaces. The method is successfully applied to a couple of sand models based on the Matsuoka-Nakai failure criterion with different kinematic constraints.

Keywords: direct integration, thermodynamic, hyperplasticity, Kinematic constraint

1 INTRODUCTION

The framework of hyperplasticity has been established, during the last two decades, mainly by Houlsby and Puzrin (e.g. Houlsby and Puzrin (2007)). Several researchers, e.g. Collins and Hilder (2002), Houlsby et al. (2017) and Dadras-Ajirloo et al. (2022) employed this framework to construct thermodynamically consistent constitutive models for different applications. The framework consists of two essential steps: 1) establishment of a free energy potential, a dissipation function and kinematic constraints; 2) derivation of yield and plastic potential surfaces using a degenerate Legendre transformation or Fenchel's duality theorem (see e.g. Houlsby (2019)). Implementation then follows the conventional integration approaches in elastoplasticity.

For simple dissipation functions and kinematic constraints, these steps are quite straightforward. However, a sophisticated choice of dissipation function and/or kinematic constraints may lead to mathematical complexities that hinder the derivation of yield and plastic potential surfaces through the degenerate Legendre transformation procedure, e.g. see Sands and Chandler (2010). Despite the great potential of the hyperplasticity framework, this mathematical complexity seems, so far, to limit its application. Thus, a direct integration scheme that represents the behaviour, without a need to establish explicit expressions for the yield and plastic potential surfaces, could be of high interest.

An alternative implementation approach, based on the optimization structure of frictional plasticity (Chandler and Sands, 2007), was proposed by Sands et al. (2011). They also introduced a graphical application of their method in order to visualise the yield surface resulted from the dissipation function and kinematic constraints (Chandler and Sands, 2009). However, their approach is, so far, limited to rigid plasticity.

In this paper we propose an alternative integration method, which works directly with the free energy potential and dissipation functions. The response of the model, in terms of stress, is found in this scheme by solving a small closed-form system of nonlinear equations that derived based on the basic principles of thermodynamics. Establishment of explicit expressions for the yield and plastic potential surfaces is not a requirement in this approach, and thus the degenerate Legendre transformation can be avoided. Besides, a simple numerical procedure is introduced to generate and visualise the shape of the yield surface. At the end, the efficiency of the method is examined through a couple of frictional models based on the Matsuoka-Nakai failure criterion with different kinematic constraints. Application to boundary value problems will follow in upcoming works.

Throughout this paper, following the conventional practice in geotechnics, compressive stress and strain are assumed to be positive. The material behaviour is thought to be rate independent. Isothermal condition, and infinitesimal strains hypothesis are adopted.

2 HYPERPLASTICITY BACKGROUND

According to the first law of thermodynamics, the incremental work done on a system is partly stored by strain energy, and partly dissipated through plastic dissipation:

$$\boldsymbol{\sigma}' : \dot{\boldsymbol{\varepsilon}} = \dot{\Psi} + \dot{\Phi}, \quad \text{where } \dot{\Phi} \geq 0 \tag{1}$$

where $\boldsymbol{\sigma}'$ and $\boldsymbol{\varepsilon}$ are, respectively, the effective stress and strain tensors, Ψ indicates the Helmholtz free energy density function, and $\dot{\Phi}$ is (the increment of) the dissipation density function, which according to the second law of thermodynamics is always non-negative. Selecting the total strain as the main state variable (Collins and Kelly, 2002), and the plastic strain ($\boldsymbol{\varepsilon}^p$) as the internal variable of the system, the free energy variation can be written:

$$\dot{\Psi} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^p} : \dot{\boldsymbol{\varepsilon}}^p \tag{2}$$

The dissipation function ($\dot{\Phi}$) is a function of plastic strain increment ($\dot{\boldsymbol{\varepsilon}}^p$). In the case of rate-independent behaviour, the dissipation function should be a homogeneous function of degree 1 with respect to the plastic strain increment, in order to fulfil the Ziegler's orthogonality postulate (Ziegler, 1983). Following the Euler's homogeneous function theorem:

$$\dot{\Phi} = \frac{\partial \dot{\Phi}}{\partial \dot{\boldsymbol{\varepsilon}}^p} : \dot{\boldsymbol{\varepsilon}}^p \tag{3}$$

Replacing (2) and (3) in Equation (1), and re-arranging the terms, we can conclude:

$$\boldsymbol{\sigma}' = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} \tag{4}$$

$$\frac{\partial \dot{\Phi}}{\partial \dot{\boldsymbol{\varepsilon}}^p} = -\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^p} \tag{5}$$

Considering Equation (3), it is clear that $\frac{\partial \dot{\Phi}}{\partial \dot{\boldsymbol{\varepsilon}}^p}$, and thus $\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^p}$ are of stress nature, and might be labelled as dissipative stress ($\boldsymbol{\chi}$):

$$\boldsymbol{\chi} = \frac{\partial \dot{\Phi}}{\partial \dot{\boldsymbol{\varepsilon}}^p} \tag{6}$$

$$\boldsymbol{\chi} = -\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^p} \tag{7}$$

Replacing (6) in (3), gives:

$$\dot{\Phi} = \boldsymbol{\chi} : \dot{\boldsymbol{\varepsilon}}^p \tag{8}$$

which must be strictly positive for any elastoplastic process and can be considered as a general indicator for the occurrence of plastic deformation.

The relation between the true stress ($\boldsymbol{\sigma}'$) and the dissipative stress depends on the form of the free energy function. Assuming, a free energy function that depends only on elastic strain (i.e. $\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p$):

$$\Psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) = \Psi(\boldsymbol{\varepsilon}^e) \tag{9}$$

Calculating the derivative of Ψ with respect to $\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}^p$ gives:

$$\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^e} \times \frac{\partial \boldsymbol{\varepsilon}^e}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^e} \tag{10}$$

$$\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^p} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^e} \times \frac{\partial \boldsymbol{\varepsilon}^e}{\partial \boldsymbol{\varepsilon}^p} = -\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^e} \tag{11}$$

Eliminating $\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^e}$ between (10) and (11), we obtain:

$$\boldsymbol{\sigma}' = \boldsymbol{\chi} \tag{12}$$

The plastic flow direction in granular materials is affected by kinematic processes, e.g. particle rearrangement. This is known as dilatancy rule in the classical theory of elastoplasticity. In the framework of hyperplasticity, this is taken into account through a kinematic constraint that is applied to the system by the modification of the original dissipation function using the standard method of Lagrange multiplier (Λ):

$$\dot{\Phi}^* = \dot{\Phi} + \Lambda c \tag{13}$$

where c is the constraint equation:

$$c(\dot{\boldsymbol{\varepsilon}}^p) = 0 \tag{14}$$

In such a case, the dissipation stress is calculated as:

$$\boldsymbol{\chi} = \frac{\partial \dot{\Phi}^*}{\partial \dot{\boldsymbol{\varepsilon}}^p} \tag{15}$$

The next step in the classical practice of hyperplasticity is to convert the final dissipation function to a yield and plastic potential surfaces using a degenerate Legendre transformation, which might involve unnecessary algebraic complexity that can potentially hinder the process. In the next section, we will show that this transformation is not a necessary step to complete the construction of a hyperplastic model.

3 DIRECT INTEGRATION SCHEME

In this section we describe a direct integration scheme to find the response of the model for a given strain increment ($\Delta\boldsymbol{\varepsilon}$). This is done by integrating a certain set of constitutive equations described in the previous section to find the unknowns: $\boldsymbol{\varepsilon}^p$, Λ, and $\boldsymbol{\sigma}'$. Considering Equations (4), (12), (14) and (15), the following residual equation can be constructed:

$$\mathbf{R} = \begin{cases} \mathbf{R}(\boldsymbol{\sigma}') = \boldsymbol{\sigma}' - \dfrac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} \\ \mathbf{R}(\boldsymbol{\varepsilon}^p) = \boldsymbol{\sigma}' - \dfrac{\partial \dot{\Phi}^*}{\partial \dot{\boldsymbol{\varepsilon}}^p} \\ R(\Lambda) = c(\Delta\boldsymbol{\varepsilon}^p) \end{cases} \tag{16}$$

where the derivatives are easily retrieved from the assigned free energy and dissipation functions. It is worth noting that hardening rules can be added to the system of Equations in (16).

The Newton-Raphson method is employed to linearize and solve the closed-form system of equations introduced in Equation (16):

$$\mathbf{J}^i_{n+1} \begin{bmatrix} \delta\boldsymbol{\sigma}' \\ \delta\boldsymbol{\varepsilon}^p \\ \delta\Lambda \end{bmatrix}^{i+1}_{n+1} = - \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ R_3 \end{bmatrix}^{i}_{n+1} \tag{17}$$

where the subscripts denote the load steps and superscripts stand for iterations, and $\mathbf{J}$ is the well-known Jacobian matrix:

$$\mathbf{J}^i_{n+1} = \begin{bmatrix} \dfrac{\partial \mathbf{R}_1}{\partial \boldsymbol{\sigma}'} & \dfrac{\partial \mathbf{R}_1}{\partial \boldsymbol{\varepsilon}^p} & \dfrac{\partial \mathbf{R}_1}{\partial \Lambda} \\ \dfrac{\partial \mathbf{R}_2}{\partial \boldsymbol{\sigma}'} & \dfrac{\partial \mathbf{R}_2}{\partial \boldsymbol{\varepsilon}^p} & \dfrac{\partial \mathbf{R}_2}{\partial \Lambda} \\ \dfrac{\partial R_5}{\partial \boldsymbol{\sigma}'} & \dfrac{\partial R_5}{\partial \boldsymbol{\varepsilon}^p} & \dfrac{\partial R_5}{\partial \Lambda} \end{bmatrix}^{i}_{n+1} \tag{18}$$

Solving the linearized system of equations (i.e. Equation (17)) in each iteration gives the increment of the unknown variables, which are updated accordingly:

$$\begin{bmatrix} \boldsymbol{\sigma}' \\ \boldsymbol{\varepsilon}^p \\ \Lambda \end{bmatrix}^{i+1}_{n+1} = \begin{bmatrix} \boldsymbol{\sigma}' \\ \boldsymbol{\varepsilon}^p \\ \Lambda \end{bmatrix}^{i}_{n+1} + \begin{bmatrix} \delta\boldsymbol{\sigma}' \\ \delta\boldsymbol{\varepsilon}^p \\ \delta\Lambda \end{bmatrix}^{i+1}_{n+1} \tag{19}$$

Iterations lasts until the residuals vanishes within a given tolerance. The solution is implicit, and thus it is unconditionally stable. The loading criterion to distinguish between elastic and elastoplastic processes, is done at this stage:

$$\begin{cases} \boldsymbol{\chi}_{n+1} : \Delta\boldsymbol{\varepsilon}^p_{n+1} > 0 \;\rightarrow\; \Delta\boldsymbol{\varepsilon}^p_{n+1} \neq 0 \\ \boldsymbol{\chi}_{n+1} : \Delta\boldsymbol{\varepsilon}^p_{n+1} \leq 0 \;\rightarrow\; \Delta\boldsymbol{\varepsilon}^p_{n+1} = 0 \end{cases} \tag{20}$$

Solution is then revised using Equation (4) by setting $\Delta\boldsymbol{\varepsilon}^p_{n+1} = 0$, when the loading criterion indicates elastic behaviour. The other variables are then modified accordingly.

3.1 *Plastic shoot*

Initial choice of the unknown variables plays a critical role in the convergence of the proposed scheme, when the dissipation function can potentially accept non-physical stress states, e.g. in case of Matsuoka-Nakai. In the classical theory of elastoplasticity, implicit integration schemes are commonly initialised using an elastic shoot with the given strain increment (known as trial stress). However, since the proposed solution scheme in this paper always searches for a possible (elastic-)plastic solution, initialising the iterative scheme by the elastic shoot might end up in a non-physical solution of the system. Thus, we propose an initial plastic shoot of the strain increment, instead of the elastic shoot. This means:

$$\boldsymbol{\sigma}'^0_{n+1} = \boldsymbol{\sigma}'_n; \quad (\boldsymbol{\varepsilon}^p)^0_{n+1} = \boldsymbol{\varepsilon}^p_n + \Delta\boldsymbol{\varepsilon}_{n+1}; \quad \Lambda^0_{n+1} = \Lambda_n \tag{21}$$

By plastic initialisation, the solution algorithm searches for the roots around the previous physical solution from the previous successful step, and thus non-physical solutions will be automatically prevented.

3.2 *Yield surface*

In hyperplasticity, yield surface is commonly found through a degenerate Legendre transformation of the dissipation function. However, in the proposed implementation, the model response is integrated directly from the free energy and dissipation functions, bypassing the transformation. In this frame, the yield surface can be generated numerically through a series of undrained simulations conducted for different initial stress states and loading paths, and finding the first stress state that fulfils the requirement for elastoplastic response expressed in Equation (20). This can be done in mean stress – deviatoric stress space, in the π−plane, and even in the full 3d principal stress space.

4 APPLICATION

In this section, the proposed method is examined through a couple of frictional models based on the Matsuoka-Nakai failure criterion with different kinematic constraints. Assuming a linear elastic behaviour for shear, and a nonlinear elastic behaviour for volumetric deformation, the free energy function might be written as:

$$\Psi = p'_{\mathrm{ref}} \kappa \exp\left(\frac{\varepsilon_v^e}{\kappa}\right) + \frac{3}{2} G \left(\varepsilon_q^e\right)^2 \tag{22}$$

where p'_{ref} is the reference pressure, κ denotes the elastic compressibility of the material, G is the shear modulus of the system, ε_v^e and ε_q^e are the elastic volumetric and deviatoric strains, respectively.

The dissipation function of Matsuoka-Nakai was introduce by Collins (2003), among the others:

$$\Phi = M_{\mathrm{smp}} \sqrt{\mathrm{tr}(\boldsymbol{\sigma}')\,\mathrm{tr}\left[\boldsymbol{\sigma}'\left(\dot{\boldsymbol{\varepsilon}}_{\mathrm{dev}}^p\right)^2\right] - \left[\mathrm{tr}\left(\boldsymbol{\sigma}'\dot{\boldsymbol{\varepsilon}}_{\mathrm{dev}}^p\right)\right]^2} \tag{23}$$

where M_{smp} is the frictional coefficient corresponding to the so-called Spatially Mobilised Plane (SMP). The dissipation function in (23) should be enriched with kinematic constraints to reach a closed-from system of equations. A couple of possible kinematic constraints are considered and discussed in the following.

4.1 Constant-volume flow

The constant-volume flow condition can be introduced to the system by the following kinematic constraint equation:

$$c(\dot{\boldsymbol{\varepsilon}}^p) = \dot{\varepsilon}_v^p = 0 \tag{24}$$

Applying this constraint to the dissipation equation results in the following residual equations:

$$\mathbf{R}(\boldsymbol{\sigma}') = \boldsymbol{\sigma}' - \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = \boldsymbol{\sigma}' - p'_{\mathrm{ref}} \exp\left(\frac{\varepsilon_v^e}{\kappa}\right)\boldsymbol{\delta} + 2G\,\boldsymbol{\varepsilon}_{\mathrm{dev}}^e \tag{25}$$

$$\mathbf{R}(\boldsymbol{\varepsilon}^p) = \boldsymbol{\sigma}' - \left(\frac{M_{\mathrm{smp}}^2}{\Delta\Phi}\left[\mathrm{tr}(\boldsymbol{\sigma}')\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p - \mathrm{tr}\left(\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p\right)\boldsymbol{\sigma}'\right] + \Lambda\boldsymbol{\delta}\right) \tag{26}$$

$$R(\Lambda) = c(\Delta\varepsilon_v^p) = \Delta\varepsilon_v^p \tag{27}$$

The residual equations were solved simultaneously using the Newton-Raphson method, as discussed in Section 3, and used for simulating several drained and undrained tests at different Lode angles. The material parameters used in the analysis were: $G = 10$ MPa, $\kappa = 0.001$, and $M_{\mathrm{smp}} = 0.408$. Figure 1 shows the numerically generated yield surfaces of the model for different M_{smp}, and the simulation results are presented in Figure 2.

4.2 Dilatant plastic flow

The incorporation of dilatancy is an important consideration in constitutive modelling of granular materials.

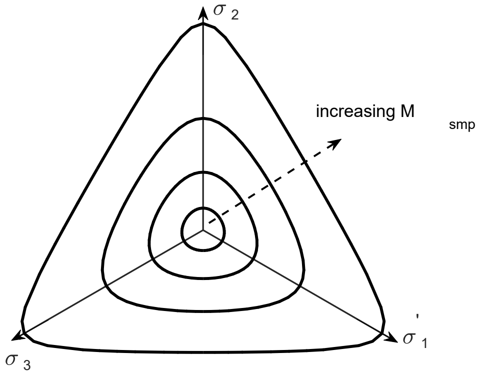

Figure 1. Model yield surface of the model in π −plane for M_{smp} = 0.1, 0.25, 0.408 and 0.65.

Equation (28) presents a simple, yet efficient, density-dependent dilatancy relation:

$$\frac{\dot{\varepsilon}_v^p}{\left(\dot{\varepsilon}_q^p\right)_{\mathrm{DKP}}} = \left\{1 - \exp\left[-\lambda_c.\left((\Delta\varepsilon_v^p)_{\mathrm{cr}} - \varepsilon_v^p\right)\right]\right\} M_{\mathrm{smp}} \tag{28}$$

where $\left(\dot{\varepsilon}_q^p\right)_{\mathrm{DKP}}$ indicates the deviatoric strain on the Dual Kinematic Plane (DKP):

$$\left(\dot{\varepsilon}_q^p\right)_{\mathrm{DKP}} = \sqrt{\frac{\mathrm{tr}\left[\boldsymbol{\sigma}'\left(\dot{\boldsymbol{\varepsilon}}_{\mathrm{dev}}^p\right)^2\right]}{\mathrm{tr}(\boldsymbol{\sigma}')}} \tag{29}$$

more information about the DKP plane can be found in Collins (2003). λ_c, in Equation (28), is a material constant, and $(\Delta\varepsilon_v^p)_{\mathrm{cr}}$ indicates the difference between the initial and the critical states of the soil in terms of ε_v^p. $(\Delta\varepsilon_v^p)_{\mathrm{cr}}$ is positive for loose materials, and negative for dense materials. By applying this dilatancy rule to the dissipation function, the following residual equation replace Equations (26) and (27):

$$\mathbf{R}(\boldsymbol{\varepsilon}^p) = \boldsymbol{\sigma}' - \left\{\left(\frac{M_{\mathrm{smp}}^2}{\Delta\Phi}\left[\mathrm{tr}(\boldsymbol{\sigma}')\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p - \mathrm{tr}\left(\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p\right)\boldsymbol{\sigma}'\right]\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p + \frac{\Lambda N}{\mathrm{tr}(\boldsymbol{\sigma}')\left(\Delta\varepsilon_q^p\right)_{\mathrm{DKP}}}\boldsymbol{\sigma}'\Delta\boldsymbol{\varepsilon}_{\mathrm{dev}}^p\right) + \Lambda\boldsymbol{\delta}\right\} \tag{30}$$

$$R(\Lambda) = \Delta\varepsilon_v^p + \left\{-1 + \exp\left[-\lambda_c.\left((\Delta\varepsilon_v^p)_{\mathrm{cr}} - \varepsilon_v^p\right)\right]\right\} M_{\mathrm{smp}}.\left(\Delta\varepsilon_q^p\right)_{\mathrm{DKP}} \tag{31}$$

Equations (25), (30) and (31) were solved simultaneously together, and used to simulate the response of the model for dense and loose sands. The results are presented in Figures 3 and 4. In these simulations, similar values as of Section 4.1 are used for G, κ and M_{smp}, and the remaining material parameters are chosen as: $\lambda_c = 10$ and $(\Delta\varepsilon_v^p)_{\mathrm{cr}} = \pm 0.05$ (for loose and dense material).

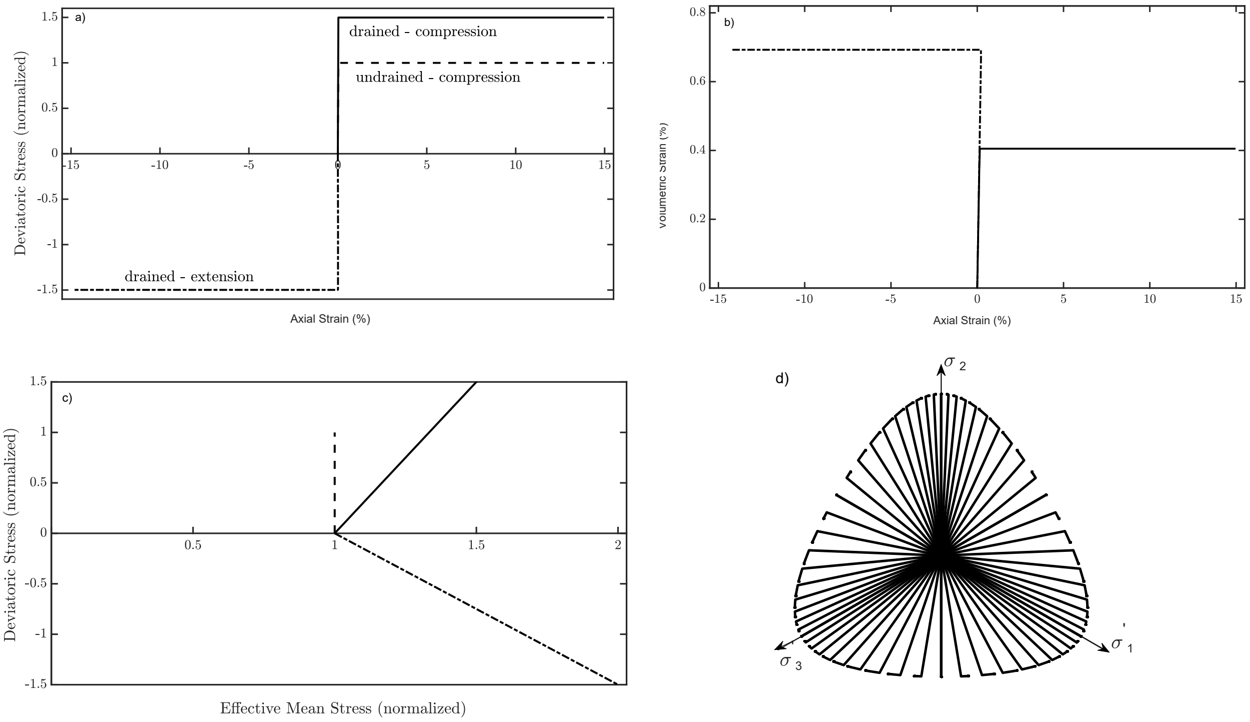

Figure 2. Response of Matsuoka-Nakai model with constant volume flow constraint, a-c) triaxial compression and extension tests with drained and undrained loading (normalized by p'_0); d) undrained tests at different Lode angles.

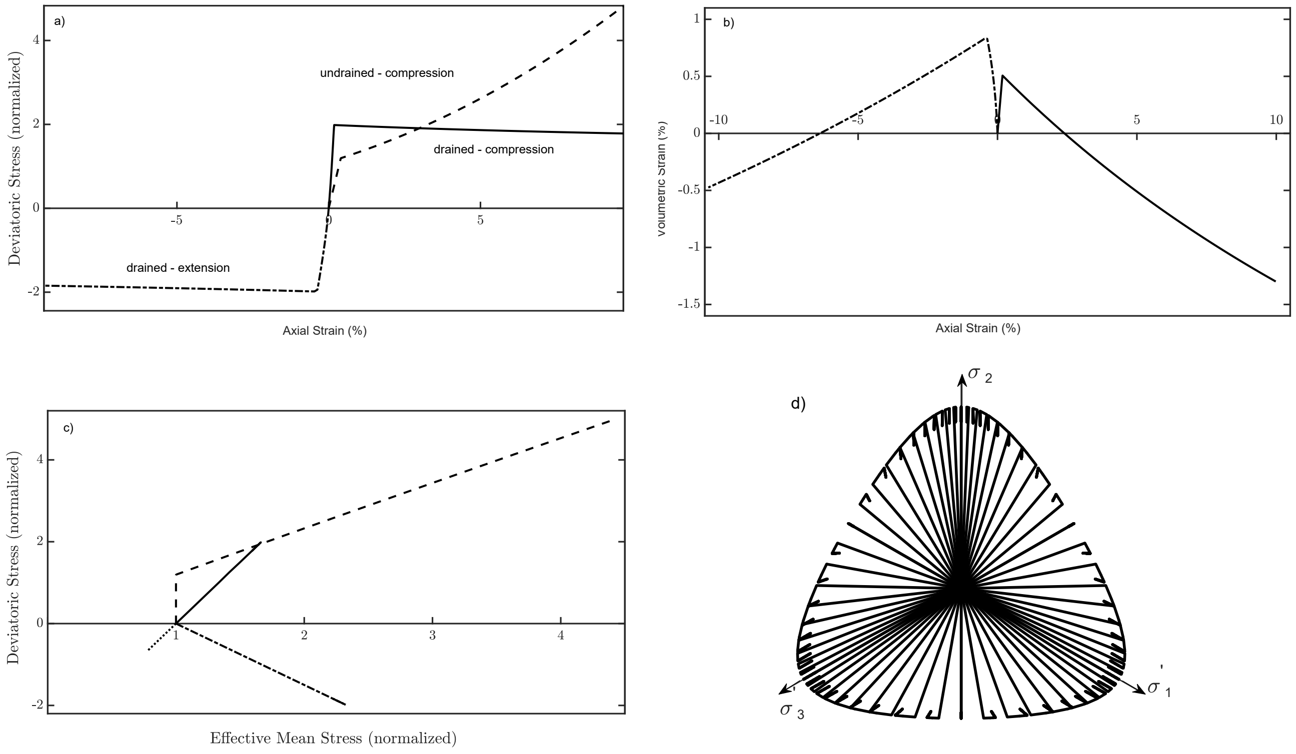

Figure 3. Response of Matsuoka-Nakai model with dilatant flow constraint for a dense sample, a-c) triaxial compression and extension tests with drained and undrained loading (normalized by p'_0); d) undrained tests at different Lode angles.

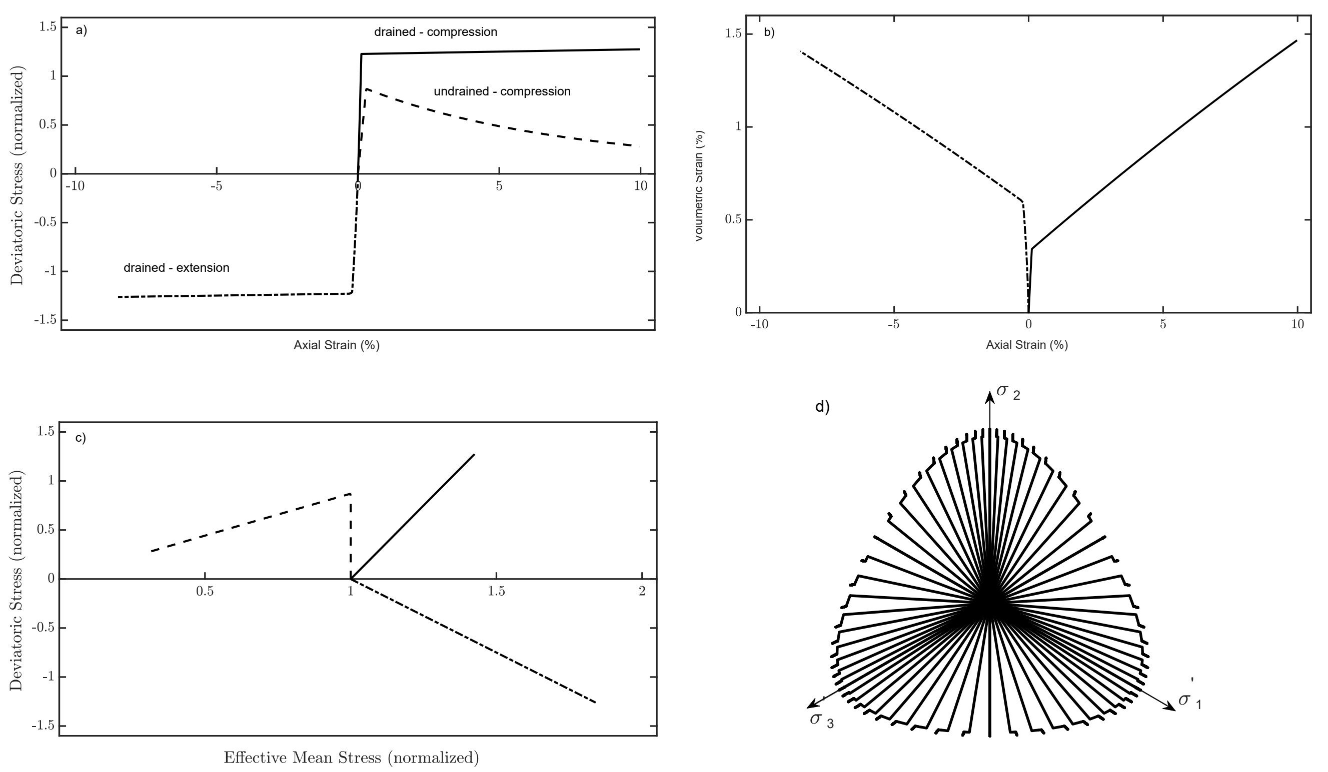

Figure 4. Response of Matsuoka-Nakai model with dilatant flow constraint for a loose sample, a-c) triaxial compression and extension tests with drained and undrained loading (normalized by p'_0); d) undrained tests at different Lode angles.

5 CONCLUSIONS

In this paper, a direct integration scheme for hyperplastic models has been proposed. The proposed method does not need any established expression for the yield and/or plastic potential surfaces. It has a relatively simple structure, and it finds the response of the material by solving a small set of nonlinear equations coming from the basic priciples of thermodynamics. The method was successfully applied to a couple of sand models, and the material response, as well as the resulted yield surfaces have been presented.

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