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NUMERICAL APPROACH TO SOME PROBLEMS IN ELASTO-PLASTICITY

SANDA CLEJA-ŢIGOIU, RAISA PAŞCAN, NADIA STOICUŢA

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3.1. INTRODUCTION

In this chapter, we present the mathematical formulation of some problems in elasto-plasticity and discuss corresponding numerical approaches to these problems. The physical research shows that plasticity and viscoplasticity are typical properties of crystalline materials. Defects, such as dislocations, generate plastic, permanent deformations and involve changes of the internal structures during the deformation process.

The basic assumptions stipulate that the material behaves like an elastic one with respect to plastically deformed configurations (the so-called relaxed configurations) and the evolution in time of the plastic distorsion, as well as the evolutions of the internal variables have to be added in order to complete the elasto-plastic behaviour of the model, see Section 3.2.

Internal variables account for the influence of the history of deformation on the current state of the material. For example, the following internal variables are used herein:

- the dislocation densities, $(\rho^{\alpha})_{\alpha=1,\dots,N}$, related to certain slip systems stand for internal variables in the models referring to crystal plasticity;

- the hardening variables, ζ_α, in a slip system, α;
- the scalar internal variable, κ, which describes the isotropic hardening in a macroscopic elasto-plastic model with small elastic strain, or the tensorial hardening variable, $\boldsymbol{\alpha}$, which defines the motion of the current yield surface in the appropriate stress space, see e.g. Cleja-Ţigoiu and Cristescu (1985).

Two types of evolution equations occur in this chapter, namely

- *rate dependent equations* – specific to viscoplasticity. In the constitutive framework of crystal plasticity the rate of plastic distortion is defined by multislip in the appropriate crystalographic systems in single crystal. The multislip mechanism is strongly related to the presence of dislocations inside the body, and the production, anihilation and motion of the dislocations; and
- *rate independent equations* – characterizing the elasto-plastic behaviour. The evolution equations are associated with certain yield surface. During an elasto-plastic process the current stress state can be on the yield surface or inside it in contrast to the rate dependent case when the current stress state is outer the appropriate flow surface.

In the following, we refer to large elasto-plastic deformation, as well as strain processes. In the finite plasticity framework funded on the physical background of the crystalline structure for metals, Cleja-Ţigoiu (1990a,b), and Cleja-Ţigoiu and Soós (1990) presented the basic assumptions for models with current relaxed configurations and internal state variables. The elasto-plastic models proposed herein are derived within the general constitutive framework already mentioned. On assuming small strains and small rotations, we subsequently derive the appropriate constitutive framework related to small elasto-plastic deformation behaviour.

The behaviour of the material is assumed to be elastic with respect to plastically deformed configurations, while the evolution equations for the plastic rate are associated with rate independent type evolution equations (and then we refer to finite elasto-plasticity) or rate dependent evolution equations in the case of elasto-viscoplasticity.

For elasto-viscoplastic models, we adopt herein the crystal plasticity framework, based on the Schmid activation condition (which is an appropriate flow surface), as described in Teodosiu and Sidoroff (1976). The material hardens with the scalar hardening parameters considered to be dependent on the scalar dislocation densities. For dislocation densities, we consider the local evolution equations associated with an appropriate slip system, following Teodosiu and Sidoroff (1976), and Teodosiu and Raphannel (1993), as well as the non-local evolution equations closely related to the paper by Bortoloni and Cermelli (2004).

In Section 3.3., we derive a variational rate boundary value problem for viscoplastic models in crystal plasticity. This is the starting point in the numerical approach to be adopted in a forthcoming paper. We intend to develop a finite element approach to solve the variational problem, which has to be coupled with an updated numerical procedure to determine the current value of the process state. We start from the paper by Teodosiu and Raphannel (1993), which is concerned with a finite element three-dimensional description of the large deformation of a polycrystalline body. The elastic anisotropy is taken into account and the plastic flow is considered to be rate dependent. The hardening law is dependent on the the dislocation densities on all planes with the evolution laws identified from single crystal experiments. The authors updated by an explicit Euler method all variables except the plastic shears for which a forward-gradient procedure was employed.

In Section 3.4., we present the numerical approach to finding the slip systems that become active during the plastic behaviour. The constitutive framework is similar to that developed in Section 3.3., where the rate boundary value problem is formulated. The elasto-plastic solution is numerically investigated for a strain controlled simple shear test. Here we show that only the first two slip systems are activated at the initial moment, while the remaining six systems become active afterwards.

Cleja-Ţigoiu (1996) considered the bifurcation of the elasto-plastic solution to the deformation of a bar made up from a single face-centred-cubic (FCC) and subjected to a uniaxial compression at the initial moment only. Firstly, a non-symmetric variational inequality (VI) was formulated for an elasto-plastic model with small elastic strains, but large elastic rotation and large deformations, within a multislip flow rule. In the initial homogeneous plastic problem, by taking into account the convexity of the activated plastic shear rates, we derive a method for solving the VI. In the very beginning of the plastic deformation, the eight glide systems become active. In the aforementioned paper, a possible solution, compatible with the VI, was built, but inferring the shear bands interfaces inside the deformed body.

In Section 3.5., a comprehensive analysis of the rigid and perfect-plastic behaviour is performed in a stress controlled test, for a homogeneous shear stress, when a single slip system was activated only, within the non-local framework to describe the evolution of the dislocation densities. The problem was initially formulated in Bortoloni and Cermelli (2004), with the mention that the authors have not given any details on the numerical method employed for solving this problem, apart from the statement that the solution was based on a finite difference method. In Section 3.5., we reconsider this problem. A numerical scheme for non-local solutions of the initial and boundary value problems is implemented using Matlab codes. This problem allows us to emphasize the nature of the numerical difficulties that could be encountered when the numerical are solved the problem concerning non-local behaviour in plastic behaviour. The system of equations to solve consists in one a partial differential equation and a differential type equation. Two methods have been proposed to solve the problem, and the domain for the material parameters has been numerical found.

In Cleja-Ţigoiu and Paşcan (2011), the initial and boundary value problem was formulated for a non-local elasto-viscoplastic model with large deformations by assuming that a single slip system is activated only and the shear stress state is homogeneous. This model takes into account the elastic part of the deformation as well. Firstly, the elastic solution is calculated in order to determine the initial condition for the elasto-viscoplastic problem at the moment when the slip system is activated. Secondly, this model deals with the hardening material. This means that the perfect plastic material is replaced by a hardening plastic material and the activation yield condition has to be accounted for. This is the key point in the numerical solution to the problem considered. The aim of this work is to analyze the influence of the evolution of the dislocation densities on the behaviour of the material when the elastic distortion is involved in the model and to establish the role played by the non-local evolution equation for the dislocation densities.

In Section 3.6., a finite element approach for the two-dimensional elasto-plastic problem is developed for the small strain elasto-plastic model. This time a rate independent evolution equation is postulated for an elasto-plastic material with isotropic hardening. A Simo-type trial algorithm is used to find the elasto-plastic moduli at every moment in the discretized interval following the approach of Simo and Hughes (1998). Using the appropriate discretized variational problem for the elastic type behaviour, the displacement vector can be found. Consequently the updated values for the stress, plastic deformation and hardening parameter can de established. Here there is a new method to find the solution for elasto-plastic model with small strain, based on the coupling of the variational problem and update algorithm for the body state.

3.2. CONSTITUTIVE FRAMEWORK

Let $\mathscr{B}$ be a body and $\chi : \mathscr{B} \times \mathbb{R} \longrightarrow \mathscr{E}$ be a motion of the body, where $\mathscr{E}$ is the three-dimensional Euclidean space. Three types of the configurations are considered herein, namely

1. the reference configuration, k;

2. the current configuration, $\chi(\cdot,t)$, at time t;

3. the current relaxed configuration, $\mathscr{K}_t$, also known as the plastically deformed configuration.

Let us consider a fixed material point $\mathbf{X}$ from the body B, in the reference configuration. For any arbitrarily given motion χ, the deformation gradient, $\mathbf{F}(\mathbf{X},t) = \nabla\chi(\mathbf{X},t)$, is defined on a certain neighbourhood of the material point $\mathbf{X}$.

Axiom 1. *The elasto-plastic model is developed based on the multiplicative decomposition of the deformation gradient into the elastic,* $\mathbf{F}^{\mathrm{e}}$*, and plastic,* $\mathbf{F}^{\mathrm{p}}$*, components, also referred sometimes to as distortions,*

$$\mathbf{F}(t) = \mathbf{F}^{\mathrm{e}}(t)\,\mathbf{F}^{\mathrm{p}}(t)\,. \tag{3.2.1}$$

Elastic response. We denote by $\widetilde{\rho}$, $\widehat{\rho}$ and $\widehat{\rho}_0$ the mass density in the relaxed, actual and reference configurations, respectively.

Axiom 2. *In general, the material behaves as an elastic material with respect to plastically deformed configurations, and the elastic type constitutive equation could be dependent on the internal state variable,* $\boldsymbol{\alpha}$*, namely*

$$\boldsymbol{\pi} = \mathbf{h}_{\mathscr{K}_t}(\mathbf{C}^{\mathrm{e}},\boldsymbol{\alpha})\,, \qquad \mathbf{C}^{\mathrm{e}} = (\mathbf{F}^{\mathrm{e}})^{\mathsf{T}}\,\mathbf{F}^{\mathrm{e}}\,. \tag{3.2.2}$$

Here $\boldsymbol{\pi}$ *represents the symmetric Piola-Kirchhoff stress, while* $\mathbf{C}^{\mathrm{e}}$ *denotes the right elastic Cauchy-Green strain tensor.*

The constitutive elastic function satisfies the following *relaxation condition*

$$\mathbf{h}_{\mathscr{K}_t}(\mathbf{S},\boldsymbol{\alpha}) = 0\,, \quad \mathbf{S}\in \mathrm{Sym} \iff \mathbf{S} = \mathbf{I}\,, \tag{3.2.3}$$

where Sym is the space of symmetric second order tensors.

If the existence of the potential φ, which represents the strain energy density per unit undeformed volume, has been accepted then:

Axiom 2*. *The elastic type constitutive equation is described with respect to the relaxed configuration, in terms of the potential, by*

$$\boldsymbol{\pi} = \widetilde{\rho}\,\frac{\partial\varphi(\mathbf{E}^{\mathrm{e}})}{\partial\mathbf{E}^{\mathrm{e}}}\,, \qquad \mathbf{E}^{\mathrm{e}} = \frac{1}{2}\left((\mathbf{F}^{\mathrm{e}})^{\mathsf{T}}\,\mathbf{F}^{\mathrm{e}} - \mathbf{I}\right)\,. \tag{3.2.4}$$

Here $\mathbf{E}^{\mathrm{e}}$ is a measure of the elastic deformation. Thus $\mathbf{C}^{\mathrm{e}} = \mathbf{I} \iff \mathbf{E}^{\mathrm{e}} = \mathbf{0}$.

We derive now the appropriate elastic type constitutive equation with respect to the reference, k, and deformed, $\chi(\cdot,t)$, configurations, respectively, and we emphasize the balance equations to be satisfied by the stresses.

In the *deformed configuration*, the balance equation for linear momentum for the equilibrium is written in terms of the Cauchy stress tensor $\mathbf{T}$

$$\operatorname{div}\mathbf{T} + \widehat{\rho}\,\mathbf{b} = 0 \quad \text{in} \quad \chi(B,t)\,, \tag{3.2.5}$$

where the body forces, $\widehat{\rho}\,\mathbf{b}$, are neglected. The balance equation for angular momentum leads to the symmetry of Cauchy stress tensor, i.e. $\mathbf{T} \in \mathrm{Sym}$.

Using the relationship between the Cauchy stress and the symmetric Piola-Kirchhoff stress tensors with respect to the relaxed (plastically deformed) configuration

$$\mathbf{T} = \frac{1}{\det \mathbf{F}^{\mathrm{e}}}\,\mathbf{F}^{\mathrm{e}}\,\boldsymbol{\pi}\,(\mathbf{F}^{\mathrm{e}})^{\mathsf{T}} \quad \text{with} \quad \widehat{\rho}\,\det \mathbf{F}^{\mathrm{e}} = \widetilde{\rho}\,, \tag{3.2.6}$$

the elastic type constitutive equation is derived in the following form

$$\mathbf{T} = \widehat{\rho}\,\mathbf{F}^{\mathrm{e}}\,\frac{\partial \varphi\,(\mathbf{E}^{\mathrm{e}})}{\partial \mathbf{E}^{\mathrm{e}}}\,(\mathbf{F}^{\mathrm{e}})^{\mathsf{T}}\,. \tag{3.2.7}$$

With respect to the *reference configuration*, the linear momentum balance equation is written in terms of the non-symmetric (or first) Piola-Kirchhoff stress tensor, $\mathbf{S}$,

$$\operatorname{div} \mathbf{S} + \widehat{\rho}_0\,\mathbf{b}_0 = 0\,, \tag{3.2.8}$$

where the body forces $\widehat{\rho}_0\,\mathbf{b}_0$ will be neglected.

The symmetry of the Cauchy stress tensor can be expressed through the first Piola-Kirchhoff stress tensor under the form

$$\mathbf{F}\mathbf{S}^{\mathsf{T}} = \mathbf{S}\mathbf{F}^{\mathsf{T}}\,. \tag{3.2.9}$$

The relationship between the first Piola-Kirchhoff stress tensor, $\mathbf{S}$, in the reference configuration and the Cauchy stress tensor, $\mathbf{T}$,

$$\mathbf{S} = (\det \mathbf{F})\,\mathbf{T}\mathbf{F}^{-\mathsf{T}} \tag{3.2.10}$$

is transformed in terms of the symmetric Piola-Kirchhoff stress tensor with respect to the relaxed configuration via (3.2.6), i.e.

$$\mathbf{S}\,(\mathbf{F}^{\mathrm{p}})^{\mathsf{T}} = (\det \mathbf{F}^{\mathrm{p}})\,\mathbf{F}^{\mathrm{e}}\,\boldsymbol{\pi}\,. \tag{3.2.11}$$

Consequently, the elastic type constitutive equation in terms of the first Piola-Kirchhoff, $\mathbf{S}$, is expressed via the potential φ introduced through (3.2.4) as

$$\mathbf{S} = \widetilde{\rho}\,\mathbf{F}^{\mathrm{e}}\,\frac{\partial \varphi\,(\mathbf{E}^{\mathrm{e}})}{\partial \mathbf{E}^{\mathrm{e}}}\,(\mathbf{F}^{\mathrm{p}})^{-\mathsf{T}}\,, \quad (\det \mathbf{F}^{\mathrm{p}})\;\widetilde{\rho} = \widehat{\rho}_0\,, \quad \mathbf{E}^{\mathrm{e}} = \frac{1}{2}\left((\mathbf{F}^{\mathrm{e}})^{\mathsf{T}}\,\mathbf{F}^{\mathrm{e}} - \mathbf{I}\right). \tag{3.2.12}$$

Rate of plastic distortion. In finite elasto-plasticity, first we present a rate independent type description for the plastic distortion and internal state variables and then we introduce rate dependent description in the *crystal plasticity setting*.

Axiom 3. (*Rate independent evolution equations*) *The variation in time of the plastic distortion and internal state variables are given, say in the stress space, by*

$$\dot{\mathbf{F}}^{\mathrm{p}}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1} = \lambda\,\mathscr{B}(\boldsymbol{\pi},\boldsymbol{\alpha})\,. \tag{3.2.13}$$

and

$$\dot{\boldsymbol{\alpha}} = \lambda\,\mathbf{l}(\boldsymbol{\pi},\boldsymbol{\alpha})\,. \tag{3.2.14}$$

We add the initial conditions

$$\mathbf{F}^{\mathrm{p}} = \mathbf{I}\,, \qquad \boldsymbol{\alpha}(t_0) = \boldsymbol{\alpha}_0\,. \tag{3.2.15}$$

The evolution equations are associated with the yield function, $\mathscr{F}$, and the plastic factor, λ, whose properties are listed below.

Axiom 4. *The function $\mathscr{F}$, which is defined in the stress space and is e.g. dependent on $\boldsymbol{\pi}$ and the internal variables, α, together with the plastic factor, λ, are defined such that they satisfy the requirements*

$$\begin{aligned} &\mathscr{F} \le 0\,, \quad \lambda \ge 0\,, \quad \lambda\mathscr{F} = 0 && (\textit{Khun-Tucker conditions}) \\ &\lambda\,\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F} = 0 && (\textit{consistency condition})\,. \end{aligned} \tag{3.2.16}$$

Remark 3.1. A strain-formulation elasto-plasticity represents an alternative formulation. For instance, it is possible to associate a yield function, $\widetilde{\mathscr{F}}$, with a given yield function, $\mathscr{F}$, in the strain space, through the composition of the latter with the elastic type constitutive function, namely

$$\widetilde{\mathscr{F}}\left(\mathbf{C}^{\mathrm{e}},\boldsymbol{\alpha}\right) := \mathscr{F}\left(\mathbf{h}\left(\mathbf{C}^{\mathrm{e}},\boldsymbol{\alpha}\right),\boldsymbol{\alpha}\right)\,. \tag{3.2.17}$$

In crystal plasticity, the rate of plastic distortion is defined by the slip in crystalographic systems. Let us denote by $(\overline{\mathbf{s}}^{\alpha},\overline{\mathbf{m}}^{\alpha})$ the $\alpha-$slip system, where $\overline{\mathbf{m}}^{\alpha}$ is the normal to the slip plane, $\overline{\mathbf{s}}^{\alpha}$ is the slip direction and $\overline{\mathbf{s}}^{\alpha}\cdot\overline{\mathbf{m}}^{\alpha} = 0$. In this case we replace Axiom 3 by an appropriate Axiom 3*.

Axiom 3*. (*Rate dependent evolution equations*) *The evolution equation for the plastic distortion is given under the form*

$$\dot{\mathbf{F}}^{\mathrm{p}}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1} = \sum_{\alpha=1}^{N} \nu^{\alpha}\left(\overline{\mathbf{s}}^{\alpha}\otimes\overline{\mathbf{m}}^{\alpha}\right)\,, \tag{3.2.18}$$

where N is the number of slip-systems, $\nu^{\alpha} = \dot{\gamma}^{\alpha}$ is the slip velocity and γ^{α} is the plastic shear on the $\alpha-$slip system.

The change in time of the plastic shear has to be defined in order to well define the evolution equation (3.2.18). Here, the viscoplastic flow rule will be introduced.

Remark 3.2. The directions $(\bar{\mathbf{s}}^\alpha, \overline{\mathbf{m}}^\alpha)$ of the $\alpha-$slip system are considered to be fixed with respect to the reference configuration as a consequence of the supposition that the relaxed configurations are isoclinic, see e.g. Mandel (1972) and Teodosiu and Sidoroff (1976), which means that the crystal lattice has the same orientation in the relaxed and reference configurations. The slip system is deformed during the plastic deformation, being defined in the deformed configuration by

$$\mathbf{F}^{\mathrm{e}}\,\bar{\mathbf{s}}^\alpha = \mathbf{s}^\alpha, \qquad (\mathbf{F}^{\mathrm{e}})^{-\mathsf{T}}\,\overline{\mathbf{m}}^\alpha = \mathbf{m}^\alpha, \tag{3.2.19}$$

where $\mathbf{s}^\alpha$ represents the glide vector in the actual configuration and $\mathbf{m}^\alpha$ is a vector parallel to the transformed normal via Nanson's formula, i.e. $(\det \mathbf{F}^{\mathrm{e}})\,(\mathbf{F}^{\mathrm{e}})^{-\mathsf{T}}\,\overline{\mathbf{m}}^\alpha$, when we push forward to the deformed configuration. Clearly, $\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0$.

Basic kinematic relationship. Using the multiplicative decomposition (3.2.1) the velocity gradient represented by $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ is related to the rate of plastic distortion, $\mathbf{L}^{\mathrm{p}}$, and the rate of elastic distortion, $\mathbf{L}^{\mathrm{e}}$, through

$$\begin{aligned} &\mathbf{L} = \mathbf{L}^{\mathrm{e}} + \mathbf{F}^{\mathrm{e}}\,\mathbf{L}^{\mathrm{p}}\,(\mathbf{F}^{\mathrm{e}})^{-1} \\ &\mathbf{L}^{\mathrm{e}} = \dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}, \quad \mathbf{L}^{\mathrm{p}} = \dot{\mathbf{F}}^{\mathrm{p}}\,(\mathbf{F}^{\mathrm{p}})^{-1}. \end{aligned} \tag{3.2.20}$$

Let us remark that in contrast with the rate of plastic distortion, which is related to the local relaxed configuration (or the plastically deformed configuration), the velocity gradient and rate of the elastic distortion are related to the current deformed configuration.

The evolution equation for plastic shears is associated with certain *yield conditions*, called here the *activation conditions*. In the literature, the Schmid activation condition has a wider utilization.

The *activation condition* is defined in a given slip system, say α, by

$$|\tau^\alpha| \geq \zeta^\alpha \tag{3.2.21}$$

with

$$\tau^\alpha := \frac{\mathbf{T}}{\widehat{\rho}}\,\mathbf{m}^\alpha \cdot \mathbf{s}^\alpha. \tag{3.2.22}$$

Here τ^α is the resolved shear stress, while ζ^α measures the critical shear stress. The yield modulus ζ^α measures the resistance to slip in the $\alpha-$slip system.

Let us remark that the activation criterium (3.2.21) together with (3.2.22) are defined in terms of the fields with respect to the deformed configuration. This criterion can be reformulated in terms of the fields pulled back to the reference configuration.

We replace the elements of a slip system in the actual configuration from the relationships (3.2.19) and the measure of Cauchy stress by the first Piola-Kirchhoff stress tensor from (3.2.6). Thus a new representation for the resolved shear stress (3.2.22) follows

$$\tau^{\alpha} = \frac{1}{\widehat{\rho}_0} \left(\mathbf{S} \left(\mathbf{F}^{\mathrm{p}} \right)^{\mathsf{T}} \overline{\mathbf{m}}^{\alpha} \right) \cdot \mathbf{F}^{\mathrm{e}} \overline{\mathbf{s}}^{\alpha} . \tag{3.2.23}$$

The viscoplastic flow takes place for the $\alpha-$slip system if and only if Schmid's law holds, i.e.

$$|\tau^{\alpha}| \geq \zeta^{\alpha} \iff \mathscr{F}^{\alpha} := |\tau^{\alpha}| - \zeta^{\alpha} \geq 0 . \tag{3.2.24}$$

The *viscoplastic flow rule* is described by:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left| \frac{\tau^{\alpha}}{\zeta^{\alpha}} \right|^n \operatorname{sign}\tau^{\alpha} \mathscr{H}\left(\mathscr{F}^{\alpha}\right), \forall \alpha = 1, \ldots, N , \tag{3.2.25}$$

where $\dot{\gamma}^{\alpha} \equiv \nu^{\alpha}$. Here $\mathscr{H}\left(\mathscr{F}^{\alpha}\right)$ is the Heaviside function composed with the activation function, $\mathscr{F}^{\alpha}$, introduced previously in (3.2.24) together with either (3.2.22) or (3.2.23).

The *hardening law* (i.e. if one assumes that the elasto-plastic material is a hardening one) is expressed either in terms of the dislocation densities according to Bortoloni and Cermelli (2004)

$$\zeta^{\alpha} = \zeta^{\alpha}\left(\rho^{\beta}\right), \qquad \beta = 1, \ldots, N , \tag{3.2.26}$$

or by certain evolution equation, say for example

$$\dot{\zeta}^{\alpha} = \sum_{\beta=1}^{N} h^{\alpha\beta} \left|\dot{\gamma}^{\beta}\right| , \tag{3.2.27}$$

where $h^{\alpha\beta}$ is the hardening matrix, see also Teodosiu and Raphannel (1993), strongly dependent on the dislocation densities.

Note that the evolution equations for the *dislocation densities* should also to be added.

3.3. VISCOPLASTIC MODELS IN CRYSTAL PLASTICITY. RATE BOUNDARY VALUE PROBLEM

In this section, we consider the description of the model with respect to the *actual configuration*, starting with the elastic type constitutive equation, which is derived from the potential φ, i.e.

$$\frac{\mathbf{T}}{\widehat{\rho}} = \mathbf{F}^{\mathrm{e}} \frac{\partial \varphi\left(\mathbf{E}^{\mathrm{e}}\right)}{\partial \mathbf{E}^{\mathrm{e}}} \left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}} , \qquad \mathbf{E}^{\mathrm{e}} = \frac{1}{2} \left(\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}} \mathbf{F}^{\mathrm{e}} - \mathbf{I} \right) . \tag{3.3.1}$$

The rate type evolution equation for the plastic distortion is described by the following multislip law

$$\dot{\mathbf{F}}^{\mathrm{p}}\,(\mathbf{F}^{\mathrm{p}})^{-1} = \sum_{\alpha=1}^{N} \nu^{\alpha}\,(\bar{\mathbf{s}}^{\alpha} \otimes \overline{\mathbf{m}}^{\alpha})\,, \qquad \nu^{\alpha} = \dot{\gamma}^{\alpha}\,, \tag{3.3.2}$$

in the plastically deformed configuration.

PROPOSITION 3.1. *We express the rate of the elastic distortion in terms of the slip systems pushed away to the deformed configuration, as defined by* (3.2.19)

$$\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1} = \dot{\mathbf{F}}\,(\mathbf{F})^{-1} - \sum_{\alpha=1}^{N} \nu^{\alpha}\,(\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha})\,. \tag{3.3.3}$$

Proof. In order to prove formula (3.3.3), we perform the transformation under the multislip flow rule, which allows us to write directly an *evolution equation for the elastic distortion*. We start from the basic kinematic relationship (3.2.20), i.e.

$$\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1} = \dot{\mathbf{F}}\,(\mathbf{F})^{-1} - \mathbf{F}^{\mathrm{e}}\left(\sum_{\alpha=1}^{N} \nu^{\alpha}\,(\bar{\mathbf{s}}^{\alpha} \otimes \overline{\mathbf{m}}^{\alpha})\right)(\mathbf{F}^{\mathrm{e}})^{-1}\,. \tag{3.3.4}$$

We note that the following relationship holds

$$\mathbf{F}^{\mathrm{e}}\,(\bar{\mathbf{s}}^{\alpha} \otimes \overline{\mathbf{m}}^{\alpha})\,(\mathbf{F}^{\mathrm{e}})^{-1} = \mathbf{F}^{\mathrm{e}}\bar{\mathbf{s}}^{\alpha} \otimes (\mathbf{F}^{\mathrm{e}})^{-\mathsf{T}}\,\overline{\mathbf{m}}^{\alpha} \equiv \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha} \tag{3.3.5}$$

since

$$\mathbf{F}^{\mathrm{e}}\,(\bar{\mathbf{s}}^{\alpha} \otimes \overline{\mathbf{m}}^{\alpha})\,(\mathbf{F}^{\mathrm{e}})^{-1}\,\mathbf{z} = \left(\mathbf{F}^{\mathrm{e}}\bar{\mathbf{s}}^{\alpha} \otimes (\mathbf{F}^{\mathrm{e}})^{-\mathsf{T}}\,\overline{\mathbf{m}}^{\alpha}\right)\mathbf{z}\,, \quad \forall \mathbf{z} \in \mathscr{V}\,. \tag{3.3.6}$$

PROPOSITION 3.2. *The change in time for* $\mathbf{s}^{\alpha}$ *and* $\mathbf{m}^{\alpha}$ *is given by*

$$\dot{\mathbf{s}}^{\alpha} = \dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\,\mathbf{s}^{\alpha}\,, \qquad \dot{\mathbf{m}}^{\alpha} = -\left(\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\right)^{\mathsf{T}}\mathbf{m}^{\alpha}\,. \tag{3.3.7}$$

Proof. The proof follows as a direct consequence of relationships (3.2.19) when we take the time derivative and account for the fixed directions of $\bar{\mathbf{s}}^{\alpha}$ and $\overline{\mathbf{m}}^{\alpha}$, namely

$$\dot{\mathbf{s}}^{\alpha} = \dot{\mathbf{F}}^{\mathrm{e}}\bar{\mathbf{s}}^{\alpha} = \dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\,\mathbf{F}^{\mathrm{e}}\bar{\mathbf{s}}^{\alpha} = \dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\,\mathbf{s}^{\alpha} \tag{3.3.8}$$

and

$$\begin{aligned}\dot{\mathbf{m}}^{\alpha} &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\,(\mathbf{F}^{\mathrm{e}})^{-1}\right)^{\mathsf{T}}\overline{\mathbf{m}}^{\alpha} = -\left((\mathbf{F}^{\mathrm{e}})^{-1}\,\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\right)^{\mathsf{T}}\overline{\mathbf{m}}^{\alpha}\\ &= -\left(\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\right)^{\mathsf{T}}(\mathbf{F}^{\mathrm{e}})^{-\mathsf{T}}\,\overline{\mathbf{m}}^{\alpha} = -\left(\dot{\mathbf{F}}^{\mathrm{e}}\,(\mathbf{F}^{\mathrm{e}})^{-1}\right)^{\mathsf{T}}\mathbf{m}^{\alpha}\,.\end{aligned} \tag{3.3.9}$$

Next, we derive the time derivative of the Cauchy stress, starting with the elastic type constitutive equation (3.3.1).

PROPOSITION 3.3. *The time derivative of the elastic type constitutive equation is given by*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{T}}{\widehat{\rho}}\right)=\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\right)\frac{\mathbf{T}}{\widehat{\rho}}+\mathscr{E}\left[\mathbf{D}\right]-\mathscr{E}\left[\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)^{\mathsf{S}}\right]+\frac{\mathbf{T}}{\widehat{\rho}}\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\right)^{\mathsf{T}}. \tag{3.3.10}$$

Here, the fourth order elastic tensor, $\mathscr{E}$, dependent on the elastic distortion has been introduced as

$$\mathscr{E}\left[\mathbf{X}\right]=\mathbf{F}^{\mathrm{e}}\left(\frac{\partial^{2}\varphi}{\partial\left(\mathbf{E}^{\mathrm{e}}\right)^{2}}\left[\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\mathbf{X}\mathbf{F}^{\mathrm{e}}\right]\right)\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}},\quad\forall\mathbf{X}\in\mathrm{Sym}. \tag{3.3.11}$$

Proof.

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{T}}{\widehat{\rho}}\right)&=\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\right)\frac{\mathbf{T}}{\widehat{\rho}}+\mathbf{F}^{\mathrm{e}}\left(\frac{\partial^{2}\varphi}{\partial(\mathbf{E}^{\mathrm{e}})^{2}}\left[\dot{\mathbf{E}}^{\mathrm{e}}\right]\right)\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\\&\quad+\mathbf{F}^{e}\frac{\partial\varphi\left(\mathbf{E}^{\mathrm{e}}\right)}{\partial\mathbf{E}^{\mathrm{e}}}\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\end{aligned} \tag{3.3.12}$$

or

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{T}}{\widehat{\rho}}\right)=\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\right)\frac{\mathbf{T}}{\widehat{\rho}}+\frac{1}{2}\mathbf{F}^{\mathrm{e}}\left(\frac{\partial^{2}\varphi}{\partial(\mathbf{E}^{\mathrm{e}})^{2}}\left[\dot{\mathbf{C}}^{\mathrm{e}}\right]\right)\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}+\frac{\mathbf{T}}{\widehat{\rho}}\left(\dot{\mathbf{F}}^{\mathrm{e}}\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\right)^{\mathsf{T}}. \tag{3.3.13}$$

On taking the time derivative of the elastic measure, $\mathbf{E}^{\mathrm{e}}$, and substituting the rate of the elastic distortion via the basic kinematic relationship (3.3.3), one obtains

$$\dot{\mathbf{C}}^{\mathrm{e}}=2\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\mathbf{D}\mathbf{F}^{\mathrm{e}}-2\left\{\mathbf{C}^{\mathrm{e}}\dot{\mathbf{F}}^{\mathrm{p}}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1}\right\}^{\mathsf{S}},\qquad\mathbf{D}=\left\{\mathbf{L}\right\}^{\mathsf{S}}. \tag{3.3.14}$$

Here, the evolution equation for the plastic distortion defined by the multislip flow rule is replaced through (3.2.18). Consequently, the following relationship holds

$$\begin{aligned}&\mathbf{C}^{\mathrm{e}}\dot{\mathbf{F}}^{\mathrm{p}}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1}=\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\mathbf{F}^{\mathrm{e}}\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\overline{\mathbf{s}}^{\alpha}\otimes\overline{\mathbf{m}}^{\alpha}\right)\\&=\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\mathbf{F}^{\mathrm{e}}\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\overline{\mathbf{s}}^{\alpha}\otimes\overline{\mathbf{m}}^{\alpha}\right)\right]\left(\mathbf{F}^{\mathrm{e}}\right)^{-1}\mathbf{F}^{\mathrm{e}}=\left(\mathbf{F}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)\right]\mathbf{F}^{\mathrm{e}},\end{aligned} \tag{3.3.15}$$

From (3.3.13) together with (3.3.15), it follows that (3.3.10) holds.

THEOREM 3.1. *The differential system which describes the evolution of the unknowns $\mathbf{T}/\widehat{\rho}$, $\mathbf{F}^{\mathrm{e}}$, $\mathbf{s}^{\alpha}$, $\mathbf{m}^{\alpha}$, γ^{α} and ρ^{α}, for a given history of the deformation gradient, $t \to \mathbf{F}(t)$, $t \in [t_0, t^*)$, is given by*

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{T}}{\widehat{\rho}}\right) - \mathbf{L}\frac{\mathbf{T}}{\widehat{\rho}} - \frac{\mathbf{T}}{\widehat{\rho}}\mathbf{L} = \mathscr{E}[\mathbf{D}] - \sum_{\alpha=1}^{N} \nu^{\alpha}\mathscr{E}\left[\{\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\}^{\mathsf{S}}\right] \\ - \sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)\frac{\mathbf{T}}{\widehat{\rho}} - \frac{\mathbf{T}}{\widehat{\rho}}\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)^{\mathsf{T}},\end{aligned} \tag{3.3.16}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{F}^{\mathrm{e}}\right)\left(\mathbf{F}^{\mathrm{e}}\right)^{-1} = \mathbf{L} - \sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right), \tag{3.3.17}$$

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left|\frac{\mathbf{T}\mathbf{m}^{\alpha}\cdot\mathbf{s}^{\alpha}}{\widehat{\rho}\,\zeta^{\alpha}}\right|^{n}\operatorname{sgn}\left(\frac{\mathbf{T}}{\widehat{\rho}}\mathbf{m}^{\alpha}\cdot\mathbf{s}^{\alpha}\right)\mathscr{H}\left(\mathscr{F}^{\alpha}\right), \quad \alpha = 1,\ldots,N, \tag{3.3.18}$$

$$\dot{\mathbf{s}}^{\alpha} = \mathbf{L}\mathbf{s}^{\alpha} - \sum_{\beta=1}^{N}\nu^{\beta}\left(\mathbf{s}^{\beta}\otimes\mathbf{m}^{\beta}\right)\mathbf{m}^{\alpha}, \quad \alpha = 1,\ldots,N, \tag{3.3.19}$$

$$\dot{\mathbf{m}}^{\alpha} = -\mathbf{L}^{\mathsf{T}}\mathbf{m}^{\alpha} + \sum_{\beta=1}^{N}\nu^{\beta}\left(\mathbf{m}^{\beta}\otimes\mathbf{s}^{\beta}\right)\mathbf{m}^{\alpha}, \quad \alpha = 1,\ldots,N, \tag{3.3.20}$$

and either

$$\dot{\rho}^{\alpha} = \frac{1}{b}\left(\frac{1}{L^{\alpha}} - 2y_c\,\rho^{\alpha}\right)|\nu^{\alpha}|, \quad L^{\alpha} = K\left(\sum_{q\neq\alpha}\rho^{q}\right)^{-1/2}, \quad \alpha = 1,\ldots,N, \tag{3.3.21}$$

or

$$\dot{\rho}^{\alpha} = D\,|\nu^{\alpha}|\left(k\,\Delta\rho^{\alpha} - \frac{\partial\psi_T}{\partial\rho^{\alpha}}\right), \quad \alpha = 1,\ldots,N, \tag{3.3.22}$$

for $\zeta^{\alpha} = \widehat{\zeta}^{\alpha}\left(\rho^{\beta}\right)$, $\beta = 1,\ldots,N$, given functions and $\nu^{\alpha} \equiv \dot{\gamma}^{\alpha}$ to be eliminated from the left-hand side of the system, with the mention that the evolution equations (3.3.21) *and* (3.3.22) *are used in Sections 3.4. and 3.5., respectively.*

Finally, the rate of the nominal stress is calculated as follows

$$\dot{\mathbf{S}}_t(\mathbf{x},t) = \widehat{\rho}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathbf{T}}{\widehat{\rho}}\right) - \frac{\mathbf{T}}{\widehat{\rho}}\mathbf{L}^{\mathsf{T}}\right], \tag{3.3.23}$$

$$\begin{aligned}\dot{\mathbf{S}}_t(\mathbf{x},t) = \widehat{\rho}\,\mathbf{L}\frac{\mathbf{T}}{\widehat{\rho}} + \widehat{\rho}\,\mathscr{E}[\mathbf{D}] \\ - \widehat{\rho}\sum_{\alpha=1}^{N}\nu^{\alpha}\left\{\mathscr{E}\left[\{\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\}^{\mathsf{S}}\right] + \left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)\frac{\mathbf{T}}{\widehat{\rho}} + \frac{\mathbf{T}}{\widehat{\rho}}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right)^{\mathsf{T}}\right\}.\end{aligned} \tag{3.3.24}$$

The weak form of the rate boundary value problem can be recast as

$$\begin{aligned}
&\int_{\Omega_t} \widehat{\rho}\nabla\mathbf{v}\frac{\mathbf{T}}{\widehat{\rho}}\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}+\int_{\Omega_t}\widehat{\rho}\mathscr{E}[\mathbf{D}]\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}-\sum_{\alpha=1}^{N}\int_{\Omega_t}\widehat{\rho}\nu^{\alpha}\mathscr{E}\left[\{\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\}^{\mathsf{S}}\right]\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}\\
&-\sum_{\alpha=1}^{N}\int_{\Omega_t}\widehat{\rho}\nu^{\alpha}\left[(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha})\frac{\mathbf{T}}{\widehat{\rho}}+\frac{\mathbf{T}}{\widehat{\rho}}(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha})^{\mathsf{T}}\right]\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}\\
&=\int_{\partial\Omega_t}\dot{\mathbf{S}}_t\,\mathbf{n}\cdot\mathbf{w}\,\mathrm{d}a+\int_{\Omega_t}\widehat{\rho}\dot{\mathbf{b}}_t\cdot\mathbf{w}\,\mathrm{d}\mathbf{x}.
\end{aligned}\tag{3.3.25}$$

Note that, on using the relative description formalism developed by Cleja-Ţigoiu (2000b), the linear momentum balance equation for the rate boundary value problem is written, in terms of the rate of the nominal stress, in the following form

$$\operatorname{div}\dot{\mathbf{S}}_t+\widehat{\rho}\,\dot{\mathbf{b}}_t=\mathbf{0}.\tag{3.3.26}$$

We suppose that the current values of $\mathbf{T}$, $\mathbf{F}^{\mathrm{e}}$, $\mathbf{s}^{\alpha}$, $\mathbf{m}^{\alpha}$, ζ^{α} and ρ^{α} are known at a certain moment t. On using (3.3.18), we eliminate ν^{α} in equation (3.3.25) and obtain the following weak formulation for finding the velocity field $\dot{\mathbf{u}}\equiv\mathbf{v}$:

$$\begin{aligned}
&\int_{\Omega_t}\widehat{\rho}\nabla\mathbf{v}\frac{\mathbf{T}}{\widehat{\rho}}\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}+\int_{\Omega_t}\widehat{\rho}\mathscr{E}[\mathbf{D}]\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}\\
&-\sum_{\alpha=1}^{N}\int_{\Omega_t}\widehat{\rho}\dot{\gamma}_0^{\alpha}\left|\frac{\mathbf{T}\mathbf{m}^{\alpha}\cdot\mathbf{s}^{\alpha}}{\zeta^{\alpha}}\right|^{n}\operatorname{sgn}(\mathbf{T}\mathbf{m}^{\alpha}\cdot\mathbf{s}^{\alpha})\,\mathscr{H}(\mathscr{F}^{\alpha})\\
&\left\{\mathscr{E}\left[\{\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\}^{\mathsf{S}}\right]+(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha})\frac{\mathbf{T}}{\widehat{\rho}}+\frac{\mathbf{T}}{\widehat{\rho}}(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha})^{\mathsf{T}}\right\}\cdot\nabla\mathbf{w}\,\mathrm{d}\mathbf{x}\\
&=\int_{\partial\Omega_t}\dot{\mathbf{S}}_t\,\mathbf{n}\cdot\mathbf{w}\,\mathrm{d}a+\int_{\Omega_t}\widehat{\rho}\dot{\mathbf{b}}_t\cdot\mathbf{w}\,\mathrm{d}\mathbf{x},\quad\forall\mathbf{w}\in\mathscr{V}_{ad}.
\end{aligned}\tag{3.3.27}$$

Comments: In Teodosiu and Raphannel (1993), the weak formulation of the boundary value problem is derived using the virtual power principle. The incremental formulation of the boundary value problem at time $t+\Delta t$ is the starting point in their numerical approach. The evaluation of the increment of the shear slip in a given system is made using an intermediate Euler algorithm. A finite element discretization is applied to the kinematic field and, consequently, the discretization of the virtual power principle leads to an appropriate algebraic system. After solving this algebraic system, the configuration of the deformed body ,as well as the state variables, namely the dislocation densities, Cauchy stress and elastic rotations, are updated at each Gauss point. The update procedure is developed by simple Euler explicit scheme, except for the shear slips increments. In the procedure adopted in this chapter, we firstly formulate the rate boundary value problem based on the relative description of the material behaviour with respect to the configuration at moment t, see the procedure developed by Cleja-Ţigoiu (2000b).

3.4. VISCOPLASTIC SIMPLE SHEAR PROBLEM IN A STRAIN CONTROLLED TEST

We formulate the problem with respect to the reference configuration. We suppose that the crystalline material has a FCC-crystalline structure and the dislocation densities occur in the model as internal state variables. The viscoplastic model and material constants are adopted from Teodosiu and Raphannel (1993). The key point of the problem consists of finding activated system at every time moment. We analyze the problem of activated slip systems in a simple shear problem with an imposed deformation process. Let us consider a peculiar case of a FCC-system which has been considered by Cleja-Ţigoiu (1996). There are $N = 12$ slip systems characterized by the corresponding elements given in Table 3.4.1. Here, the slip systems $\{(\bar{\mathbf{s}}^\alpha, \overline{\mathbf{m}}^\alpha)\}$,

Table 3.4.1 – *The slip directions* $\mathbf{s}^\alpha$ *and the slip planes* $\mathbf{m}^\alpha$

$\bar{\mathbf{s}}^1 = \frac{1}{\sqrt{2}}[1,\bar{1},0]$	$\overline{\mathbf{m}}^1 = \frac{1}{\sqrt{3}}(1,1,1)$	$\bar{\mathbf{s}}^7 = \frac{1}{\sqrt{2}}[1,\bar{1},0]$	$\overline{\mathbf{m}}^7 = \frac{1}{\sqrt{3}}(\bar{1},\bar{1},1)$
$\bar{\mathbf{s}}^2 = \frac{1}{\sqrt{2}}[\bar{1},0,1]$	$\overline{\mathbf{m}}^2 = \frac{1}{\sqrt{3}}(1,1,1)$	$\bar{\mathbf{s}}^8 = \frac{1}{\sqrt{2}}[\bar{1},0,1]$	$\overline{\mathbf{m}}^8 = \frac{1}{\sqrt{3}}(1,\bar{1},1)$
$\bar{\mathbf{s}}^3 = \frac{1}{\sqrt{2}}[0,\bar{1},1]$	$\overline{\mathbf{m}}^3 = \frac{1}{\sqrt{3}}(1,1,1)$	$\bar{\mathbf{s}}^9 = \frac{1}{\sqrt{2}}[0,\bar{1},1]$	$\overline{\mathbf{m}}^9 = \frac{1}{\sqrt{3}}(\bar{1},1,1)$
$\bar{\mathbf{s}}^4 = \frac{1}{\sqrt{2}}[1,0,1]$	$\overline{\mathbf{m}}^4 = \frac{1}{\sqrt{3}}(\bar{1},\bar{1},1)$	$\bar{\mathbf{s}}^{10} = \frac{1}{\sqrt{2}}[1,0,1]$	$\overline{\mathbf{m}}^{10} = \frac{1}{\sqrt{3}}(\bar{1},1,1)$
$\bar{\mathbf{s}}^5 = \frac{1}{\sqrt{2}}[0,1,1]$	$\overline{\mathbf{m}}^5 = \frac{1}{\sqrt{3}}(\bar{1},\bar{1},1)$	$\bar{\mathbf{s}}^{11} = \frac{1}{\sqrt{2}}[0,1,1]$	$\overline{\mathbf{m}}^{11} = \frac{1}{\sqrt{3}}(1,\bar{1},1)$
$\bar{\mathbf{s}}^6 = \frac{1}{\sqrt{2}}[1,1,0]$	$\overline{\mathbf{m}}^6 = \frac{1}{\sqrt{3}}(1,\bar{1},1)$	$\bar{\mathbf{s}}^{12} = \frac{1}{\sqrt{2}}[1,1,0]$	$\overline{\mathbf{m}}^{12} = \frac{1}{\sqrt{3}}(\bar{1},1,1)$

$\alpha = 1,\ldots,12$, are considered such that $\bar{\mathbf{s}}^\alpha$ and $\overline{\mathbf{m}}^\alpha$ are constant, orthonormal vectors, i.e. $\|\bar{\mathbf{s}}^\alpha\| = \|\overline{\mathbf{m}}^\alpha\| = 1$, $\bar{\mathbf{s}}^\alpha \cdot \overline{\mathbf{m}}^\alpha = 0$.

3.4.1. FORMULATION OF THE PROBLEM

On assuming a strain controlled test corresponding to a homogeneous process, $t \longrightarrow \mathbf{F}(t)$, we solve the following problem:
Find the Piola-Kirchhoff stress, $\mathbf{S}$, plastic distortion, $\mathbf{F}^p$, dislocation densities, ρ^α, and hardening parameters, τ_C^α, which satisfy the following relationships:

- The balance equation together with the symmetry condition

$$\operatorname{div}\mathbf{S}=0\,,\quad \mathbf{F}\mathbf{S}^{\mathsf{T}}=\mathbf{S}\mathbf{F}^{\mathsf{T}}\,. \tag{3.4.1}$$

- The elastic type constitutive equation

$$\mathbf{S}=\widehat{\rho}_0\,\mathbf{F}\,(\mathbf{F}^{\mathrm{p}})^{-1}\,[\lambda\,(\operatorname{tr}\mathbf{E}^{\mathrm{e}})\,\mathbf{I}+2\,\mu\,\mathbf{E}^{\mathrm{e}}]\,(\mathbf{F}^{\mathrm{p}})^{-\mathsf{T}}\,, \tag{3.4.2}$$

  where

$$\mathbf{E}^{\mathrm{e}}=\frac{1}{2}\left[(\mathbf{F}^{\mathrm{p}})^{-\mathsf{T}}\,\mathbf{C}\,(\mathbf{F}^{\mathrm{p}})^{-1}-\mathbf{I}\right],\quad \text{with}\quad \mathbf{C}=\mathbf{F}^{\mathsf{T}}\,\mathbf{F}, \tag{3.4.3}$$

  which corresponds to a linear elastic behaviour with respect to the plastically deformed configuration. In this case, the elastic potential is given by

$$\varphi\,(\mathbf{E}^{\mathrm{e}})=\frac{1}{2}\lambda\,(\operatorname{tr}\mathbf{E}^{\mathrm{e}})^2+\mu\,\mathbf{E}^{\mathrm{e}}\cdot\mathbf{E}^{\mathrm{e}}\,,$$

  where λ and μ are the elastic material constants.

- The evolution equation defining the variation in time of the plastic distortion

$$\dot{\mathbf{F}}^{\mathrm{p}}=\sum_{\alpha=1}^{12}\nu^{\alpha}\,(\bar{\mathbf{s}}^{\alpha}\otimes\overline{\mathbf{m}}^{\alpha})\,\mathbf{F}^{\mathrm{p}}\,, \tag{3.4.4}$$

  with the slip velocities described via the relationships given in (3.2.25), namely

$$\nu^{\alpha}:=\dot{\gamma}^{\alpha}=\dot{\gamma}_0^{\alpha}\left|\frac{\tau^{\alpha}}{\tau_C^{\alpha}}\right|^n\operatorname{sgn}(\tau^{\alpha})\,\mathscr{H}\,(\mathscr{F}^{\alpha})\,,\qquad \alpha=1,\ldots,N. \tag{3.4.5}$$

- The Schmid law describing the activation condition with the resolved shear stress, τ^{α}, expressed in terms of the first Piola-Kirchhoff stress in the $\alpha-$slip system

$$\begin{gathered}|\tau^{\alpha}|\geq\tau_C^{\alpha}\iff\mathscr{F}^{\alpha}:=|\tau^{\alpha}|-\tau_C^{\alpha}\geq 0\,,\\ \tau^{\alpha}=\frac{1}{\widehat{\rho}_0}\left(\mathbf{S}\,(\mathbf{F}^{\mathrm{p}})^{\mathsf{T}}\,\overline{\mathbf{m}}^{\alpha}\right)\cdot(\mathbf{F}^{\mathrm{e}}\,\bar{\mathbf{s}}^{\alpha})\,.\end{gathered} \tag{3.4.6}$$

  Here, $\zeta^{\alpha}:=\tau_C^{\alpha}=\tau_C^{\alpha}\left(\rho^{\beta}\right)$ is the hardening parameter which has the meaning of the critical shear stress in the $\alpha-$slip system and is dependent on all of the dislocation densities, ρ^{β}, $\beta=1,\ldots,N$.

- The hardening laws introduced for each slip system through τ_C^α expressed in terms of the dislocations densities, i.e.

$$\tau_C^\alpha = \mu b \left(\sum_{u=1}^{12} a^{\alpha u} \rho^u \right)^{1/2} , \tag{3.4.7}$$

  where the hardening matrix, $\left(a^{\alpha\beta}\right)$, describes the interactions between dislocations, b is the intensity of the Burgers vector and μ is the elastic shear modulus.

- The evolution equation for τ_C^α obtained by taking the time derivative of equation (3.4.7), namely

$$\dot{\tau}_C^\alpha = \sum_{u=1}^{12} h^{\alpha u} \left| \nu^u \right| . \tag{3.4.8}$$

  The elements of the matrix $(h^{\alpha u})$ have the following expressions

$$h^{\alpha u} = \frac{\mu}{2} a^{\alpha u} \left(\sum_q a^{\alpha q} \rho^q \right)^{-1/2} \left[\frac{1}{K} \left(\sum_{q \neq u} \rho^q \right)^{1/2} - 2 y_c \rho^u \right] . \tag{3.4.9}$$

- The evolution law for the dislocation densities as considered by Teodosiu and Raphannel (1993), i.e.

$$\dot{\rho}^\alpha = \frac{1}{b} \left(\frac{1}{L^\alpha} - 2 y_c \rho^\alpha \right) \left| \nu^\alpha \right| , \tag{3.4.10}$$

  where

$$L^\alpha = K \left(\sum_{q \neq \alpha} \rho^q \right)^{-1/2} . \tag{3.4.11}$$

- Initial conditions to be added. The initial values for the critical shear stress, $\tau_{C_0}^\alpha = \tau_{C_0}$, are provided from (3.4.7) and correspond to $\rho^\alpha = \rho_0$.

Problem: Given the deformation gradient

$$\mathbf{F}(t) = \begin{bmatrix} 1 & 0 & 0 \\ F_{21}(t) & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} , \tag{3.4.12}$$

find the homogeneous process $\mathbf{F}^{\mathrm{p}}$, τ_C^α and ρ^α, satisfying at every time t the differential equation system (DES) described by (3.4.4)–(3.4.6) and (3.4.8)–(3.4.11), where $\mathbf{S}$ is eliminated via the algebraic equation (3.4.2).
The initial conditions associated with the problem are the following:

$$\mathbf{F}^{\mathrm{p}}(t_0) = \mathbf{I}, \quad \tau_C^\alpha(t_0) = \tau_{C_0} , \quad \rho^\alpha(t_0) = \rho_0 . \tag{3.4.13}$$

Remarks:

- The differential system is strongly time-dependent, where the time-dependent definition domain is related to the activated systems. Note that the explicit dependence on time appears through the current value of the deformation gradient $\mathbf{F}(t)$.

- The *maximal number of the unknowns* is 9 (plastic distortion) + 12 (hardening parameters) + 12 (plastic shears) = 33.

- The differential system can be formally written in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{F}^{\mathrm{p}}, \tau_C^{\alpha}, \rho^{\alpha}\right) = f\left(\mathbf{F}(t), \mathbf{F}^{\mathrm{p}}, \tau_C^{\alpha}, \rho^{\alpha}; \mathbf{S}\right) \mathscr{H}\left(\mathscr{F}^{\alpha}\right), \tag{3.4.14}$$

  where $\mathbf{S} = \mathbf{S}\left(\mathbf{F}(t), \mathbf{F}^{\mathrm{p}}\right)$ and $\mathscr{F}^{\alpha} = \mathscr{F}^{\alpha}\left(\mathbf{F}(t), \mathbf{F}^{\mathrm{p}}, \tau_C^{\alpha}; \mathbf{S}\right)$, for a given history of the deformation gradient, $t \longrightarrow \mathbf{F}(t)$.

3.4.2. DESCRIPTION OF THE ALGORITHM AND NUMERICAL RESULTS

In the following, we describe the algorithm used for solving numerically the problem presented in the previous section. A Mathcad code was employed to obtain the numerical results. Next, we define the Mathcad matrix, vector and scalar functions used in the proposed numerical algorithm.

- The vector function $\mathbf{L}(\boldsymbol{\rho})$, given by (3.4.11), can be expressed as

$$\mathbf{L}(\boldsymbol{\rho}) = K \Big/ \sqrt{\mathbf{M}\,\boldsymbol{\rho}}\ ,$$

  where $\mathbf{M} = \left(M_{ij}\right)_{1 \le i,j \le 12}$ is the matrix that allows for the elimination of the elements with the same index, i.e.

$$M_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \neq j \end{cases},$$

  while $\boldsymbol{\rho} = \left(\rho_1 \ldots \rho_{12}\right)^{\mathsf{T}}$ and $\mathbf{L} = \left(L_1 \ldots L_{12}\right)^{\mathsf{T}}$ are column vectors.

- The matrix function

$$\mathbf{E}^{\mathrm{e}}\left(t, \mathbf{F}^{\mathrm{p}}\right) = \frac{1}{2}\left[\left(\left(\mathbf{F}^{\mathrm{p}}\right)^{-1}\right)^{\mathsf{T}} \mathbf{F}(t)^{\mathsf{T}}\, \mathbf{F}(t)\, \left(\mathbf{F}^{\mathrm{p}}\right)^{-1} - \mathbf{I}\right]$$

  is calculated according to formula (3.4.2).

- The stress is given by the elastic type constitutive equation, see (3.4.3), i.e.

$$\mathbf{S}(t,\mathbf{F}^{\mathrm{p}}) = \mathbf{F}(t)\,(\mathbf{F}^{\mathrm{p}})^{-1}\left(\lambda\left(\operatorname{tr}\mathbf{E}^{\mathrm{e}}(t,\mathbf{F}^{\mathrm{p}})\right)\mathbf{I} + 2\,\mu\,\mathbf{E}^{\mathrm{e}}(t,\mathbf{F}^{\mathrm{p}})\right)\left((\mathbf{F}^{\mathrm{p}})^{-1}\right)^{\mathsf{T}}.$$

- The matrices $\mathbf{m}$ and $\mathbf{s}$ define the vectors $\sqrt{3}\,\overline{\mathbf{m}}^{\alpha}$ and $\sqrt{2}\,\overline{\mathbf{s}}^{\alpha}$, $\alpha = 1,\ldots,12$, respectively, i.e.

$$\mathbf{m} = \begin{bmatrix} 1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

and

$$\mathbf{s} = \begin{bmatrix} 1 & -1 & 0 & 1 & 0 & 1 & 1 & -1 & 0 & 1 & 0 & 1 \\ -1 & 0 & -1 & 0 & 1 & 1 & -1 & 0 & -1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

- The scalar function τ is calculated according to equation (3.4.6), i.e.

$$\tau(t,\mathbf{F}^{\mathrm{p}},u) = \frac{1}{\sqrt{6}}\left[\mathbf{F}(t)\,(\mathbf{F}^{\mathrm{p}})^{-1}\left(\lambda\left(\operatorname{tr}\mathbf{E}^{\mathrm{e}}(t,\mathbf{F}^{\mathrm{p}})\right)\mathbf{I} + 2\,\mu\,\mathbf{E}^{\mathrm{e}}(t,\mathbf{F}^{\mathrm{p}})\right)\mathbf{m}^{\langle u\rangle}\right]$$
$$\cdot\left[\mathbf{F}(t)\,(\mathbf{F}^{\mathrm{p}})^{-1}\,\mathbf{s}^{\langle u\rangle}\right],$$

where $\mathbf{m}^{\langle u\rangle}$ denotes the u-th column of the matrix $\mathbf{m}$.

- According to equation (3.4.9), the scalar function h is given by

$$h(\alpha,u,\boldsymbol{\rho}) = \frac{\mu}{2}\,a_{\alpha u}\left(\sum_{q=1}^{12} a_{\alpha q}\,\rho_q\right)^{-1/2}\cdot\left(\frac{1}{\left(\mathbf{L}(\boldsymbol{\rho})\right)_u} - 2\,y_c\,\rho_u\right).$$

- The scalar function defining the rate of plastic shear is introduced as depending on four parameters, namely

$$\nu(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,u) = \nu_0\left(\frac{|\tau(t,\mathbf{F}^{\mathrm{p}},u)|}{(\boldsymbol{\tau}_c)_u}\right)^{n}\operatorname{sgn}\left[\tau(t,\mathbf{F}^{\mathrm{p}},u)\right]\Phi\left(|\tau(t,\mathbf{F}^{\mathrm{p}},u)| - (\boldsymbol{\tau}_c)_u\right),$$

where Φ is the Heaviside function

$$\Phi(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0. \end{cases}$$

- The scalar function describing the differential equation (3.4.8) is introduced as

$$\mathrm{d}\tau_c\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,\boldsymbol{\rho},\alpha\right)=\sum_{\alpha=1}^{12}h\left(\alpha,u,\boldsymbol{\rho}\right)\left|\nu\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,u\right)\right|.$$

- In order to describe the evolution equation for $\mathbf{F}^{\mathrm{p}}$, first we introduce the following matrix type functions which enable the computation of the tensorial product denoted by $\mathbf{s}\otimes\mathbf{m}$

$$\left(\mathbf{s}\otimes\mathbf{m}\right)(u)=\frac{1}{\sqrt{6}}\begin{bmatrix}\left(\mathbf{s}^{\langle u\rangle}\right)_1\left(\mathbf{m}^{\langle u\rangle}\right)_1 & \left(\mathbf{s}^{\langle u\rangle}\right)_1\left(\mathbf{m}^{\langle u\rangle}\right)_2 & \left(\mathbf{s}^{\langle u\rangle}\right)_1\left(\mathbf{m}^{\langle u\rangle}\right)_3\\ \left(\mathbf{s}^{\langle u\rangle}\right)_2\left(\mathbf{m}^{\langle u\rangle}\right)_1 & \left(\mathbf{s}^{\langle u\rangle}\right)_2\left(\mathbf{m}^{\langle u\rangle}\right)_2 & \left(\mathbf{s}^{\langle u\rangle}\right)_2\left(\mathbf{m}^{\langle u\rangle}\right)_3\\ \left(\mathbf{s}^{\langle u\rangle}\right)_3\left(\mathbf{m}^{\langle u\rangle}\right)_1 & \left(\mathbf{s}^{\langle u\rangle}\right)_3\left(\mathbf{m}^{\langle u\rangle}\right)_2 & \left(\mathbf{s}^{\langle u\rangle}\right)_3\left(\mathbf{m}^{\langle u\rangle}\right)_3\end{bmatrix}$$

$$\mathrm{d}\mathbf{F}^{\mathrm{p}}\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c\right)=\left(\sum_{u=1}^{12}\nu\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,u\right)\left(\mathbf{s}\otimes\mathbf{m}\right)(u)\right)\mathbf{F}^{\mathrm{p}}.$$

- The evolution equations describing the variation in time of the dislocation densities can be characterized by

$$\mathrm{d}\rho\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,\boldsymbol{\rho},u\right)=\frac{1}{b}\left(\frac{1}{\left(\mathbf{L}(\boldsymbol{\rho})\right)_u}-2y_c\,\rho_u\right)\left|\nu\left(t,\mathbf{F}^{\mathrm{p}},\boldsymbol{\tau}_c,u\right)\right|.$$

- The initial values for the hardening parameters defining the initial activation conditions are calculated starting with (3.4.7)

$$\boldsymbol{\tau}_{C_0}=\left(\mu b\left(\sum_{u=1}^{12}a_{1,u}\,\rho_0\right)^{1/2}\ldots\mu b\left(\sum_{u=1}^{12}a_{12,u}\,\rho_0\right)^{1/2}\right)^{\mathsf{T}}.$$

- The moment at which the activation condition is reached, $t=t^*$, as well as the systems which became active, are determined by solving the following equations:

$$\left|\tau\left(t,\mathbf{F}^{\mathrm{p}},u\right)\right|-\left(\boldsymbol{\tau}_{C_0}\right)_u=0,\quad u=1,\ldots,12.$$

  We denote by $\mathbf{t}^*=\left(t_1^*\ldots t_{12}^*\right)^{\mathsf{T}}$ the vector of solutions and choose $t^*=\min\limits_{1\le j\le 12}t_j^*$.

- The DES given by (3.4.4), (3.4.8) and (3.4.10), together with the associated initial conditions (3.4.13), is solved for the unknowns $\mathbf{F}^{\mathrm{p}}$, τ_C^{α} and ρ^{α} in $[t^*,T]$ using the Runge-Kutta method adapted to the formulated system with vector and matrix valued unknowns. Note that here the explicit dependence on time appears through the current value of the shear component, F_{21}, that has been identified with the time, t, namely $t\equiv F_{21}$.

Remark 3.3. During the deformation process there are various slip systems which could be activated. The control over these slip systems is managed by the Heaviside function, see formula (3.4.5).

Remark 3.4. The values of n allow a large increase in the expression $\left|\tau^{\alpha}/\tau_C^{\alpha}\right|^n$ in equation (3.4.5). This is the rationale for introducing the *breaking condition* in the algorithm with a threshold, r_τ, suggested by a material failure condition.

ALGORITHM

$t_1 = t^*$
$\Delta t = 10^{-5}$
$r_\tau = 300$
$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\mathbf{F}_1^{\mathrm{p}} = \mathbf{I}$
$\boldsymbol{\tau}_{C_1} = \boldsymbol{\tau}_{C_0}$
$\boldsymbol{\rho}_1 = \rho_0 \, (1,\ldots,1)^{\mathsf{T}}$
$i = 1$
while 1
break if $t_i > T$
break if $\left(\dfrac{\left|\tau\left(t_i, \mathbf{F}_i^{\mathrm{p}}, 1\right)\right|}{\left(\boldsymbol{\tau}_{c_i}\right)_1} \right)^n \geq r_\tau$
$\vdots$
break if $\left(\dfrac{\left|\tau\left(t_i, \mathbf{F}_i^{\mathrm{p}}, 12\right)\right|}{\left(\boldsymbol{\tau}_{c_i}\right)_{12}} \right)^n \geq r_\tau$
$\mathbf{k}1 = \mathrm{d}\,\mathbf{F}^{\mathrm{p}}\left(t_i, \mathbf{F}_i^{\mathrm{p}}, \boldsymbol{\tau}_{c_i}\right)$
for $u = 1,\ldots,12$
$m1_u = \mathrm{d}\,\boldsymbol{\tau}_c\left(t_i, \mathbf{F}_i^{\mathrm{p}}, \boldsymbol{\tau}_{c_i}, \boldsymbol{\rho}_i, u\right)$
$n1_u = \mathrm{d}\,\rho\left(t_i, \mathbf{F}_i^{\mathrm{p}}, \boldsymbol{\tau}_{c_i}, \boldsymbol{\rho}_i, u\right)$
end
$\mathbf{k}2 = \mathrm{d}\,\mathbf{F}^{\mathrm{p}}\left(t_i + \dfrac{\Delta t}{2}, \mathbf{F}_i^{\mathrm{p}} + \dfrac{\Delta t}{2}\mathbf{k}1, \boldsymbol{\tau}_{c_i} + \dfrac{\Delta t}{2}\mathbf{m}1\right)$
for $u = 1,\ldots,12$
$m2_u = \mathrm{d}\,\tau_c\left(t_i + \dfrac{\Delta t}{2}, \mathbf{F}_i^{\mathrm{p}} + \dfrac{\Delta t}{2}\mathbf{k}1, \boldsymbol{\tau}_{c_i} + \dfrac{\Delta t}{2}\mathbf{m}1 + \rho_i + \dfrac{\Delta t}{2}\mathbf{n}1, u\right)$
$n2_u = \mathrm{d}\,\rho\left(t_i + \dfrac{\Delta t}{2}, \mathbf{F}_i^{\mathrm{p}} + \dfrac{\Delta t}{2}\mathbf{k}1, \boldsymbol{\tau}_{c_i} + \dfrac{\Delta t}{2}\mathbf{m}1 + \rho_i + \dfrac{\Delta t}{2}\mathbf{n}1, u\right)$
end

$$\mathbf{k}3 = \mathrm{d}\,\mathbf{F}^{\mathrm{p}}\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}2, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}2\right)$$

for $u = 1, \ldots, 12$

$$m3_u = \mathrm{d}\,\tau_c\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}2, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}2 + \rho_i + \frac{\Delta t}{2}\,\mathbf{n}2, u\right)$$

$$n3_u = \mathrm{d}\,\rho\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}2, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}2 + \rho_i + \frac{\Delta t}{2}\,\mathbf{n}2, u\right)$$

end

$$\mathbf{k}4 = \mathrm{d}\,\mathbf{F}^{\mathrm{p}}\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}3, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}3\right)$$

for $u = 1, \ldots, 12$

$$m4_u = \mathrm{d}\,\tau_c\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}3, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}3 + \rho_i + \frac{\Delta t}{2}\,\mathbf{n}3, u\right)$$

$$n4_u = \mathrm{d}\,\rho\left(t_i + \frac{\Delta t}{2}, \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{2}\,\mathbf{k}3, \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{2}\,\mathbf{m}3 + \rho_i + \frac{\Delta t}{2}\,\mathbf{n}3, u\right)$$

end

$$t_{i+1} = t_i + \Delta t$$

$$\mathbf{F}^{\mathrm{p}}_{i+1} = \mathbf{F}^{\mathrm{p}}_i + \frac{\Delta t}{6}\,(\mathbf{k}1 + 2\,\mathbf{k}2 + 2\,\mathbf{k}3 + \mathbf{k}4)$$

$$\boldsymbol{\tau}_{c_{i+1}} = \boldsymbol{\tau}_{c_i} + \frac{\Delta t}{6}\,(\mathbf{m}1 + 2\,\mathbf{m}2 + 2\,\mathbf{m}3 + \mathbf{m}4)$$

$$\boldsymbol{\rho}_{i+1} = \boldsymbol{\rho}_i + \frac{\Delta t}{6}\,(\mathbf{n}1 + 2\,\mathbf{n}2 + 2\,\mathbf{n}3 + \mathbf{n}4)$$ The numerical values for the mate-

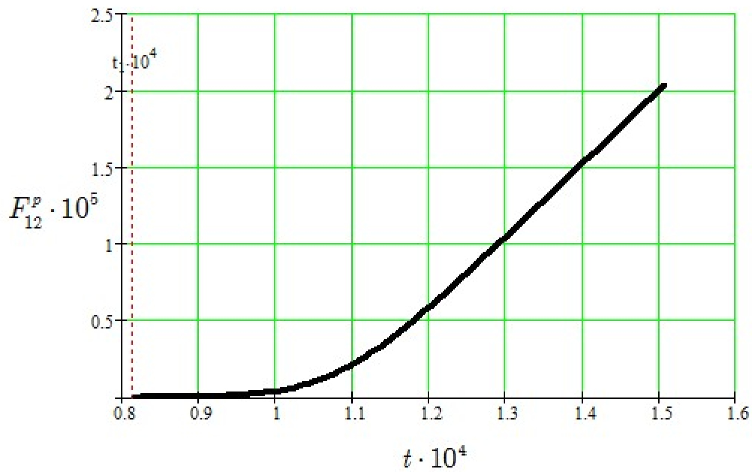

Fig. 3.4.1 – The evolution of the component F^{p}_{12} of the plastic distortion $\mathbf{F}^{\mathrm{p}}$.

rial parameters and model constants considered by Teodosiu and Raphannel (1993)

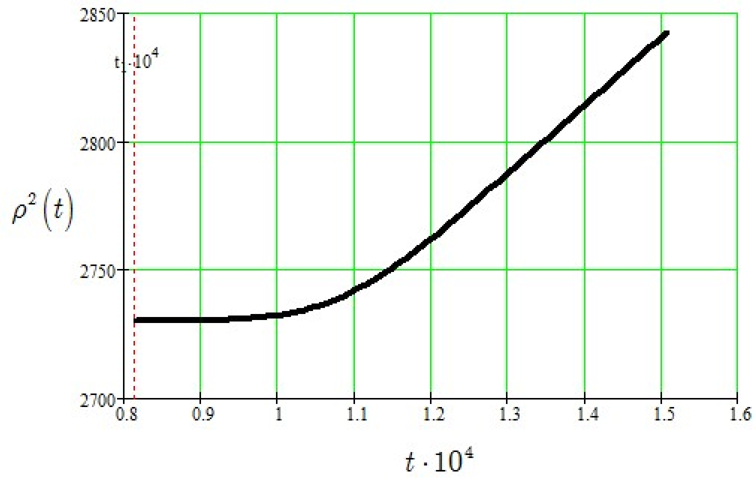

Fig. 3.4.2 – The evolution of the dislocation density ρ^2 in the second slip system.

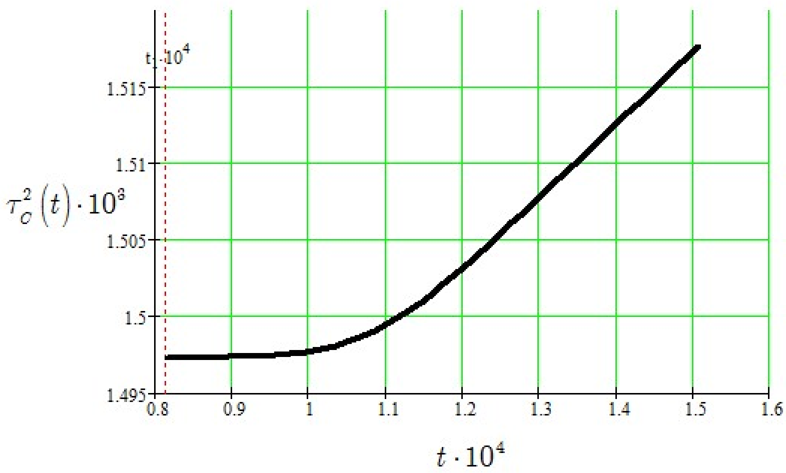

Fig. 3.4.3 – The evolution of the hardening function τ_C^2 related to the second slip system.

have been used herein, namely $y_c = 0.5 \times 10^{-6}\,\text{mm}$, $n = 20$, $\nu_0 \equiv \dot{\gamma}_0 = 10^{-3}\,\text{s}^{-1}$, $b = 2.57 \times 10^{-7}\,\text{mm}$, $\rho_0 = 2{,}730\,\text{mm}^{-2}$, $K = 75$, $a^{\alpha u} = 0.42$ for $\alpha = u$, $a^{\alpha u} = 0.52$ for $\alpha \neq u$, $\mu = 45\,\text{GPa}$, $\nu = 0.3$, $E = 2\mu(1+\nu)$, $\lambda = \nu E/[(1+\nu)(1-2\nu)]$, $\widehat{\rho}_0 = 1$, $\mathbf{a} = (a_{ij})$, where $a_{ij} = 0.42$ for $i = j$ and $a_{ij} = 0.52$ for $i \neq j$, and $T = 0.1$.

From the numerical results obtained, the following conclusions can be drawn:

1. The slip systems $\left(\bar{\mathbf{s}}^2, \overline{\mathbf{m}}^2\right)$ and $\left(\bar{\mathbf{s}}^4, \overline{\mathbf{m}}^4\right)$ become active at $t = t_2^*$.

2. The remaining six slip systems $(\bar{\mathbf{s}}^\alpha, \overline{\mathbf{m}}^\alpha)$, $\alpha \in \{3, 5, 8, 9, 10, 11\}$, are activated at $t_2^* + \Delta t$. Once a system becomes active, it will remain active at the following moments.

The numerical values obtained using the algorithm described above are the following: $(\boldsymbol{\tau}_{C_1})_i = 1.497 \times 10^{-3}$, $i = 1, \ldots, 12$, $t_1^* = t_6^* = t_7^* = t_{12}^* = 0.011$, $t_2^* = t_4^* = 8.142 \times 10^{-5}$, $t_8^* = t_{10}^* = 8.166 \times 10^{-5}$, $t_9^* = t_{11}^* = 8.158 \times 10^{-5}$.

Conclusions: It should be mentioned that there is no evolution of the function ρ for a non-activated slip system. The dislocation densities for the activated slip systems are almost identical and they have small deviations only. A possible explanation for this is given by the fact that the components of the matrix **a** describing the dislocation interactions have almost the same values for any activated slip systems. The shear components of the Piola-Kirchhoff stress tensor **S** are larger than the normal components. For example, at $t = 1.5 \times 10^{-4}$ one obtains

$$\mathbf{S}(t) = \begin{pmatrix} 2.4 \times 10^{-7} & 4.9 \times 10^{-3} & 0 \\ 4.9 \times 10^{-3} & 9.1 \times 10^{-7} & 0 \\ 0 & 0 & 9.5 \times 10^{-7} \end{pmatrix},$$

while the plastic distortion is given by

$$\mathbf{F}^{\mathrm{p}}(t) = \begin{pmatrix} 1 & F_{12}^{\mathrm{p}} & 0 \\ F_{21}^{\mathrm{p}} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where $F_{12}^{\mathrm{p}} = F_{21}^{\mathrm{p}}$. The numerically retrieved evolution of the fields F_{12}^{p}, ρ^2 and τ_C^2, as functions of time, are presented in Figs. 3.4.1 − 3.4.3, respectively.

3.5. SIMPLE SHEAR IN A STRESS CONTROLLED TEST, NON-LOCAL MODEL

We consider a body $\mathscr{B}$ made up from a material assumed to be *rigid-perfect plastic*, within the constitutive framework of finite crystal plasticity, involving the dislocation densities whose evolution in time is described by non-local equations associated with the appropriate slip systems. For instance the non-local evolution for the dislocation densities considered by Bortoloni and Cermelli (2004)

$$\dot{\rho}^\alpha = D\,|\nu^\alpha| \left(k\Delta\rho^\alpha - \frac{\partial \psi_T}{\partial \rho^\alpha} \right), \quad \alpha = 1, \ldots, N, \tag{3.5.1}$$

where

$$\psi_T = \psi_T\left(\rho^\beta\right), \beta = 1, \ldots, N, \tag{3.5.2}$$

is a dislocation energy, while D and k are constant. It should be mentioned that, in the evolution equation (3.2.4), the diffusivity is proportional to the modulus of the slip velocity.

Problem statement: Let the domain occupied by the body be a layer, namely

$$B = \left\{(x,y,z) \in \mathbb{R}^3 : 0 \leq z \leq L\right\}. \tag{3.5.3}$$

Consider the homogeneous shear stress state

$$\mathbf{S} = S_{13}(t)\,(\mathbf{i} \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{i}), \tag{3.5.4}$$

where **i**, **j** and **k** are unit vectors, and $S_{13}(t) > 0$, for all $t > t_0$. We consider a single

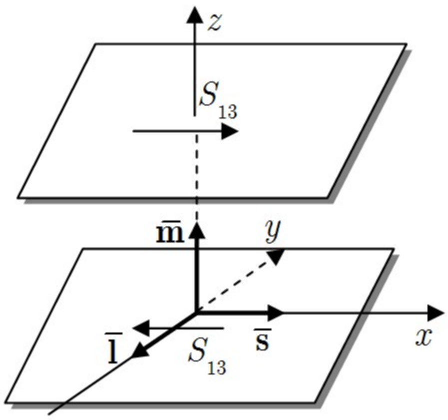

Fig. 3.5.1 – The domain occupied by the body B and the direction of the Burgers vector and slip plane normal.

slip system with the slip direction $\overline{\mathbf{s}} = \mathbf{i}$ in a plane whose outward unit normal vector is $\overline{\mathbf{m}} = \mathbf{k}$.

For the fixed slip system given by (3.4.4) with the initial condition $\mathbf{F}^{\mathrm{p}}(t_0) = \mathbf{I}$, the plastic distortion is derived to be a shear deformation

$$\mathbf{F}^{\mathrm{p}} = \mathbf{I} + \gamma\,(\overline{\mathbf{s}} \otimes \overline{\mathbf{m}}), \tag{3.5.5}$$

where $\dot{\gamma} = \nu$.

The rigid behaviour means $\mathbf{F}^{\mathrm{e}} = \mathbf{I}$, while the perfect plastic behaviour leads to $\zeta^\alpha = \zeta^\alpha(\rho_0)$. Thus $\mathbf{F}^{\mathrm{p}} = \mathbf{F}$. For the homogeneous stress state, the balance equation (3.4.13) is satisfied.

By direct calculation, the resolved shear stress can be expressed as

$$\begin{aligned} \tau &= \left\{ S_{13}(t)\,(\mathbf{i}\otimes\mathbf{k}+\mathbf{k}\otimes\mathbf{i})\,[\mathbf{I}+\gamma\,(\bar{\mathbf{s}}\otimes\overline{\mathbf{m}})]^{\mathsf{T}}\,\overline{\mathbf{m}} \right\} \cdot \left\{ \mathbf{F}\,[\mathbf{I}+\gamma\,(\bar{\mathbf{s}}\otimes\overline{\mathbf{m}})]^{-1}\,\bar{\mathbf{s}} \right\} \\ &= S_{13}(t)\,F_{11}\,, \end{aligned} \tag{3.5.6}$$

and, consequently, from (3.4.5) the rate of plastic shear is obtained as

$$\dot{\gamma} = \left| \frac{S_{13}(t)\,F_{11}}{\zeta(\rho)} \right|^n \operatorname{sgn}(S_{13}(t)\,F_{11})\,\mathscr{H}(|\tau| - \zeta(\rho))\,. \tag{3.5.7}$$

According to the hypotheses assumed, a perfect plastic material leads to $|\tau| = \zeta(\rho_0)$, while the rigid behaviour actually means that $\mathbf{F} = \mathbf{F}^{\mathrm{p}}$. Therefore, the slip system is activated only if the following relationship holds

$$|\tau| \equiv |S_{13}(t)| = \zeta(\rho_0)\,. \tag{3.5.8}$$

In the case of a single slip system, the non-local evolution equation for the dislocation density (3.5.1) becomes

$$\dot{\rho} = D \left| \frac{S_{13}(t)\,F_{11}}{\zeta(\rho)} \right|^n \left(k\Delta\rho - \frac{\partial\psi_T}{\partial\rho} \right) \mathscr{H}(|\tau| - \zeta(\rho))\,, \tag{3.5.9}$$

where D and k are material constants, whilst $\psi_T = \psi_T(\rho)$ and $\zeta = \zeta(\rho)$ are constitutive functions to be prescribed.

Problem: Given a shear stress function (3.3.9), find the unknown piecewise C^1 functions

$$\begin{aligned} \rho(\cdot,\cdot) &: B \times [t_0, T) \longrightarrow [0,\infty)\,, \qquad (z,t) \longmapsto \rho = \rho(z,t)\,, \\ \gamma(\cdot,\cdot) &: B \times [t_0, T) \longrightarrow [0,\infty)\,, \qquad (z,t) \longmapsto \gamma = \gamma(z,t)\,, \end{aligned} \tag{3.5.10}$$

satisfying the following equations:

1. The evolution equation for γ:

$$\dot{\gamma} = \left| \frac{S_{13}(t)}{\zeta(\rho)} \right|^n \operatorname{sgn}(S_{13}(t))\,. \tag{3.5.11}$$

2. The evolution equation for the dislocation density:

$$\dot{\rho} = D \left| \frac{S_{13}(t)}{\zeta(\rho)} \right|^n \left(k\Delta\rho - \frac{\partial\psi_T}{\partial\rho} \right), \tag{3.5.12}$$

where $S_{13} = S_{13}(t)$, $\zeta = \zeta(\rho)$, $\psi_T = \psi_T(\rho)$, k and D are given.

3. Initial conditions:

$$\gamma(z,0) = 0\,, \tag{3.5.13}$$

$$\rho(z,0) = \rho_0(z)\,. \tag{3.5.14}$$

4. Boundary conditions:

$$\frac{\partial \rho}{\partial z}(0,t) = \frac{\partial \rho}{\partial z}(L,t) = 0\,. \tag{3.5.15}$$

The constitutive functions and constant parameters used in the present computations were taken from Bortoloni and Cermelli (2004), namely

$$\zeta(\rho) = \frac{d\left(\rho^3 - 2\,\rho_r\,\rho^2 + \rho_r^2\,\rho + 1\right)}{3}\,, \tag{3.5.16}$$

where the function $\zeta(\rho)$ attains the global minimum at $\rho = \rho_r$ and a local maximum at $\rho = \rho_r/3$, whilst d and ρ_r are such that $\rho_r = \rho_m/2$.

Figure 3.5.2 presents the graph of the function given by (3.5.16). The energy of

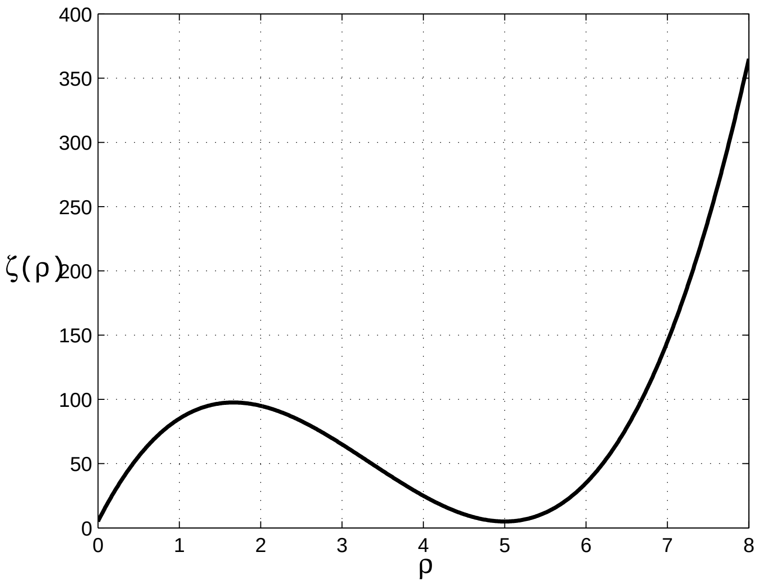

Fig. 3.5.2 – The curve $\zeta = \zeta(\rho)$.

the dislocation function, ψ_T, is defined by

$$\psi_T(\rho) = \frac{c}{4}\,\left[\rho\,(\rho - \rho_m)\right]^2\,. \tag{3.5.17}$$

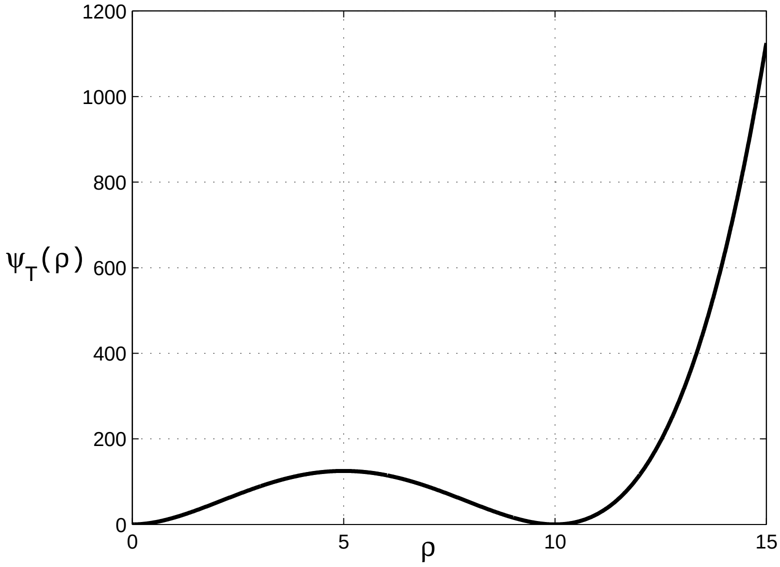

Fig. 3.5.3 – The curve $\psi_T = \psi_T(\rho)$.

The evolution equations (3.5.11) and (3.5.12) become

$$\dot{\rho} = D \left| \frac{S_{13}}{d\,(\rho^3 - 2\,\rho_r\,\rho^2 + \rho_r^2\,\rho + 1)/3} \right|^n \operatorname{sgn}(S_{13}) \times \left(k\,\frac{\partial^2 \rho}{\partial z^2} - c\,\rho^3 + \frac{3c}{2}\,\rho_m\,\rho^2 - \frac{c}{2}\,\rho_m^2\,\rho \right) \tag{3.5.18}$$

and

$$\dot{\gamma} = \left| \frac{S_{13}}{d\,(\rho^3 - 2\,\rho_r\,\rho^2 + \rho_r^2\,\rho + 1)/3} \right|^n \operatorname{sgn}(S_{13})\,, \tag{3.5.19}$$

respectively. We propose two methods for solving the system (3.5.18)–(3.5.19) with respect to the unknowns γ and ρ. The numerical algorithms are shortly presented below, while their numerical implementation was realized through Matlab codes.

I. Direct method: We first solve the partial differential equation (3.5.18) and obtain its solution $\rho = \rho(z,t)$. Then we solve the ordinary differential equation (3.5.19) with the initial condition (3.5.13), its solution being calculated by the formula

$$\gamma(z,t) = \int_0^t \left| \frac{S_{13}(\xi)}{d\,(\rho(z,\xi)^3 - 2\,\rho_r\,\rho(z,\xi)^2 + \rho_r^2\,\rho(z,\xi) + 1)/3} \right|^n \operatorname{sgn}(S_{13}(\xi))\,\mathrm{d}\xi\,. \tag{3.5.20}$$

The following numerical data were used: $L = 2$, $T = 0.2$, $k = 0.1$, $\rho_m = 10$ and $c = 0.8$. We consider a function $\rho_0(z)$ exhibiting an oscillating behaviour in the vicinity of the minimum value, $\rho = \rho_{min} = 5$, and at the same time compatible with the boundary values.

We solve numerically the partial derivative equation by using the predefined function pdepe. Consider $\{t_i\}_{1\leq i\leq M}$ and $\{z_j\}_{1\leq j\leq N}$ two discretizations of the intervals $[0,L]$ and $[0,T]$, respectively. A table containing the numerical data can be created $\{\rho_{ij}\}_{\substack{1\leq i\leq M\\ 1\leq j\leq N}}$, where $\rho_{ij} = \rho(z_j, t_i)$. By using the trapezoidal method we calculate numerically the integral (3.5.20), i.e.

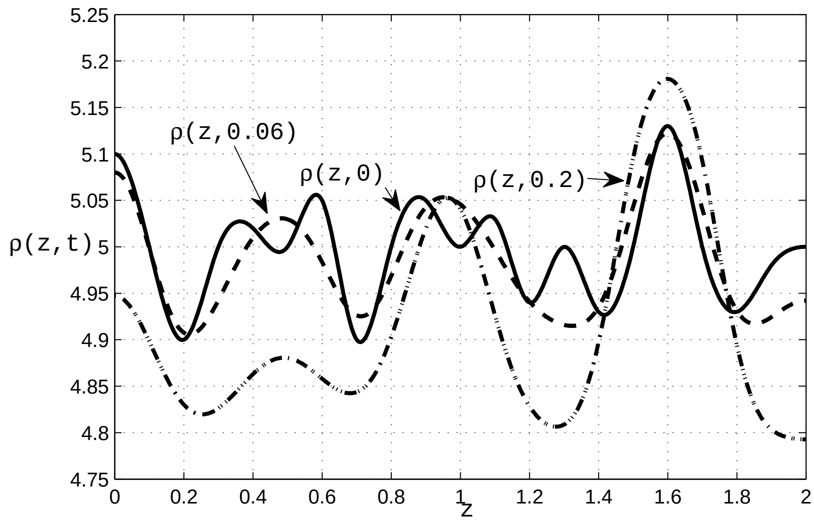

Fig. 3.5.4 – The dislocation density $\rho = \rho(z,t)$ as a function of the spatial coordinate z, for various moments $t \in [0,T]$, where $T = 0.2$.

- For $i = 1$:

$$\gamma_{i,j} = 0, \quad 1 \leq j \leq N.$$

- For $2 \leq i \leq M$:

$$\gamma_{i,j} = \gamma_{i-1,j} + \frac{1}{2}\left(\left|\frac{S_{13}(t_{i-1})}{d\,(\rho_{i-1,j}^3 - 2\,\rho_r\,\rho_{i-1,j}^2 + \rho_r^2\,\rho_{i-1,j} + 1)/3}\right|^n + \left|\frac{S_{13}(t_i)}{d\,(\rho_{i,j}^3 - 2\,\rho_r\,\rho_{i,j}^2 + \rho_r^2\,\rho_{i,j} + 1)/3}\right|^n\right)(t_i - t_{i-1}), \quad 1 \leq j \leq N.$$

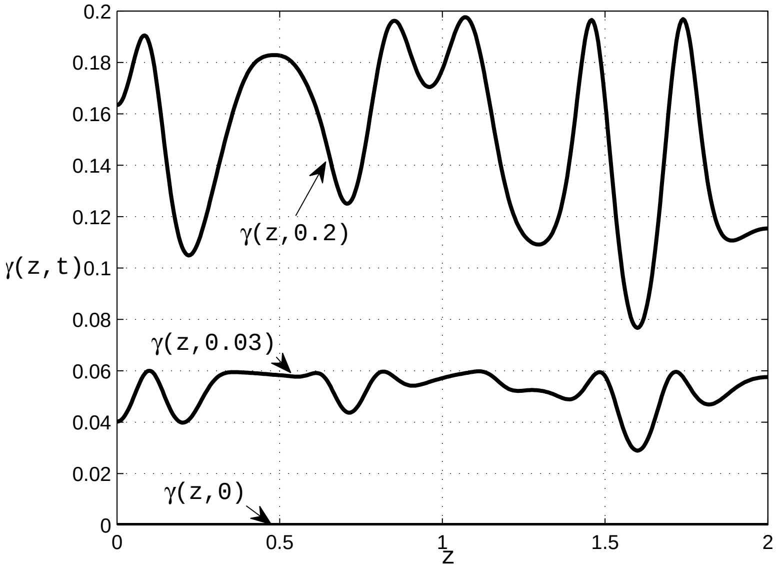

Fig. 3.5.5 – The plastic shear deformation $\gamma = \gamma(z,t)$ as a function of the spatial coordinate z, for various moments $t \in [0,T]$, where $T = 0.2$.

II. Time discretization method: In the case of the general problem, one needs to solve numerically a system containing the partial differential equation (3.5.18) and the ordinary differential equation (3.5.19). Further, we propose an algorithm that accounts for the coupling of the two equations mentioned above:

- For $i = 1$:
$$\gamma_{i,j} = 0\,, \quad \rho_{ij} = \rho_0\left(z_j\right)\,, \quad 1 \le j \le N\,.$$

- For $2 \le i \le M$:

  (i) Compute the unknown $\gamma_{i,j}$, $1 \le j \le N$, as follows:
$$\gamma_{i,j} = \gamma_{i-1,j} + \left| \frac{S_{13}\left(t_{i-1}\right)}{d\left(\rho^3_{i-1,j} - 2\,\rho_r\,\rho^2_{i-1,j} + \rho^2_r\,\rho_{i-1,j} + 1\right)/3} \right|^n \left(t_i - t_{i-1}\right)\,.$$

  (ii) The unknown ρ_{ij}, $1 \le j \le N$, is computed as follows: The partial differential equation (3.5.18) is solved for $t \in \left[t_{i-1}, t_i\right]$ with the boundary conditions (3.5.15) and the updated initial condition $\rho\left(z, t_{i-1}\right) = \rho^{i-1}(z)$, where $\rho^{i-1}(z)$ has been obtained by interpolating the data $\rho_{i-1,j}$ from the previous step.

The solutions obtained following the methods described above are identical. Figures 3.5.4 and 3.5.5 show the evolution of the dislocation density, ρ, and plastic shear deformation, γ, as functions of the spatial coordinate z, for various moments $t \in [0,T]$, where $T = 0.2$. The proposed numerical methods lead to the following conclusions: Not every initial non-periodic function $\rho_0(z)$ evolves into a periodic scalar dislocation density as compared with the statement made by Bortoloni and Cermelli (2004).

3.6. MATHEMATICAL MODEL OF AN ELASTO-PLASTIC MATERIAL WITH ISOTROPIC HARDENING

3.6.1. CONSTITUTIVE FRAMEWORK FOR SMALL ELASTO-PLASTIC STRAINS

Let $\Omega \subset \mathbb{R}^d$ be an open bounded set occupied by a solid body with a smooth boundary, $\Gamma \equiv \partial\Omega$, where usually $d \in \{1,2,3\}$ denotes the dimension of the problem considered. We also assume that $I = [0,T)$, $T > 0$, is the time interval on which the problem associated with the solid body Ω is formulated.

Let the deformation gradient introduced in terms of the motion of the body in Section 3.2. be expressed through the displacement gradient

$$\mathbf{F}(\mathbf{X},t) = \mathbf{I} + \mathbf{H}(\mathbf{X},t)\,, \quad \mathbf{H}(\mathbf{X},t) = \nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X},t)\,, \quad \mathbf{u}(\mathbf{X},t) := \chi(\mathbf{X},t) - \mathbf{X}\,. \tag{3.6.1}$$

By definition, the body $\mathscr{B}$ undergoes small deformations if

$$\delta = \sup_{\mathbf{X}\in\mathscr{B},\, t\in\mathbb{R}} |\mathbf{H}(\mathbf{X},t)| \ll 1\,. \tag{3.6.2}$$

On assuming that both the elastic, $\mathbf{F}^{\mathrm{e}}$, and the plastic, $\mathbf{F}^{\mathrm{p}}$, components of the deformation gradient, $\mathbf{F}$, which appear in the multiplicative decomposition (3.2.1), can be decomposed in a similar manner as that given by equations (3.6.1) and (3.6.2), i.e.

$$\begin{aligned} &\mathbf{F}^{\mathrm{e}}(\mathbf{X},t) = \mathbf{I} + \mathbf{H}^{\mathrm{e}}(\mathbf{X},t)\,, && \sup_{\mathbf{X}\in\mathscr{B},\, t\in\mathbb{R}} |\mathbf{H}^{\mathrm{e}}| \ll 1\,, \\ &\mathbf{F}^{\mathrm{p}}(\mathbf{X},t) = \mathbf{I} + \mathbf{H}^{\mathrm{p}}(\mathbf{X},t)\,, && \sup_{\mathbf{X}\in\mathscr{B},\, t\in\mathbb{R}} |\mathbf{H}^{\mathrm{p}}| \ll 1\,, \end{aligned} \tag{3.6.3}$$

where the tensors $\mathbf{H}$, $\mathbf{H}^{\mathrm{e}}$ and $\mathbf{H}^{\mathrm{p}}$ have the same order of magnitude, say δ.

As a consequence of the multiplicative decomposition (3.2.1), when tensors of order $O(\delta^{m+1})$ are neglected with respect to tensors of order $O(\delta^m)$, for $m \geq 0$, then the following approximation formulae hold:

$$\begin{aligned} &\mathbf{H} = \mathbf{H}^{\mathrm{e}} + \mathbf{H}^{\mathrm{p}}\,, && \varepsilon = \varepsilon^{\mathrm{e}} + \varepsilon^{\mathrm{p}}\,, \\ &\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathsf{T}}\right)\,, && \varepsilon^{\mathrm{e}} = \frac{1}{2}\left(\mathbf{H}^{\mathrm{e}} + (\mathbf{H}^{\mathrm{e}})^{\mathsf{T}}\right)\,, \quad \varepsilon^{\mathrm{p}} = \frac{1}{2}\left(\mathbf{H}^{\mathrm{p}} + (\mathbf{H}^{\mathrm{p}})^{\mathsf{T}}\right)\,. \end{aligned} \tag{3.6.4}$$

Using the relationships between the Cauchy stress tensor, $\mathbf{T}$, and the symmetric Piola-Kirchhoff stress tensor with respect to the relaxed (plastically deformed) configuration, $\boldsymbol{\pi}$, see equation (3.2.6), as well as the first Piola-Kirchhoff stress tensor with respect to the reference configuration, $\mathbf{S}$, see expression (3.2.10), one can emphasize that these stress tensors become equal, namely

$$\boldsymbol{\pi} \simeq \mathbf{S} \simeq \mathbf{T}. \tag{3.6.5}$$

Consequently, the small deformation counter-parts of finite deformation can be emphasized:

Stress measure	$\boldsymbol{\pi} = \mathbf{S} = \mathbf{T} = \boldsymbol{\sigma}$
Yield function	$\mathscr{F}(\boldsymbol{\sigma}, \boldsymbol{\alpha})$ with $\boldsymbol{\alpha} = k \in \mathbb{R}$
Elastic strain (3.2.4)	$\mathbf{E}^{\mathrm{e}} = \boldsymbol{\varepsilon}^{\mathrm{e}}$
Rate of the plastic component (3.2.13)	$\dot{\mathbf{F}}^{\mathrm{p}} \left(\mathbf{F}^{\mathrm{p}}\right)^{-1} = \dot{\mathbf{H}}^{\mathrm{p}}$
Symmetric part of the rate of the plastic component	$\frac{1}{2}\left[\dot{\mathbf{F}}^{p}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1} + \left(\dot{\mathbf{F}}^{p}\left(\mathbf{F}^{\mathrm{p}}\right)^{-1}\right)^{\mathsf{T}}\right] = \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$
Evolution equation (3.2.13)	for $\mathscr{B}(\boldsymbol{\pi}, k) = \partial_{\boldsymbol{\sigma}}\mathscr{F}$
	$\Longleftrightarrow\ \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \lambda\, \partial_{\boldsymbol{\sigma}}\mathscr{F}$
Basic kinematic relationship	$\dot{\mathbf{H}} = \dot{\mathbf{H}}^{\mathrm{e}} + \dot{\mathbf{H}}^{\mathrm{p}}$.

1. The rate of the strain tensor, $\dot{\boldsymbol{\varepsilon}}$, can be decomposed into the sum of the rates of elastic and plastic parts, denoted by $\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}}$ and $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, respectively

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} + \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}. \tag{3.6.6}$$

2. The irreversible properties of the material are described in terms of the yield function $\mathscr{F}(\cdot,\cdot) : \mathrm{Sim} \times \mathbb{R} \longrightarrow \mathbb{R}_{\leq 0}$ which depends on the stress, $\boldsymbol{\sigma}$, and hardening scalar variable, k, i.e.

$$\mathscr{F}(\boldsymbol{\sigma}, k) = \|\mathrm{dev}(\boldsymbol{\sigma})\| - [H\,k + \sigma_Y], \tag{3.6.7}$$

where $H > 0$ is the hardening constant and σ_Y represents the initial yield constant in terms of the deviatoric part of the stress tensor defined as

$$\mathbf{s} \equiv \mathrm{dev}(\boldsymbol{\sigma}) = \boldsymbol{\sigma} - \mathrm{tr}(\boldsymbol{\sigma})\,\mathbf{I}.$$

3. The rate of the plastic strain tensor is described by the associated flow rule:

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \lambda \frac{\partial \mathscr{F}(\boldsymbol{\sigma}, k)}{\partial \boldsymbol{\sigma}} \quad \text{or, equivalently} \quad \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \lambda\,\mathbf{n}, \ \ \mathbf{n} = \frac{\mathrm{dev}(\boldsymbol{\sigma})}{\|\mathrm{dev}(\boldsymbol{\sigma})\|}. \tag{3.6.8}$$

4. The so-called plastic factor, λ, is a function defined through the Kuhn-Tucker and consistency conditions

$$\lambda \geq 0\,, \quad \mathscr{F} \leq 0\,, \quad \lambda \mathscr{F} = 0\,, \quad \lambda \dot{\mathscr{F}} = 0\,. \tag{3.6.9}$$

5. The elastic type constitutive equation is expressed in terms of the Cauchy stress tensor or via its associated rate form, i.e.

$$\begin{aligned} &\boldsymbol{\sigma} = \mathscr{E}\left(\boldsymbol{\varepsilon}^{\mathrm{e}}\right), \\ &\dot{\boldsymbol{\sigma}} = \mathscr{E}\big(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}\big) = \mathscr{E}\big(\boldsymbol{\varepsilon}(\dot{\mathbf{u}}) - \lambda \mathbf{n}\big), \end{aligned} \tag{3.6.10}$$

where the fourth order elastic tensor $\mathscr{E}$ is given by

$$\mathscr{E} = k_a \mathbf{I} \otimes \mathbf{I} + 2\mu \mathbf{I}_{dev}\,. \tag{3.6.11}$$

In the isotropic case, the bulk modulus is given by $k_a = \lambda_a + \dfrac{2}{3}\,\mu$, where λ_a and μ are the Lamé constants.

6. The rate of the isotropic hardening variable, k, is given by

$$\dot{k} = \sqrt{\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} \cdot \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}} = \lambda\,. \tag{3.6.12}$$

7. We add the *initial condition*

$$\boldsymbol{\sigma}(0) = \mathbf{0}\,, \quad \boldsymbol{\varepsilon}(0) = \mathbf{0}\,, \quad \boldsymbol{\varepsilon}^{\mathrm{p}}(0) = \mathbf{0}\,, \quad k(0) = 0\,. \tag{3.6.13}$$

Remark 3.5. The plastic factor, $\lambda(\cdot,\cdot) : \Omega \times I \to \mathbb{R}$, on the yield surface, $\mathscr{F}(\boldsymbol{\sigma}, k) = 0$, is calculated according to the following formula

$$\lambda = \frac{\langle \beta \rangle}{h}\,\mathscr{H}(\mathscr{F})\,, \tag{3.6.14}$$

where

$$\beta = \mathbf{n} \cdot \mathscr{E}\big(\boldsymbol{\varepsilon}(\dot{\mathbf{u}})\big) \quad \text{and} \quad h = \mathbf{n} \cdot \mathscr{E}(\mathbf{n}) + H\,. \tag{3.6.15}$$

Here, $h > 0$ is the hardening parameter, while $\mathscr{H}$ denotes the Heaviside function.

In the following, we consider $d = 2$, i.e. $\Omega \subset \mathbb{R}^2$ is a two-dimensional domain, while the following notations are made:

- $\mathbb{R}_{\leq 0} = \left\{x \in \mathbb{R} \middle| x \leq 0\right\}$;
- Lin is the set of second-order tensors, while $\mathrm{Lin}^+ \subset \mathrm{Lin}$ contains elements with a positive determinant;

- $\langle x \rangle = \frac{1}{2}(x + |x|)$, $\forall x \in \mathbb{R}$, is the so-called ramp function.

We start from the *equilibrium equation*, i.e.

$$\operatorname{div} \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad \text{in} \quad \Omega \times I, \tag{3.6.16}$$

where $\mathbf{b}(\cdot,\cdot) : \Omega \times I \longrightarrow \mathbb{R}^2$, $\mathbf{b} = (b_1, b_2)^{\mathsf{T}}$ are the body forces.

The *boundary conditions* are formulated on the boundary $\Gamma = \Gamma_u \cup \Gamma_\sigma$, $\Gamma_u \cap \Gamma_\sigma = \varnothing$, and are given by

$$\begin{cases} \boldsymbol{\sigma}\widetilde{\mathbf{n}} = \mathbf{f} & \text{on} \quad \Gamma_\sigma \times I \\ \mathbf{u} = \mathbf{0} & \text{on} \quad \Gamma_u \times I, \end{cases} \tag{3.6.17}$$

where $\widetilde{\mathbf{n}}$ is the outward normal vector and $\mathbf{f}(\cdot) : \Omega \longrightarrow \mathbb{R}^2$ is a given vector function.

We are now able to formulate the following problem (P):

Find the real valued functions $\mathbf{u}$, $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^{\mathrm{p}}$ and k defined on $\Omega \times I$ that satisfy the equilibrium equation (3.6.16), the boundary conditions (3.6.17), and the differential type equations (3.6.8), (3.6.10) and (3.6.12), together with (3.6.14) and (3.6.15).

We divide problem (P) into the following two problems:

$$(P_1): \begin{cases} \mathscr{F}(\boldsymbol{\sigma}, k) = \|\operatorname{dev}(\boldsymbol{\sigma})\| - [H\,k + \sigma_Y] \\ \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \lambda\,\mathbf{n} \\ \dot{\boldsymbol{\sigma}} = \mathscr{E}\big(\boldsymbol{\varepsilon}(\dot{\mathbf{u}}) - \lambda\,\mathbf{n}\big) \\ \dot{k} = \lambda \\ \lambda = \dfrac{\big\langle \mathbf{n} \cdot \mathscr{E}\big(\boldsymbol{\varepsilon}(\dot{\mathbf{u}})\big) \big\rangle}{\mathbf{n} \cdot \mathscr{E}(\mathbf{n}) + H}\,\mathscr{H}(\mathscr{F}) \\ \boldsymbol{\sigma}(0) = \mathbf{0}, \quad \boldsymbol{\varepsilon}(0) = \mathbf{0} \\ \boldsymbol{\varepsilon}^{\mathrm{p}}(0) = \mathbf{0}, \quad k(0) = 0 \end{cases} \qquad (P_2): \begin{cases} \boldsymbol{\sigma} = \mathscr{E}\big(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}\big) \\ \operatorname{div} \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} & \text{in} \quad \Omega \times I \\ \boldsymbol{\sigma}\widetilde{\mathbf{n}} = \mathbf{f} & \text{on} \quad \Gamma_\sigma \times I \\ \mathbf{u} = \mathbf{0} & \text{on} \quad \Gamma_u \times I. \end{cases}$$

To solve numerically problem (P), we realize a coupling of problem (P_1) and a modified version of problem (P_2) following a certain strategy to be discussed further.

1. We present the variational formulation for a modified problem (P_2), which refers to a non-linear elastic material, in which

   $$\boldsymbol{\sigma} = \widetilde{\mathscr{E}}(\boldsymbol{\varepsilon})$$

   and the elastic coefficients matrix depends on both the material point $\mathbf{x} \in \Omega$ and the time t. Here, the time t is considered to be a parameter.

   The finite element method is used to solve the variational formulation for a modified problem (P_2) at any fixed time t.

2. We formulate the Radial Return Method to solve problem (P_1) for the elasto-plastic model with isotropic hardening. At every time t, an implicit finite relationship between the current values of the stress and (total) strain tensors results. Then the elasto-plastic fourth order tensor $\mathscr{E}^{\mathrm{ep}}$ can be associated with the model.

3. We realize the coupling of the Radial Return method with finite element method with the variational formulation for the problem (P_2) by choosing $\widetilde{\mathscr{E}} \equiv \mathscr{E}^{\mathrm{ep}}$.

We recall the representation of the tensorial fields involved in this model:

- The displacement field $\mathbf{u}(\cdot,\cdot) : \overline{\Omega} \times I \longrightarrow \mathbb{R}^2$, $\mathbf{u}(x,t) = u_i(x,t)\,\mathbf{e}_i$;
- The stress tensor $\boldsymbol{\sigma}(\cdot,\cdot) : \Omega \times I \longrightarrow \mathrm{Sym}$, $\boldsymbol{\sigma}(x,t) = \sigma_{ij}(x,t)\,(\mathbf{e}_i \otimes \mathbf{e}_j)$;
- The infinitesimal strain tensor

$$\boldsymbol{\varepsilon}(\cdot,\cdot) : \Omega \times I \longrightarrow \mathrm{Sym}, \quad \boldsymbol{\varepsilon}(x,t) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j}\right)(\mathbf{e}_i \otimes \mathbf{e}_j)\,.$$

The elastic domain in the stress space is given by

$$E = \left\{(\boldsymbol{\sigma}, \boldsymbol{\alpha}, k) \in \mathrm{Sym} \times \mathrm{Sym} \times \mathbb{R}^2 \middle| \mathscr{F}(\boldsymbol{\sigma}, \boldsymbol{\alpha}, k) \leq 0\right\}\,. \tag{3.6.18}$$

Following standard conventions, the components, ε_{ij}, of the strain tensor are collected in vector form as:

$$\boldsymbol{\varepsilon} = (\varepsilon_{11}, \varepsilon_{22}, 2\,\varepsilon_{12})^{\mathsf{T}} \quad \text{and} \quad \boldsymbol{\varepsilon}^{\mathrm{p}} = \left(\varepsilon^{\mathrm{p}}_{11}, \varepsilon^{\mathrm{p}}_{22}, 2\,\varepsilon^{\mathrm{p}}_{12}\right)^{\mathsf{T}}\,. \tag{3.6.19}$$

In the following, we introduce the basic assumptions of the elasto-plastic model with isotropic hardening, see e.g. Paraschiv-Munteanu *et al.* (2004):

Next, we define the weak solution of the elastic problem (P_2), namely

$$(P_2): \quad \begin{cases} \boldsymbol{\sigma} = \mathscr{E}(\boldsymbol{\varepsilon}) & \\ \operatorname{div}\boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} & \text{in} \quad \Omega \times I \\ \boldsymbol{\sigma}\,\mathbf{n} = \mathbf{f} & \text{on} \quad \Gamma_\sigma \times I \\ \mathbf{u} = \mathbf{0} & \text{on} \quad \Gamma_u \times I\,. \end{cases} \tag{3.6.20}$$

The set of kinematically admissible velocity field is denoted by:

$$\mathscr{V}_{ad} = \left\{ w : \Omega \times I \longrightarrow \mathbb{R}^2 \middle| \frac{\partial w_i}{\partial x_j} \in L^2(\Omega)\,,\ i,j = 1,2;\ w_i\big|_{\Gamma_u} = g_i\,,\ i = 1,2 \right\}\,, \tag{3.6.21}$$

where $L^2(\Omega)$ is the space of square integrable functions in Ω and $H^1(\Omega)$ is the Sobolev space.

The variational problem associated with the elastic problem P_2 can be written as: Find the displacement field $\mathbf{u}$ which is the solution to the variational problem

$$a(\mathbf{u},\mathbf{w}) = L(\mathbf{w}), \quad \forall \mathbf{w} \in \mathscr{V}_{ad}, \tag{3.6.22}$$

where $a(\cdot,\cdot) : \mathscr{V}_{ad} \times \mathscr{V}_{ad} \longrightarrow \mathbb{R}$ is a bilinear and symmetric form, while L is a linear functional given by

$$a(\mathbf{u},\mathbf{w}) = \int_{\Omega} \mathscr{E}[\varepsilon(\mathbf{u})] \cdot \varepsilon(\mathbf{w}) \mathrm{d}\mathbf{x} \tag{3.6.23}$$

and

$$L(\mathbf{w}) = \int_{\Gamma_\sigma} \mathbf{f} \cdot \mathbf{w} \, \mathrm{d}\Gamma_\sigma + \int_{\Omega} \mathbf{b} \cdot \mathbf{w} \, \mathrm{d}\mathbf{x}. \tag{3.6.24}$$

Hypothesis: We assume that the material properties are given such that

$$a(\cdot,\cdot) : \mathscr{V}_{ad} \times \mathscr{V}_{ad} \longrightarrow \mathbb{R}$$

is a bilinear, symmetric, continuous and coercive form.

3.6.2. VARIATIONAL FORMULATION–DISCRETIZATION BY THE FINITE ELEMENT METHOD

The finite element method (FEM) is used for solving the variational elasto-plastic problem with isotropic hardening (Simo and Hughes, 1998). In this section, we present the general FEM procedure Fish and Belytschko (2007) and using the operator assembly of the external and internal vector forces elaborated by Hughes (1987). The following notation is made: $dsp = 2$ is the dimension of the space; *nel* is the total number of network elements; *nt_nod* is the total number of nodes belonging to the network; *nne* is the number of nodes on each element; *ngl* is the number of the degrees of freedom; $n\_eq = nt\_nod \times ngl$ is the total number of equations.

We apply the FEM to the domain $\Omega \subset \mathbb{R}^2$ which is divided into elements, say $\Omega = \bigcup_{e=1}^{nel} \Omega_e$, each element having four nodes $nne = 4$. Since $d = dsp = 2$, the number of degrees of freedom is 2 for each node in the network.

We make the transition from the physical coordinates (x_1, x_2) to the parent coordinates (ξ, η) that ensures the continuity between the network elements. We consider that a certain domain Ω_e is formed by four nodes, characterized by the following physical coordinates:

$$\begin{cases} \mathbf{x}_1^{\mathrm{e}} = \begin{bmatrix} (x_1)_1^{\mathrm{e}} & (x_1)_2^{\mathrm{e}} & (x_1)_3^{\mathrm{e}} & (x_1)_4^{\mathrm{e}} \end{bmatrix}^{\mathsf{T}} \\ \mathbf{x}_2^{\mathrm{e}} = \begin{bmatrix} (x_2)_1^{\mathrm{e}} & (x_2)_2^{\mathrm{e}} & (x_2)_3^{\mathrm{e}} & (x_2)_4^{\mathrm{e}} \end{bmatrix}^{\mathsf{T}}. \end{cases} \tag{3.6.25}$$

Switching from the reference coordinates to the parent coordinates, Fish and Belytschko (2007) introduced the following transformation

$$x_1^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{x}_1^{\mathrm{e}}, \quad x_2^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{x}_2^{\mathrm{e}}, \tag{3.6.26}$$

where the vector $\mathbf{N}(\xi,\eta)$ is given by

$$\mathbf{N}(\xi,\eta) = \left[\begin{array}{cccc} N_1(\xi,\eta) & N_2(\xi,\eta) & N_3(\xi,\eta) & N_4(\xi,\eta) \end{array}\right] \tag{3.6.27}$$

and the element of the vector $\mathbf{N}(\xi,\eta)$ are:

$$\begin{aligned} N_1(\xi,\eta) &= \frac{1}{4}(1-\xi)(1-\eta), \quad N_2(\xi,\eta) = \frac{1}{4}(1+\xi)(1-\eta), \\ N_3(\xi,\eta) &= \frac{1}{4}(1+\xi)(1+\eta), \quad N_4(\xi,\eta) = \frac{1}{4}(1-\xi)(1+\eta). \end{aligned} \tag{3.6.28}$$

For each element, the displacements along directions *OX* and *OY* are denoted by $u_1^{\mathrm{e}}(\xi,\eta,t)$ and $u_2^{\mathrm{e}}(\xi,\eta,t)$, respectively, and are calculated using the formula:

$$\mathbf{u}^{\mathrm{e}}(\xi,\eta,t) = \mathbf{N}(\xi,\eta)\,\mathbf{u}^{\mathrm{e}}(t), \tag{3.6.29}$$

where the nodal displacement vector is given by

$$\mathbf{u}^{\mathrm{e}}(t) = \left[\left(u_1(t)\right)_1^{\mathrm{e}}\ \left(u_2(t)\right)_1^{\mathrm{e}}\ \left(u_1(t)\right)_2^{\mathrm{e}}\ \left(u_2(t)\right)_2^{\mathrm{e}}\ \left(u_1(t)\right)_3^{\mathrm{e}}\ \left(u_2(t)\right)_3^{\mathrm{e}}\ \left(u_1(t)\right)_4^{\mathrm{e}}\ \left(u_2(t)\right)_4^{\mathrm{e}}\right]^{\mathsf{T}};$$

$\left(u_k(t)\right)_i^{\mathrm{e}}$, $k = 1,2$, $i = \overline{1,nne}$; $\mathbf{u}^{\mathrm{e}}(\xi,\eta,t) = [u_1^{\mathrm{e}}(\xi,\eta,t)\ u_2^{\mathrm{e}}(\xi,\eta,t)]^{\mathsf{T}}$, $e = \overline{1,nel}$; and $\mathbf{N}(\chi)$, $\chi = (\xi,\eta)$, is the shape function matrix given by

$$\mathbf{N}(\chi) = \begin{bmatrix} N_1(\chi) & 0 & N_2(\chi) & 0 & N_3(\chi) & 0 & N_4(\chi) & 0 \\ 0 & N_1(\chi) & 0 & N_2(\chi) & 0 & N_3(\chi) & 0 & N_4(\chi) \end{bmatrix}. \tag{3.6.30}$$

The weight function vector is approximated by the same shape functions as the displacement fields

$$\mathbf{w}^{\mathrm{e}}(\xi,\eta,t) = \mathbf{N}(\xi,\eta)\,\mathbf{w}^{\mathrm{e}}(t), \tag{3.6.31}$$

where $w^{\mathrm{e}}(t)$ is given by a relationship similar to (3.6.29). In a similar manner, we approximate the internal forces, $\mathbf{b}$, and the forces given by the natural boundary conditions, $\mathbf{f}$, for each element

$$\mathbf{b}^{\mathrm{e}}(\xi,\eta,t) = \mathbf{N}(\xi,\eta)\,\mathbf{b}^{\mathrm{e}}(t), \quad \mathbf{f}^{\mathrm{e}}(\xi,\eta,t) = \mathbf{N}(\xi,\eta)\,\mathbf{f}^{\mathrm{e}}(t). \tag{3.6.32}$$

The FEM approximation of the strains reads

$$[\varepsilon_{\mathbf{u}}]^{\mathrm{e}}(\xi,\eta,t) = \mathbf{B}^{\mathrm{e}}(\xi,\eta)\,\mathbf{u}^{\mathrm{e}}(t), \quad [\varepsilon_{\mathbf{w}}]^{\mathrm{e}}(\xi,\eta,t) = \mathbf{B}^{\mathrm{e}}(\xi,\eta)\,\mathbf{w}^{\mathrm{e}}(t). \tag{3.6.33}$$

On using the change of variables (3.6.26), one can easily determine the Jacobian of the transformation, J^{e}, for each element, i.e.

$$J^{\mathrm{e}} = \begin{bmatrix} \dfrac{\partial N_1(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_2(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_3(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_4(\xi,\eta)}{\partial \xi} \\ \dfrac{\partial N_1(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_2(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_3(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_4(\xi,\eta)}{\partial \eta} \end{bmatrix} \begin{bmatrix} (x_1)_1^{\mathrm{e}} & (x_2)_1^{\mathrm{e}} \\ (x_1)_2^{\mathrm{e}} & (x_2)_2^{\mathrm{e}} \\ (x_1)_3^{\mathrm{e}} & (x_2)_3^{\mathrm{e}} \\ (x_1)_4^{\mathrm{e}} & (x_2)_4^{\mathrm{e}} \end{bmatrix}. \tag{3.6.34}$$

On assuming that $\det(J^{\mathrm{e}}) \neq 0$, then there exists a unique inverse matrix, $(J^{\mathrm{e}})^{-1}$, satisfying the following relationship

$$\begin{bmatrix} B_{11}^{\mathrm{e}} & B_{12}^{\mathrm{e}} & B_{13}^{\mathrm{e}} & B_{14}^{\mathrm{e}} \\ B_{21}^{\mathrm{e}} & B_{22}^{\mathrm{e}} & B_{23}^{\mathrm{e}} & B_{24}^{\mathrm{e}} \end{bmatrix} = (J^{\mathrm{e}})^{-1} \begin{bmatrix} \dfrac{\partial N_1(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_2(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_3(\xi,\eta)}{\partial \xi} & \dfrac{\partial N_4(\xi,\eta)}{\partial \xi} \\ \dfrac{\partial N_1(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_2(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_3(\xi,\eta)}{\partial \eta} & \dfrac{\partial N_4(\xi,\eta)}{\partial \eta} \end{bmatrix}, \tag{3.6.35}$$

where the strain-displacement matrix $\mathbf{B}^{\mathrm{e}}(\xi,\eta)$ is defined by

$$\mathbf{B}^{\mathrm{e}} = \begin{bmatrix} B_{11}^{\mathrm{e}} & 0 & B_{12}^{\mathrm{e}} & 0 & B_{13}^{\mathrm{e}} & 0 & B_{14}^{\mathrm{e}} & 0 \\ 0 & B_{21}^{\mathrm{e}} & 0 & B_{22}^{\mathrm{e}} & 0 & B_{23}^{\mathrm{e}} & 0 & B_{24}^{\mathrm{e}} \\ B_{21}^{\mathrm{e}} & B_{11}^{\mathrm{e}} & B_{22}^{\mathrm{e}} & B_{12}^{\mathrm{e}} & B_{23}^{\mathrm{e}} & B_{13}^{\mathrm{e}} & B_{24}^{\mathrm{e}} & B_{14}^{\mathrm{e}} \end{bmatrix}. \tag{3.6.36}$$

Expressions (3.6.29), (3.6.31)–(3.6.33), at $t = t_{n+1}$, now read as

$$\begin{aligned} &\mathbf{u}_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{u}_{n+1}^{\mathrm{e}}, \qquad && \mathbf{w}_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{w}_{n+1}^{\mathrm{e}}, \\ &\mathbf{b}_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{b}_{n+1}^{\mathrm{e}}, && \mathbf{f}_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{N}(\xi,\eta)\,\mathbf{f}_{n+1}^{\mathrm{e}}, \\ &[\varepsilon_{\mathbf{u}}]_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{B}^{\mathrm{e}}(\xi,\eta)\,\mathbf{u}_{n+1}^{\mathrm{e}}, && [\varepsilon_{\mathbf{w}}]_{n+1}^{\mathrm{e}}(\xi,\eta) = \mathbf{B}^{\mathrm{e}}(\xi,\eta)\,\mathbf{w}_{n+1}^{\mathrm{e}}. \end{aligned} \tag{3.6.37}$$

On accounting for the above expressions and the fact that $\Omega = \bigcup_{e=1}^{nel} \Omega_e$, the variational formulation (3.6.22), at $t = t_{n+1}$, may be recast as

$$\begin{aligned} &\sum_{e=1}^{nel} \left\{ \left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}} \int_{-1}^{1}\int_{-1}^{1} \left[\left[\mathbf{B}^{\mathrm{e}}(\xi,\eta)\right]^{\mathsf{T}} \boldsymbol{\sigma}\left([\mathbf{u}]_{n+1}^{\mathrm{e}}\right)(\xi,\eta)\, |J^{\mathrm{e}}(\xi,\eta)| \right] \mathrm{d}\xi\mathrm{d}\eta \right\} \\ &= \sum_{i=1}^{2}\sum_{e=1}^{nel} \left\{ \left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}} \int_{-1}^{1} \left[\left[\mathbf{N}^{\mathrm{e}}(\xi,-(2i-3))\right]^{\mathsf{T}} \mathbf{N}^{\mathrm{e}}(\xi,-(2i-3))\,\mathbf{f}_{n+1}^{\mathrm{e}} \left(J_1\right)_i^{\mathrm{e}} \right] \mathrm{d}\xi \right\} \\ &+ \sum_{i=1}^{2}\sum_{e=1}^{nel} \left\{ \left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}} \int_{-1}^{1} \left[\left[\mathbf{N}^{\mathrm{e}}(-(2i-3),\eta)\right]^{\mathsf{T}} \mathbf{N}^{\mathrm{e}}(-(2i-3),\eta)\,\mathbf{f}_{n+1}^{\mathrm{e}} \left(J_2\right)_i^{\mathrm{e}} \right] \mathrm{d}\eta \right\} \\ &+ \sum_{e=1}^{nel} \left\{ \left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}} \int_{-1}^{1}\int_{-1}^{1} \left[\left[\mathbf{N}^{\mathrm{e}}(\xi,\eta)\right]^{\mathsf{T}} \mathbf{N}^{\mathrm{e}}(\xi,\eta)\,\mathbf{b}_{n+1}^{\mathrm{e}}\, |J^{\mathrm{e}}(\xi,\eta)| \right] \mathrm{d}\xi\mathrm{d}\eta \right\}. \end{aligned} \tag{3.6.38}$$

We introduce the following notation

$$\mathbf{f}^{\mathrm{int}}\left([u]_{n+1}^{\mathrm{e}}\right)=\int_{-1}^{1}\int_{-1}^{1}\left[\left[\mathbf{B}^{\mathrm{e}}(\xi,\eta)\right]^{\mathsf{T}}\boldsymbol{\sigma}\left([\mathbf{u}]_{n+1}^{\mathrm{e}}\right)(\xi,\eta)\,|J^{\mathrm{e}}(\xi,\eta)|\right]\mathrm{d}\,\xi\mathrm{d}\eta\,, \tag{3.6.39a}$$

$$\left[\left(\mathbf{f}_1^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}=\int_{-1}^{1}\left[\left[\mathbf{N}^{\mathrm{e}}(\xi,-(2i-3))\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(\xi,-(2i-3))\,\mathbf{f}_{n+1}^{\mathrm{e}}\left(J_1\right)_i^{\mathrm{e}}\right]\mathrm{d}\,\xi\,, \tag{3.6.39b}$$

$$\left[\left(\mathbf{f}_2^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}=\int_{-1}^{1}\left[\left[\mathbf{N}^{\mathrm{e}}(-(2i-3),\eta)\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(-(2i-3),\eta)\,\mathbf{f}_{n+1}^{\mathrm{e}}\left(J_2\right)_i^{\mathrm{e}}\right]\mathrm{d}\eta\,, \tag{3.6.39c}$$

$$\left[\left(\mathbf{f}_3^{\mathrm{ext}}\right)\right]_{n+1}^{\mathrm{e}}=\int_{-1}^{1}\int_{-1}^{1}\left[\left[\mathbf{N}^{\mathrm{e}}(\xi,\eta)\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(\xi,\eta)\,\mathbf{b}_{n+1}^{\mathrm{e}}\,|J^{\mathrm{e}}(\xi,\eta)|\right]\mathrm{d}\,\xi\mathrm{d}\eta\,, \tag{3.6.39d}$$

$$\left(\mathbf{J}_1\right)^{\mathrm{e}}=\left[\ \left(J_1\right)_1^{\mathrm{e}}\quad\left(J_1\right)_2^{\mathrm{e}}\ \right]^{\mathsf{T}},\quad\left(\mathbf{J}_2\right)^{\mathrm{e}}=\left[\ \left(J_2\right)_1^{\mathrm{e}}\quad\left(J_2\right)_2^{\mathrm{e}}\ \right]^{\mathsf{T}}, \tag{3.6.40a}$$

$$\left(J_1\right)_1^{\mathrm{e}}=\frac{1}{2}\sqrt{\left[(x_1)_3^{\mathrm{e}}-(x_1)_4^{\mathrm{e}}\right]^2+\left[(x_2)_3^{\mathrm{e}}-(x_2)_4^{\mathrm{e}}\right]^2}\,, \tag{3.6.40b}$$

$$\left(J_1\right)_2^{\mathrm{e}}=\frac{1}{2}\sqrt{[(x_1)_1^{\mathrm{e}}-(x_1)_2^{\mathrm{e}}]^2+[(x_2)_1^{\mathrm{e}}-(x_2)_2^{\mathrm{e}}]^2}\,, \tag{3.6.40c}$$

$$\left(J_2\right)_1^{\mathrm{e}}=\frac{1}{2}\sqrt{\left[(x_1)_2^{\mathrm{e}}-(x_1)_3^{\mathrm{e}}\right]^2+\left[(x_2)_2^{\mathrm{e}}-(x_2)_3^{\mathrm{e}}\right]^2}\,, \tag{3.6.40d}$$

$$\left(J_2\right)_2^{\mathrm{e}}=\frac{1}{2}\sqrt{[(x_1)_1^{\mathrm{e}}-(x_1)_4^{\mathrm{e}}]^2+[(x_2)_1^{\mathrm{e}}-(x_2)_4^{\mathrm{e}}]^2}\,. \tag{3.6.40e}$$

The integrals involved in the expressions above are solved by the two-point Gauss method, ie $ng=2$ in the interpolations below. Consequently, expressions (3.6.39) become

$$\left[\left(\mathbf{f}^{\mathrm{int}}\right)\right]_{n+1}^{\mathrm{e}}\cong\sum_{i=1}^{ng}\sum_{i=1}^{ng}A_iA_j\left[\left[\mathbf{B}^{\mathrm{e}}(\xi_i,\eta_j)\right]^{\mathsf{T}}\,[\boldsymbol{\sigma}]_{n+1}^{\mathrm{e}}(\xi_i,\eta_j)\,\left|J^{\mathrm{e}}(\xi_i,\eta_j)\right|\right], \tag{3.6.41a}$$

$$\left[\left(\mathbf{f}_1^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}\cong\sum_{i=j}^{ng}A_j\left[\left[\mathbf{N}^{\mathrm{e}}(\xi_j,-(2i-3))\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(\xi_j,-(2i-3))\,\mathbf{f}_{n+1}^{\mathrm{e}}\left(J_1\right)_i^{\mathrm{e}}\right], \tag{3.6.41b}$$

$$\left[\left(\mathbf{f}_2^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}\cong\sum_{i=j}^{ng}A_j\left[\left[\mathbf{N}^{\mathrm{e}}(-(2i-3),\eta_j)\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(-(2i-3),\eta_j)\,\mathbf{f}_{n+1}^{\mathrm{e}}\left(J_2\right)_i^{\mathrm{e}}\right], \tag{3.6.41c}$$

$$\left[\left(\mathbf{f}_3^{\mathrm{ext}}\right)\right]_{n+1}^{\mathrm{e}}\cong\sum_{i=1}^{ng}\sum_{i=1}^{ng}A_iA_j\left[\left[\mathbf{N}^{\mathrm{e}}(\xi_i,\eta_j)\right]^{\mathsf{T}}\mathbf{N}^{\mathrm{e}}(\xi_i,\eta_j)\,\mathbf{b}_{n+1}^{\mathrm{e}}\left|J^{\mathrm{e}}(\xi_i,\eta_j)\right|\right], \tag{3.6.41d}$$

where the coefficients in the formulae above are given by

$$A_1=A_2=1\,,\quad\xi_1=\eta_1=-\frac{1}{\sqrt{3}}\,,\quad\xi_2=\eta_2=\frac{1}{\sqrt{3}}\,. \tag{3.6.42}$$

According to relations (3.6.41), expressions (3.6.38) can be written as

$$
\begin{aligned}
&\sum_{e=1}^{nel}\left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\left(\mathbf{f}^{\mathrm{int}}\right)\right]_{n+1}^{\mathrm{e}}=\sum_{i=1}^{2}\sum_{e=1}^{nel}\left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\left(\mathbf{f}_1^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}\\
&+\sum_{i=1}^{2}\sum_{e=1}^{nel}\left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\left(\mathbf{f}_2^{\mathrm{ext}}\right)_i^{\mathrm{e}}\right]_{n+1}+\sum_{e=1}^{nel}\left(\mathbf{w}_{n+1}^{\mathrm{e}}\right)^{\mathsf{T}}\left[\left(\mathbf{f}_3^{\mathrm{ext}}\right)\right]_{n+1}^{\mathrm{e}}.
\end{aligned}
\tag{3.6.43}
$$

The *key point of coupling problems* consists of considering an appropriate expression for $[\sigma]_{n+1}^{\mathrm{e}}$ in (3.6.38). Such an expression is that obtained by the Radial Return Algorithm, which is presented in the following section.

After the assembly operator $\overset{nel}{\underset{e=1}{A}}$, originally introduced by Hughes (1987), is applied to expressions (3.6.39), one obtains the matrix of internal forces and the vectors of external forces

$$
\begin{aligned}
&\left(\mathbf{F}^{\mathrm{int}}\right)_{n+1}=\overset{nel}{\underset{e=1}{A}}\left[\left(\mathbf{f}^{\mathrm{int}}\right)\right]_{n+1}^{\mathrm{e}}, && \left(\mathbf{F}_1^{\mathrm{ext}}\right)_{n+1}=A_{e=1}^{nel}\left[\left(\mathbf{f}_1^{\mathrm{ext}}\right)_1^{\mathrm{e}}+\left(\mathbf{f}_1^{\mathrm{ext}}\right)_2^{\mathrm{e}}\right]_{n+1},\\
&\left(\mathbf{F}_3^{\mathrm{ext}}\right)_{n+1}=A_{e=1}^{nel}\left[\left(\mathbf{f}_1^{\mathrm{ext}}\right)_3^{\mathrm{e}}\right]_{n+1}, && \left(\mathbf{F}_2^{\mathrm{ext}}\right)_{n+1}=A_{e=1}^{nel}\left[\left(\mathbf{f}_2^{\mathrm{ext}}\right)_1^{\mathrm{e}}+\left(\mathbf{f}_2^{\mathrm{ext}}\right)_2^{\mathrm{e}}\right]_{n+1}.
\end{aligned}
\tag{3.6.44}
$$

Consequently, the variational formulation (3.6.38) has been transformed by the discretization procedure into the following non-linear system

$$
G\left(\mathbf{u}_{n+1},\mathbf{w}_{n+1}\right)\equiv\mathbf{w}_{n+1}^{\mathsf{T}}\left[\left(\mathbf{F}^{\mathrm{int}}\right)_{n+1}-\left(\mathbf{F}^{\mathrm{ext}}\right)_{n+1}\right]=0,\quad \forall w\in\mathscr{V}_{ad},
\tag{3.6.45}
$$

where $\left(\mathbf{F}^{\mathrm{ext}}\right)_{n+1}=\sum_{i=1}^{3}\left(\mathbf{F}_i^{\mathrm{ext}}\right)_{n+1}$.

The system of non-linear equations (3.6.45) is the result of the dicretization by the FEM applied to the variational formulation

$$
G\left(\mathbf{u}_{n+1}\right)\equiv\left(\mathbf{F}^{\mathrm{int}}\right)_{n+1}-\left(\mathbf{F}^{\mathrm{ext}}\right)_{n+1}=0.
\tag{3.6.46}
$$

3.6.3. THE RADIAL RETURN ALGORITHM

The numerical integration of the equations corresponding to problem (P_1) is based on the Radial Return Algorithm proposed by Simo and Hughes (1998). This method allows us to find the elasto-plastic moduli and then the *modified problem* (P_2) is solved by the Newton method. Only at this level the coupling of the variational problem with the Radial Return Algorithm is achieved. The elastic-plastic moduli permits the replacement of the stress vector by the displacement vector in the variational problem at a given time.

In order to find the numerical solution of elastic-plastic problems, we follow the methodology proposed by Krieg and Key (1976). First, we replace the continuous time interval $\bar{I} = [0,T]$ by the sequence of discrete times $t_0, t_1, \ldots, t_N$, with $0 = t_0 < t_1 < \ldots < t_N = T$. We denote by $X_{n+1} := X(t_{n+1})$ the numerical approximation of the exact value $X(t_{n+1})$ at time $t_{n+1} = t_n + \Delta t$.

The discrete form of the elastic type constitutive equation (3.6.10) at time t_{n+1} is given by

$$[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}(\xi,\eta) = \mathscr{E}\big([\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}(\xi,\eta) - [\boldsymbol{\varepsilon}^{\mathrm{p}}]^{\mathrm{e}}_{n+1}(\xi,\eta)\big). \tag{3.6.47}$$

For the sake of simplicity, we drop the variables (ξ,η) in what follows. We apply the backward Euler method to the differential relations (3.6.8) and (3.6.12) and hence we obtain

$$[\boldsymbol{\varepsilon}^{\mathrm{p}}]^{\mathrm{e}}_{n+1} = [\boldsymbol{\varepsilon}^{\mathrm{p}}]^{\mathrm{e}}_{n} + [\lambda^*]^{\mathrm{e}}_{n+1}\,\frac{[\mathbf{s}]^{\mathrm{e}}_{n+1}}{\big\|[\mathbf{s}]^{\mathrm{e}}_{n+1}\big\|}, \quad [k]^{\mathrm{e}}_{n+1} = [k]^{\mathrm{e}}_{n} + [\lambda^*]^{\mathrm{e}}_{n+1}, \tag{3.6.48}$$

where $[\lambda^*]^{\mathrm{e}}_{n+1} = [\lambda]^{\mathrm{e}}_{n+1}\,\Delta t = [\lambda]^{\mathrm{e}}_{n+1}\,(t_{n+1} - t_n)$ and

$$\mathscr{F}\left([\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}, [k]^{\mathrm{e}}_{n+1}\right) \le 0, \quad [\lambda^*]^{\mathrm{e}}_{n+1} \ge 0, \quad [\lambda^*]^{\mathrm{e}}_{n+1}\,\mathscr{F}\left([\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}, [k]^{\mathrm{e}}_{n+1}\right) = 0, \tag{3.6.49}$$

$$\begin{aligned} &\mathscr{F}\left([\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}, [k]^{\mathrm{e}}_{n+1}\right) = \left\|\operatorname{dev}[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}\right\| - F\left([k]^{\mathrm{e}}_{n+1}\right), \\ &F\left([k]^{\mathrm{e}}_{n+1}\right) = H\left([k]^{\mathrm{e}}_{n} + [\lambda^*]^{\mathrm{e}}_{n+1}\right) + \sigma_Y. \end{aligned} \tag{3.6.50}$$

We introduce the *trial (elastic) stress* tensor through

$$\left\{[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}} = k_a\,\mathrm{tr}\left([\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}\right)\mathbf{I} + 2\mu\left(\operatorname{dev}[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1} - [\boldsymbol{\varepsilon}^{\mathrm{p}}]^{\mathrm{e}}_{n}\right). \tag{3.6.51}$$

From equations (3.6.51) and (3.6.47), it follows

$$[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1} = \left\{[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}} - 2\mu\,[\lambda^*]^{\mathrm{e}}_{n+1}\,\frac{[\mathbf{s}]^{\mathrm{e}}_{n+1}}{\big\|[\mathbf{s}]^{\mathrm{e}}_{n+1}\big\|}. \tag{3.6.52}$$

The deviatoric part of (3.6.50) is characterized by

$$\begin{aligned} &[\mathbf{s}]^{\mathrm{e}}_{n+1} = \left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}} - 2\mu\,[\lambda^*]^{\mathrm{e}}_{n+1}\,\frac{[\mathbf{s}]^{\mathrm{e}}_{n+1}}{\big\|[\mathbf{s}]^{\mathrm{e}}_{n+1}\big\|}, \\ &\left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}} = 2\mu\left(\operatorname{dev}[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1} - [\boldsymbol{\varepsilon}^{\mathrm{p}}]^{\mathrm{e}}_{n}\right). \end{aligned} \tag{3.6.53}$$

To determine the expression for the plastic factor $[\lambda^*]^{\mathrm{e}}_{n+1}$, we look at the sign of the following expression

$$\mathscr{F}^{\mathsf{T}}\left(\left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}}, [k]^{\mathrm{e}}_{n}\right),$$

where the plasticity test function is given by

$$\mathscr{F}^{\mathsf{T}}\left([\mathbf{s}]^{\mathrm{e}}_{n+1}, [k]^{\mathrm{e}}_{n}\right) = \left\|[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\| - \left(H\,[k]^{\mathrm{e}}_{n} + \sigma_Y\right). \tag{3.6.54}$$

- If $\mathscr{F}^{\mathsf{T}}\left(\left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}}, [k]^{\mathrm{e}}_{n}\right) \leq 0$ then $[\lambda^*]^{\mathrm{e}}_{n+1} = 0$.
- If $\mathscr{F}^{\mathsf{T}}\left(\left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}}, [k]^{\mathrm{e}}_{n}\right) > 0$ then the expression for the plastic factor, $[\lambda^*]^{\mathrm{e}}_{n+1}$, is obtained by imposing the condition to have the current value at time t_{n+1} on the yield surface, i.e. $\mathscr{F}^{\mathsf{T}}\left(\left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}}, [k]^{\mathrm{e}}_{n+1}\right) = 0$. Consequently, one obtains

$$[\lambda^*]^{\mathrm{e}}_{n+1} = \frac{\left\| \left\{[\mathbf{s}]^{\mathrm{e}}_{n+1}\right\}^{\mathsf{T}} \right\| - \left(H\,[k]^{\mathrm{e}}_{n} + \sigma_Y\right)}{H + 2\mu}. \tag{3.6.55}$$

To obtain a complete representation and the meaning of the Radial Return Algorithm, we show how the elasto-plastic moduli can be defined. After the elasto-plastic moduli have been associated with the algorithm, see $\mathscr{E}^{\mathrm{ep}}$ given by equation (3.6.58), we look at the expression (3.6.47) which is a non-linear system with respect to the unknown $\mathbf{u}_{n+1}$. The system can be solved using Newton-Raphson method. Following the Newton-Raphson method, the solution $\mathbf{u}_{n+1}$ is obtained on the based of the following iterative relations:

$$\mathbf{u}^{j+1}_{n+1} = \mathbf{u}^{j}_{n+1} - \beta_j \left[K\left(\mathbf{u}^{j}_{n+1}\right)\right]^{-1} G\left(\mathbf{u}^{j}_{n+1}\right), \tag{3.6.56}$$

where $\beta_j \in (0,1]$ and the Jacobian of the function G is given by the following expression

$$\begin{aligned}
\left[K\left(\mathbf{u}_{n+1}\right)\right]_{i,k} &= \frac{\partial G_i\left(\mathbf{u}_{n+1}\right)}{\partial\left(\mathbf{u}_{n+1}\right)_k} = \mathop{A}_{e=1}^{nel} \frac{\partial\left[\left(\mathbf{f}^{\mathrm{int}}\right)_i\right]^{\mathrm{e}}_{n+1}}{\partial\left(\mathbf{u}_{n+1}\right)_k} \\
&= \mathop{A}_{e=1}^{nel} \left\{ \int_{-1}^{1}\int_{-1}^{1} \left[\left(\mathbf{B}^{\mathrm{e}}(\xi,\eta)\right)^{\mathsf{T}} \frac{\partial[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}}{\partial[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}} \frac{\partial[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}}{\partial\left(\mathbf{u}^{\mathrm{e}}_{n+1}\right)_k} \left|J^{\mathrm{e}}(\xi,\eta)\right| \right] \mathrm{d}\xi\,\mathrm{d}\eta \right\} \\
&= \mathop{A}_{e=1}^{nel} \left\{ \int_{-1}^{1}\int_{-1}^{1} \left[\left(\mathbf{B}^{\mathrm{e}}(\xi,\eta)\right)^{\mathsf{T}} [\mathscr{E}^{ep}]^{\mathrm{e}}_{n+1}\, \mathbf{B}^{\mathrm{e}}(\xi,\eta) \left|J^{\mathrm{e}}(\xi,\eta)\right| \right] \mathrm{d}\xi\,\mathrm{d}\eta \right\}.
\end{aligned} \tag{3.6.57}$$

The elasto-plastic moduli are given by the following relationship

$$[\mathscr{E}^{\mathrm{ep}}]^{\mathrm{e}}_{n+1} = \frac{\partial[\boldsymbol{\sigma}]^{\mathrm{e}}_{n+1}}{\partial[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}}. \tag{3.6.58}$$

One refers to (3.6.58) as to the algorithmic tangent modulus, a notion first introduced by Simo and Hughes (1998).

If we differentiate the algorithmic constitutive equation (3.6.52) with respect to $[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}$ then we obtain the following expression for $\mathscr{E}^{\mathrm{ep}}$

$$[\mathscr{E}^{\mathrm{ep}}]^{\mathrm{e}}_{n+1} = k_a\,\mathbf{I}\otimes\mathbf{I} + 2\mu\,\mathbf{I}_{dev} - 2\mu\left([\mathbf{n}]^{\mathrm{e}}_{n+1} \otimes \frac{\partial[\lambda^*]^{\mathrm{e}}_{n+1}}{\partial[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}} + [\lambda^*]^{\mathrm{e}}_{n+1} \frac{\partial[\mathbf{n}]^{\mathrm{e}}_{n+1}}{\partial[\boldsymbol{\varepsilon}_{\mathbf{u}}]^{\mathrm{e}}_{n+1}} \right). \tag{3.6.59}$$

Consequently, the expression for the elastic-plastic moduli is given by

$$[\mathscr{E}^{\mathrm{ep}}]^{\mathrm{e}}_{n+1} = \begin{cases} \mathscr{E} & \text{if} \quad \mathscr{F} \le 0 \\ k_a \, \mathbf{I} \otimes \mathbf{I} + 2\mu \, [\theta_1]^{\mathrm{e}}_{n+1} \, I_{dev} - 2\mu \, [\theta_2]^{\mathrm{e}}_{n+1} \, [\mathbf{n}]^{\mathrm{e}}_{n+1} \otimes [\mathbf{n}]^{\mathrm{e}}_{n+1} & \text{if} \quad \mathscr{F} > 0 \end{cases} \tag{3.6.60}$$

where $\mathscr{F} = \mathscr{F}^{\mathsf{T}} \left(\left\{ [\mathbf{s}]^{\mathrm{e}}_{n+1} \right\}^{\mathsf{T}}, [k]^{\mathrm{e}}_{n} \right)$ and

$$[\theta_1]^{\mathrm{e}}_{n+1} = 1 - \frac{2\mu \, [\lambda^*]^{\mathrm{e}}_{n+1}}{\| \left\{ [\mathbf{s}]^{\mathrm{e}}_{n+1} \right\}^{\mathsf{T}} \|}, \quad [\theta_2]^{\mathrm{e}}_{n+1} = \frac{2\mu}{H + 2\mu} - \frac{2\mu \, [\lambda^*]^{\mathrm{e}}_{n+1}}{\| \left\{ [\mathbf{s}]^{\mathrm{e}}_{n+1} \right\}^{\mathsf{T}} \|}. \tag{3.6.61}$$

Bearing in mind the proven relationships, one can assemble the Radial Return Mapping Algorithm in the following form:

$$\left\{ [\boldsymbol{\sigma}]^{\mathrm{e},j+1}_{n+1}, [\varepsilon^{\mathrm{p}}]^{\mathrm{e},j+1}_{n+1}, [k]^{\mathrm{e},j+1}_{n+1} \right\} = \text{Radial Return} \left\{ \mathbf{u}^{\mathrm{e},j}_{n+1}, [\varepsilon^{\mathrm{p}}]^{\mathrm{e}}_{n}, [k]^{\mathrm{e}}_{n} \right\}. \tag{3.6.62}$$

Next, we list the steps of the RADIAL RETURN MAPPING ALGORITHM:

1. Compute the trial elastic stress for the prescribed strain $[\varepsilon_{\mathbf{u}}]^{\mathrm{e},j+1}_{n+1} = [\mathbf{B}]^{\mathrm{e}} \, \mathbf{u}^{\mathrm{e},j}_{n+1}$:

$$\left\{ [\mathbf{s}]^{\mathrm{e},j+1}_{n+1} \right\}^{\mathsf{T}} = 2\mu \left(\operatorname{dev} [\varepsilon_{\mathbf{u}}]^{\mathrm{e},j+1}_{n+1} - [\varepsilon^{\mathrm{p}}]^{\mathrm{e}}_{n} \right);$$

$$\left\{ [\boldsymbol{\sigma}]^{\mathrm{e},j+1}_{n+1} \right\}^{\mathsf{T}} = k_a \, \mathrm{tr} \left([\varepsilon_{\mathbf{u}}]^{\mathrm{e},j+1}_{n+1} \right) \mathbf{I} + \left\{ [\mathbf{s}]^{\mathrm{e},j+1}_{n+1} \right\}^{\mathsf{T}}.$$

2. Check the yield condition for $\mathscr{F}^{\mathsf{T},j+1}_{n+1} = \mathscr{F}^{\mathsf{T}} \left(\left\{ [\mathbf{s}]^{\mathrm{e}}, j+1_{n+1} \right\}, [k]^{\mathrm{e}}_{n} \right)$:

   if $\mathscr{F}^{tr,j+1}_{n+1} \le 0$ then

$$[\boldsymbol{\sigma}]^{\mathrm{e},j+1}_{n+1} = \left\{ [\boldsymbol{\sigma}]^{\mathrm{e},j+1}_{n+1} \right\}^{\mathsf{T}}; \quad [\varepsilon^{\mathrm{p}}]^{\mathrm{e},j+1}_{n+1} = [\varepsilon^{\mathrm{p}}]^{\mathrm{e}}_{n};$$

$$[k]^{\mathrm{e},j+1}_{n+1} = [k]^{\mathrm{e}}_{n}; \qquad [\mathscr{E}^{\mathrm{ep}}]^{\mathrm{e},j+1}_{n+1} = \mathscr{E};$$

else

$$[\mathbf{n}]_{n+1}^{e,j+1} = \frac{\left\{[\mathbf{s}]_{n+1}^{e,j+1}\right\}^{\mathsf{T}}}{\left\|\left\{[\mathbf{s}]_{n+1}^{e,j+1}\right\}^{\mathsf{T}}\right\|}; \quad [\lambda^*]_{n+1}^{e,j+1} = \frac{\left\|\left\{[\mathbf{s}]_{n+1}^{e,j+1}\right\}^{\mathsf{T}}\right\| - (H\,[k]_n^e + \sigma_Y)}{H + 2\mu};$$

$$[\sigma]_{n+1}^{e,j+1} = [\sigma]_n^{e,j+1} - 2\mu\,[\lambda^*]_{n+1}^{e,j+1}\,[\mathbf{n}]_{n+1}^{e,j+1};$$

$$[\varepsilon^p]_{n+1}^{e,j+1} = [\varepsilon^p]_n^{e,j+1} + [\lambda^*]_{n+1}^{e,j+1}\,[\mathbf{n}]_{n+1}^{e,j+1}; \quad [k]_{n+1}^{e,j+1} = [k]_n^e + [\lambda^*]_{n+1}^{e,j+1};$$

$$[\theta_1]_{n+1}^{e,j+1} = 1 - \frac{2\mu\,[\lambda^*]_{n+1}^{e,j+1}}{\left\|\left\{[\mathbf{s}]_{n+1}^{e,j+1}\right\}^{\mathsf{T}}\right\|}; \quad [\theta_2]_{n+1}^{e,j+1} = \frac{2\mu}{H+2\mu} - \frac{2\mu\,[\lambda^*]_{n+1}^{e,j+1}}{\left\|\left\{[\mathbf{s}]_{n+1}^{e,j+1}\right\}^{\mathsf{T}}\right\|};$$

$$[\mathscr{E}^{ep}]_{n+1}^{e,j+1} = k_a\,\mathbf{I}\otimes\mathbf{I} + 2\mu\,[\theta_1]_{n+1}^{e,j+1}\,\mathbf{I}_{dev} - 2\mu\,[\theta_2]\,[\mathbf{n}]_{n+1}^{e,j+1}\otimes[\mathbf{n}]_{n+1}^{e,j+1}\,.$$

return.

The GENERAL ALGORITHM for problem (P) consists of the following steps:

1. Initialize the vectors $\mathbf{n} = \mathbf{0}$; $[\mathbf{u}]_1^0 = \mathbf{0}$; $[\varepsilon^p]_0 = \mathbf{0}$; $[k]_0 = 0$;
2. Perform a for loop with respect to $n = \overline{0,N}$ in order to compute the time increment $t_{n+1} = t_n + \Delta t$, $t_0 = 0$.
   - 2.1. Perform a while loop with respect to the index variable, $j = 1,2,\ldots$, meaning that the Newton-Raphson method is applied.
     - 2.1.1. Perform a for loop with respect to the number of elements of the FEM mesh used, $e = \overline{1,nel}$.

- First, the local vectors $[\mathbf{u}]_{n+1}^{e,j}$, $[\varepsilon^p]_n^e$ and $[k]_n^e$ are extracted from the global vectors $[\mathbf{u}]_{n+1}^{j}$, $[\varepsilon^p]_n$ and $[k]_n$, respectively.
- Then, the procedure Radial Return is applied.
- Next, the local Jacobian matrix, and the local vectors of internal and external forces are calculated, followed by the assembly of these items.
- Further, $\mathbf{u}_{n+1}^{j+1}$ is determined via Newton's method:

$$\mathbf{u}_{n+1}^{j+1} = \mathbf{u}_{n+1}^{j} - \beta_j\,[\Delta\mathbf{u}]_{n+1}^{j}; \quad [\Delta\mathbf{u}]_{n+1}^{j} = \left[K\left(\mathbf{u}_{n+1}^{j}\right)\right]^{-1} G\left(\mathbf{u}_{n+1}^{j}\right).$$

- Evaluate the error $[\mathrm{ERR}]_{n+1}^{j} = \dfrac{[\Delta \mathbf{u}]_{n+1}^{j}}{\left\| \mathbf{u}_{n+1}^{j} \right\|}$:

  if $[\mathrm{ERR}]_{n+1}^{j} < \mathrm{TOL}$ then

  $\mathbf{u}_{n+2} \longleftarrow \mathbf{u}_{n+1}^{j+1}\,; \quad [\varepsilon^{\mathrm{p}}]_{n+1} = [\varepsilon^{\mathrm{p}}]_{n+1}^{j+1}\,;$

  $[k]_{n+1} = [k]_{n+1}^{j+1}\,; \quad [\boldsymbol{\sigma}]_{n+1} = [\boldsymbol{\sigma}]_{n+1}^{j+1}\,;$

  return

  else

  $j \longleftarrow j+1\,;$ go to 2.2.1.

  endif

3.6.4. NUMERICAL APPLICATION

In order to illustrate the efficiency of the proposed algorithm for solving two-dimensional elasto-plastic problems, we choose the trapezoidal panel domain illustrated in Fig. 3.6.1 and given by

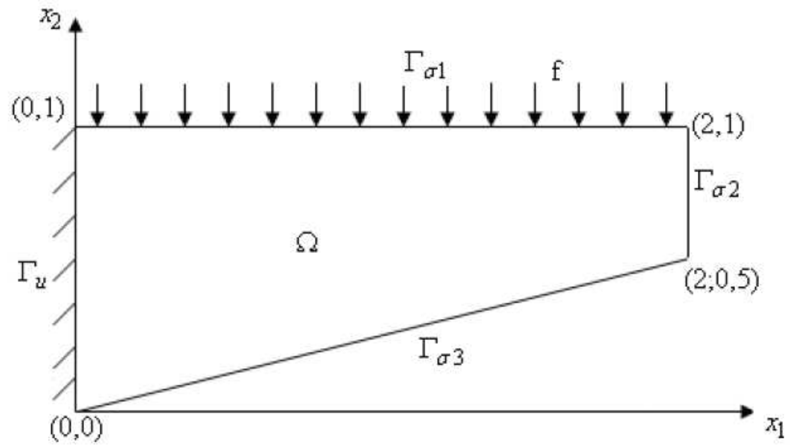

Fig. 3.6.1 – Problem definition for the numerical example considered.

$$\Omega = \left\{ (x_1, x_2) \in \mathbb{R}^2 \middle| 0 \le x_1 \le 2,\ \frac{x_1}{4} \le x_2 \le 1 \right\}. \tag{3.6.1}$$

In the absence of body forces, we assume that the vertical left edge is fixed, the bottom and right edges are free of traction, i.e. $\mathbf{f} = \mathbf{0}$, and a vertical traction $\mathbf{f} = 100 \sin t$ is applied on the top edge. The example investigated in this section aims at highlighting the efficiency of the numerical algorithm when solving problem (P).

The material considered in this example is steel DP 600, whose parameters are given by, see e.g. Brogiatto *et al.* (2008),

$$\begin{aligned} &E = 182{,}000.00\,\mathrm{MPa}\,; \quad \nu = 0.30\,; \quad \sigma_Y = 349.40\,\mathrm{MPa}\,; \\ &\lambda_a = 10{,}500.00\,; \quad \mu_a = 70{,}000.00\,; \quad H = 3\,. \end{aligned} \tag{3.6.2}$$

It should be mentioned that the trapezoidal panel domain was divided into 16 el-

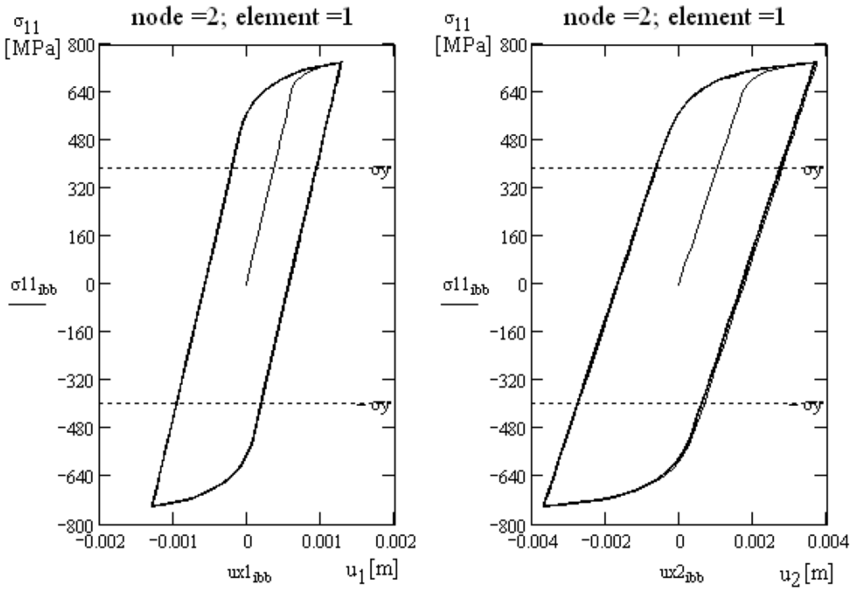

Fig. 3.6.2 – The stress σ_{11} as a function of the displacement u.

ements, each of these having four nodes, with the total number of nodes equal to 25. More precisely, the FEM parameters for the domain under investigation are the following: $dsp = 2$; $nel = 16$; $nt_{nod} = 25$; $nne = 4$; $ngl = 2$; $n_{eq} = nt_{nod} \times ngl = 50$.

Fig. 3.6.2 illustrates the tension σ_{11} as a function of the displacement $\mathbf{u}$ and, consequently, it shows the deformed image of the plate in comparison with the initial state, see e.g. Fig. 3.6.3.

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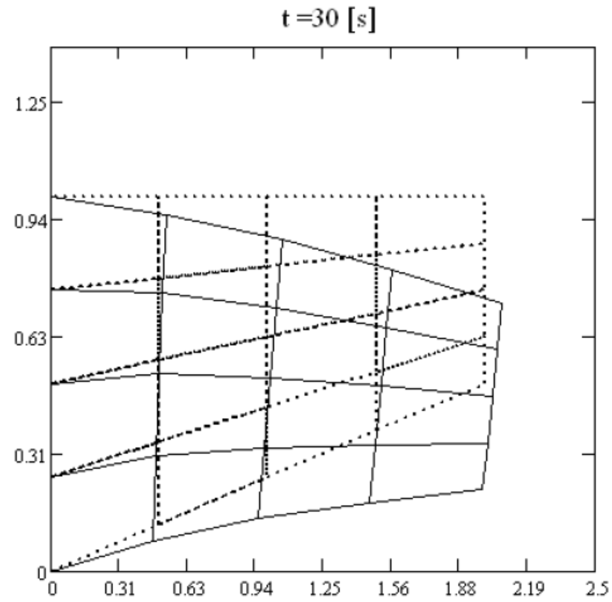

Fig. 3.6.3 – Deformed and undeformed meshes (with the scaling factor 10).

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