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# A NEW VARIATIONAL THEORY AND A COMPUTATIONAL ALGORITHM FOR COUPLED ELASTOPLASTIC DAMAGE MODELS

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Abstract--A model of elastoplasticity with hardening coupled with ductile damage which allows anisotropic change of the shape of the damage domain is presented. The assumption for the development of the constitutive model consists in assigning the elastic and damage domains and the free energy. The general variational formulation for the elastoplastic model coupled with damage is derived as well as a mixed principle which is useful from the computational standpoint. Accordingly a solution algorithm is then derived and examples are presented. *C* 1997 Elsevier Science Ltd.

## 1. INTRODCCTION

The formulation of elastoplastic models with damage has been the object of an abundant literature in which the concepts of the damage mechanics have been applied to model creep damage, fatigue damage with creep interaction, elasticity coupled with damage, isotropic plastic damage and inelastic behaviour. Among others see Lemaitre and Chaboche (1978), Krajcinovic and Fonseka (1981), llankambau and Krajcinovic (1987), Stevens and Liu (1992), Carole *et al.* (1994), Fichant *et al.* (1995), Laschet (1995), Habraken *et al. (1995),* Konke (1995).

The constitutive theories of inelastic behaviour most commonly adopted are the elastoplasticity and the continuum damage mechanics (COM) (Lemaitre and Chaboche, 1990, Lubliner, 1990). They have been used to represent different phenomena: the elastoplastic theory describes the slips of the material at the microscale : the CDM is concerned with the evolution of a material with distributed microdefects.

A material can show both elastoplastic and damage behaviour so that some elastoplastic theories coupled with damage have been proposed, see, e.g., the models presented by Simo and Ju (1987), Ju (1989), Hansen and Schreyer (1994).

However, it appears that restrictive assumptions are adopted in the damage elastoplastic models. As examples, the yield and damage functionals proposed by Hansen and Schreyer (1994) are assumed to be homogeneous of degree one. The effective strains are introduced in addition to the effective stresses and the plasticity variables for a damaged material evolve in the effective strain space and are associative in the effective stress space.

The force conjugate to the elastoplastic microcrack evolution turns out to be the elastic strain energy in Simo and Ju (1987), Lemaitre and Chaboche (1990), Hansen and Schreyer (1994).

Moreover, the damage functional presented in Simo and Ju (1987), Ju (1989) coincides with the damage energy release rate and the damage threshold turns out to be equal to the damage multiplier.

As a rule, the principle of equivalent strain is always considered in the model as an additional hypothesis of the constitutive model and is introduced in an unrelated form with respect to the constitutive relations derived from the free energy.

This paper presents a general formulation which encompasses in a unitary model a family of damage elastoplastic constitutive models with hardening. More relaxed hypotheses with respect to the ones adopted in the literature will be assumed.

Since plastic and damage constitutive relations are expressed in terms of multivalued laws, the natural framework to develop a consistent analysis of the damage elastoplastic model and of its finite step counterpart requires the recourse to the methods of the convex analysis (Rockafellar, ]970, Hiriart-Hurruty and Lemarechal, 1993). The main results of convex analysis and ofsaddle functionals, used in the paper, are collected in the appendices.

An outline ofthe paper is as follows. **In** Section 2, an elastoplastic model with hardening is addressed as an extension of the generalized standard material proposed by Halphen and Nguyen (1975). A novel energy-based damage model is presented and, subsequently, elastoplasticity is coupled with damage.

The additive slip of the strain in an elastic-damage and plastic-damage part is assumed; this approach is physically more appealing than the use of the stress split formulation, e.g. Simo and Ju (1987), Hansen and Schreyer (1994).

The damage behaviour is described in terms of two pairs of dual variables. A pair of damage variables is scalar and is suitable for characterizing isotropic damage processes. The other pair of damage variables is tensorial and is introduced in order to model anisotropic change in the shape of the damage domain.

The existence of a convex plastic domain and of a convex damage domain is assumed. A standard behaviour is postulated for the evolution of the plastic and damage variables. Both the yield and damage functionals are required to be convex.

For what concern the normality rule for a damage elastoplastic material, note that local stresses in a damage material are redistributed to the undamaged microbounds with the effect of increasing the stresses effectively acting on the material. Accordingly, we assume that plastic flows in the actual space occur by means of the effective stresses.

The coupling between plasticity and damage is also provided by the expression of the free energy which yields the force associated with the elastoplastic microcrack evolution as the sum of the elastic strain energy and of the hardening potential.

The principle of strain equivalence (see Lemaitre and Chaboche, 1990) is not introduced at the beginning of the model as an additional hypothesis but it follows from the expression of the free energy. It is further shown how a different choice of the free energy can lead to the principle of equivalent elastic energy introduced by Cordebois and Sidoroff (1979).

**In** Section 3, the damage elastoplastic model is cast in an operator form corresponding to a backward Euler scheme. The damage elastoplastic operator is proved to be conservative so that the potential theory for monotone operator (Romano *et al.*, 1993d) can be invoked to evaluate the related variational formulation in the complete set of state variables.

The utility of this approach relies on the possibility of deriving all the variational principles in a different number of state variables by enforcing Fenchel's equalities; for nonlinear elastic problems and for plasticity with hardening see Romano *et* at. *(1992),* (1993b,c).

Variational formulations provide valuable tools to establish existence and uniqueness results for the solution of problems in structural mechanics and to evaluate approximate solutions. Uniqueness is ensured if the functional to be minimized turns out to be strictly convex (or concave). By contrast, the question of existence is a considerable challenge and it will not be of concern in this paper.

The variational formulation in stresses and kinematic damage internal variables is derived. It is proved that the relevant maximum problem provides a consistent basis for developing a computational algorithm which is a generalization of the one proposed by Simo and Ju (1987), Ju (1989).

**In** Section 4 the possibility of solving in cascade plasticity and damage is proved to derive from the variational principle in stresses and kinematic damage internal variables. The maximization of the potential can be equivalently enforced in the effective stress space so that the solution of the elastoplastic constitutive problem for a given increment of total strain is obtained. This maximization can be achieved following the elastic predictor-plastic corrector scheme in the effective stress space.

Afterwards the damage problem is solved by maximizing the potential in the space of the damage variables. This problem can be directly solved without any iteration for a large class of damage functionals and damage threshold function.

The elastoplastic predictor is enforced in the effective stress and in the actual strain spaces. Hence it appears reasonable to assume that the consistent tangent operator relates the increment of the actual strain to the increment of the effective stress. Accordingly, following the general methodology presented in Marotti de Sciarra and Rosati (1995), the tangent operator consistent with the Euler backward scheme is derived in Section 5.

In Section 6, the formulation presented in this paper is applied to an aluminum alloy in the case of uniaxial monotone increasing strains and cyclic strains.

## 2. CONSTITUTIVE MODELS

Let us denote by  $\mathscr{D}$  the linear space of strains and by  $\mathscr{P}$  the dual space of stresses  $\sigma$ . Assuming small deformations the total strain  $\varepsilon \in \mathcal{L}$  is additively decomposed into an elastic *e* and a plastic part *p.*

A time-independent mechanical behaviour of the body is assumed so that the time *t* is conceived as a monotonically increasing parameter which merely orders successive events.

#### *2.1. Elastoplastic model*

Plastic phenomena are described in terms of kinematic internal variables  $\alpha$  and static internal variables  $\chi$  which belong to the dual linear spaces X and X', respectively; the variables  $\alpha$  account for structural rearrangements at the microscale (Reddy and Martin, 1991. Comi *ct al.,* 1992, Romano *et al.,* 1993c).

The elastoplastic constitutive model here addressed is an extension of the *generalized standard material* (GSM) proposed by Halphen and Nguyen (1975).

To encompass in a unitary framework the perfect plasticity as well as the hardening behaviour we introduce the generalized vectors (Nguyen, 1977):

$$
\mathbf{e} = (e, \alpha) \quad \mathbf{p} = (p, -\alpha) \quad \mathbf{\varepsilon} = (e, 0) \quad \mathbf{\sigma} = (\sigma, \chi)
$$

where e, **p** and  $\varepsilon$  belong to the product space  $\mathcal{L}_a = \mathcal{L} \times X$  and  $\sigma$  belongs to  $\mathcal{S}_a = \mathcal{S} \times X'$ . In the sequel, the label generalized will be omitted.

The duality pairing between product spaces will be denoted by  $\prec$ ;  $\succ$  and is defined as follows  $\langle \sigma, \mathbf{e} \rangle = \langle \sigma, e \rangle + \langle \chi, \chi \rangle$ . For simplicity, the bilinear forms in the spaces  $\mathcal{S} \times \mathcal{D}$ and  $X' \times X$  have been denoted by the same symbol. They have the mechanical meaning of virtual work performed by the stresses (internal static variables) for the strains (internal kinematic variables), Panagiotopoulos (1985).

In this model the existence of a convex elastic domain  $C \subseteq \mathcal{S}_{\alpha}$ , containing the origin in its interior, is postulated.

The yield criterion, which defines the current yield surface, can be expressed in terms of a convex yield functional  $f: \mathcal{S}_d \mapsto \mathfrak{R} \cup \{ +\infty \}$  so that the elastic domain C is defined in terms of the stresses  $\sigma$  as follows:

$$
\mathbf{C} = \{\pmb{\sigma} \in \mathcal{S}_a : f(\pmb{\sigma}) \leq 0\}
$$

Different kinds of hardening usually adopted in the literature can be accommodated in the model by suitably defining the expressions of the yield functional f and of the static internal variable  $\chi$ ; see, e.g., Marotti de Sciarra and Rosati (1995).

2.1.1. *The normality rule.* The main aspect of standard plasticity is the multivaluedness of the relation between plastic flows  $\dot{\mathbf{p}}$  and stresses  $\boldsymbol{\sigma}$ . In fact, a convex cone of plastic flows is associated with a given stress belonging to the boundary of the elastic domain. Vice versa,

for any plastic flow there exists a convex set of stresses belonging to the face of the elastic domain which the plastic flow is normal to.

Hence, the natural framework to develop a consistent analysis of the elastoplastic continuous model and of its finite step counterpart requires the recourse to the methods of the convex analysis. Some basic notions of convex analysis adopted in this paper are summarized in Appendix A; for more details see Hiriart-Hurruty and Lemarechal (1993).

In standard plasticity, the plastic flow  $\dot{\mathbf{p}}$  belongs to the normal cone to the elastic domain C at the point  $\sigma$ :

$$
\dot{\mathbf{p}} \in N_C(\boldsymbol{\sigma}) = \partial ||_C(\boldsymbol{\sigma}) \Leftrightarrow \boldsymbol{\sigma} \in \partial D_n(\dot{\mathbf{p}}),
$$

where  $D<sub>p</sub>$  is the support functional (see Appendix A) of the elastic domain:

$$
D_p(\mathbf{\dot{p}})=\sup\{\prec\tau,\mathbf{\dot{p}}\succ\div\tau\in\mathbf{C}\}.
$$

The superimposed dot denotes differentiation with respect to a (pseudo-)time  $t$  which merely orders the events.

For any pair  $(\hat{\mathbf{p}}, \sigma)$  which fulfils the plastic flow rule, the following equality holds:

$$
\sqcup_{\mathcal{C}}(\boldsymbol{\sigma})+D_{p}(\boldsymbol{\dot{p}})=D_{p}(\boldsymbol{\dot{p}})=\langle \boldsymbol{\sigma},\boldsymbol{\dot{p}}\rangle
$$

zero being the indicator of  $C$  since  $\sigma$  belongs to the elastic domain.

*Remark* 2.1. The value  $D_p(\mathbf{p})$  is the plastic dissipation associated with the flow  $\mathbf{p}$  and the latter equality above represents the *principle of the maximum plastic dissipation.*

Further, note that the dissipation  $D<sub>p</sub>$  turns out to be nonnegative if the null stress belongs to the interior of **C** (Romano *et al.*, 1993a).

The indicator of  $C$  can be written in terms of the yield functional  $f$  as follows:

$$
\sqcup_{\mathcal{C}}(\sigma)=(\sqsubset_{\mathfrak{R}}\neg f)(\sigma),
$$

where  $\mathfrak{R}^-$  is the cone of the nonpositive scalars.

The subdifferential of the indicator  $\mathcal{L}_c$  can thus be evaluated according to the former subdifferential rule reported in Appendix A in which we set  $m = \bigsqcup_{\Re}$ :

$$
\hat{c}\bigcup_{C}(\boldsymbol{\sigma})=\hat{c}\bigcup_{\mathfrak{R}}\left[f(\boldsymbol{\sigma})\right]\hat{c}f(\boldsymbol{\sigma})=N_{\mathfrak{R}}\left[f(\boldsymbol{\sigma})\right]\hat{c}f(\boldsymbol{\sigma}).
$$

The symbol  $\hat{c}$  denotes the subdifferential operator (see Appendix A) and the subdifferentials  $\partial_{\Box} \mathbf{F}_{\mathbf{F}}[f(\boldsymbol{\sigma})]$  and  $\partial f(\boldsymbol{\sigma})$  are performed with respect to the relevant arguments.

The flow rule can then be written in terms of the convex yield functional  $f$  as follows:

$$
\dot{\mathbf{p}} \in N_C(\boldsymbol{\sigma}) \Leftrightarrow \dot{\mathbf{p}} \in \lambda \,\partial f(\boldsymbol{\sigma}),
$$

where the plastic multiplier  $\lambda$  fulfils the condition  $\lambda \in N_{\Re}$  [ $f(\boldsymbol{\sigma})$ ].

Note that the loading/unloading condition  $\lambda \in N_{\mathcal{R}^-}[f(\sigma)]$  is equivalent to the Kuhn-Tucker relations:

$$
\lambda \geqslant 0 \quad f(\pmb{\sigma}) \leqslant 0 \quad \lambda f(\pmb{\sigma}) = 0.
$$

Assuming a differentiable convex yield functional *j,* the flow rule can be written as follows:

New theory for elastic damage mode  
\n
$$
\dot{\mathbf{p}} = \lambda \, d f(\sigma) \Leftrightarrow \begin{cases} \dot{p} = \lambda \, d_{\sigma} f(\sigma, \chi) \\ \dot{\alpha} = -\lambda \, d_{\chi} f(\sigma, \chi) \end{cases}
$$

where  $\lambda \geq 0$ ,  $f(\sigma) \leq 0$  and  $\lambda f(\sigma) = 0$ .

#### *2.2. Damage model*

When a material becomes damaged, the stress at the subscale is redistributed to the undamaged material microbonds over the effective section of resistance. The true stresses corresponding to the undamaged material microbonds are then higher than the nominal stresses.

In the continuum damage mechanics the stress calculated over the effective area is called the *effective stress;* it has been first introduced by Kachanov (\ 956) and is the basis on which the elastoplasticity is coupled with damage.

The effective stress  $\hat{\sigma}$  can be related to the actual stress  $\sigma$  by means of an effectivestress operator *M,* depending on a damage parameter *D* which characterizes the state of damage of the material, in the form :

$$
\hat{\sigma}=M(D)\sigma.
$$

The operator *M* takes account of the area of the microvoids and microcracks, stress concentrations due to the microcracks and the interactions between neighbouring defects.

Since the mechanical behaviour of the microcracks depends on their orientation, damage is an anisotropic phenomenon. Nevertheless damage theories based on a scalar parameter are extensively used in the applications due to their simplicity on one side and their agreement with the experimental behaviour of real models on the other side. For example isotropic theories can be used for concrete up to a stress level which approximately coincides with the outset of major cracking (Lubliner *et al., 1989).*

The scalar formulation (Simo and Ju, 1987, Ju, 1989, Lemaitre and Chaboche, 1990, Hansen and Schreyer, 1994) is the most common model of damage. The damage parameter *D* reduces to a scalar damage parameter  $\delta_1 \in \mathcal{R}$  and hence the operator *M* is defined as  $1/(1-\delta_1)$ . Correspondingly the effective stress is given by:

$$
\hat{\sigma} = \frac{\sigma}{1-\delta_i},
$$

where the damage parameter  $\delta_1$  belongs to the interval [0,  $\delta_c$ ]. The scalar  $\delta_c$  is given and is assumed to belong to the interval ]0. 1[.

The value  $\delta_1 = 0$  corresponds to the undamaged material whereas a non-zero value  $\delta_1 \in ]0, \delta_c[$  corresponds to a damage state; the value  $\delta_1 = \delta_c < 1$  corresponds to the local rupture.

In this paper the scalar damage parameter  $\delta_1$  is considered as an internal kinematic variable which governs the state of damage. The related dual static internal variable is indicated as  $\xi_1 \in \mathbb{R}$  and describes the shift of the centre of the damage domain G. The expression of  $\xi_1$  will be derived in Section 2.4.

In analogy with the elastoplastic behaviour, we introduce the static damage variable  $\xi_2$ , belonging to the space  $Y'_2$ , which describes the shape and size of the damage surface. Note that  $\zeta_2$  is not a scalar variable so that anisotropic changes of the damage domain G can be accommodated in the proposed model.

The dual kinematic internal variable is denoted by  $\delta_2$  and belongs to the space  $Y_2$  dual of  $Y_2'$ . Its expression will be provided in Section 2.4 in terms of  $\zeta_2$ .

At this time the spaces associated with the plastic and damage variables will remain unspecified to allow the following framework to be applied to a large class of elastoplastic damage theories. For an explicit expression of the damage variables see, e.g. Simo and Ju (1987), Zhu and Cescotto (\995).

We can now collect two sets of internal variables for damage as follows:



Fig. 1. A one-dimensional example of: (a) Young function; (b) nonnegative monotone concave function.

**(b)**

 $\delta = (\delta_1, \delta_2)$   $\xi = (\xi_1, \xi_2)$ 

where the kinematic damage variable  $\delta$  belongs to the product space  $Y_a = \Re \times Y_2$  and the static damage variable  $\xi$  belongs to the dual space  $Y'_a = \Re \times Y'_a$ .

**In** a similar way to the arguments leading to the plastic dissipative potential, it can be assumed that there exists a surface which separates the damaging domain from the undamaging domain. Hence, to model the irreversibility of the damage behaviour, the existence of a damage convex domain G in the space  $Y_a$ , containing the origin in its interior, is postulated.

The damage criterion is thus expressed in terms of a damage mode  $g_1 : \mathbb{R} \mapsto \mathbb{R} \cup \{+\infty\}$ and of a nonnegative monotone concave function (current damage threshold)  $g_2: Y_2 \mapsto \mathfrak{R} \cup \{+\infty\}$ . The damage mode is assumed to be a Young function (see Appendix A), i.e., an extended real-valued function defined in [0,  $+ \infty$  [which is nonnegative monotone convex with  $g_1(0) = 0$ ; a one-dimensional example of  $g_1$  and  $g_2$  is given in Fig. 1. Accordingly, the damage domain is defined as the level set of  $g_1$  at the value  $g_2(\xi_2)$ :

$$
\mathbf{G} = \{ (\xi_1, \xi_2) \in \mathfrak{R} \times Y_2 : g_1(-\xi_1) \leq g_2(\xi_2) \},
$$

and turns out to be convex.

**(a)**

*Remark* 2.2. The assumption that  $g_1$  is a convex function defined in  $[0, +\infty)$  is not restrictive. **In** fact, the constitutive model developed in Section 2.4 will provide a nonpositive static damage internal variable  $\xi_1$  so that only the non-negative part of  $g_1$  is of interest.

2.2.1. *Damage flow rule.* To describe the growth and expansion of microcracks and damage surfaces, the evolution of the damage variable  $\delta$  must be specified.

We recall that the normal cone to the convex set G at the point  $\xi$  is given by:

$$
N_G(\xi) = \{\boldsymbol{\delta} \in Y_a : \langle \boldsymbol{\zeta} - \boldsymbol{\xi}, \boldsymbol{\delta} \rangle \leq 0 \quad \forall \boldsymbol{\zeta} \in \mathbf{G}\},
$$

and coincides with the subdifferential of the indicator of G at  $\xi$ :

$$
N_G(\xi) = \partial \Box_G(\xi).
$$

The evolution of the damage variables is provided by the normality rule to the set  $\mathbf{G}$ :

$$
\dot{\delta} \in N_G(\xi) = \partial \Box_G(\xi) \Leftrightarrow \xi \in \partial D_d(\dot{\delta})
$$

where  $D_d$  is the support functional of the damage domain  $G$ :

$$
D_d(\delta) = \sup \{ \langle \xi, \delta \rangle : \zeta \in G \}.
$$

Defining the damage function as  $g(\xi_1, \xi_2) = g_1(-\xi_1) - g_2(\xi_2)$ , the indicator of G can be written in terms of the damage function  $g$  as follows:

$$
\sqcup_G(\xi)=(\sqcup_{\Re} \cdot g)(\xi)
$$

where  $\mathfrak{R}^-$  represents the cone of the nonpositive scalars.

The former subdifferential rule, reported in Appendix A, allows us to perform the subdifferential of  $|\cdot|_G$  in the form:

$$
\partial \Box_G(\xi) = \partial \Box_{\mathfrak{R}^+}[g(\xi)] \partial g(\xi) = N_{\mathfrak{R}^+}[g(\xi)] \partial g(\xi).
$$

Hence the damage flow rule can be written in terms of a damage multiplier  $\mu$  as follows:

$$
\dot{\delta} \in N_G(\xi) \Leftrightarrow \dot{\delta} \in \mu \,\hat{c}g(\xi)
$$

where  $\mu \in N_{\mathfrak{R}^-}[g(\xi)]$ , that is:

$$
\mu \geq 0
$$
  $g(\xi_1, \xi_2) \leq 0$   $\mu g(\xi_1, \xi_2) = 0$ 

which represent the damage loading/unloading conditions.

The above conditions ensure that no further damage takes place if  $g(\xi_1, \xi_2) < 0$  since it turns out to be  $\mu = 0$  and hence  $\dot{\delta} = 0$ . If, on the contrary,  $q(\xi_1, \xi_2) = 0$  the damage multiplier  $\mu$  can be nonvanishing and damage phenomena can occur.

Resorting to the additivity of the subdifferential, the flow rule can be rewritten as follows:

$$
\dot{\delta} \in \mu \, \partial g(\xi) \Leftrightarrow \begin{cases} \dot{\delta}_1 \in \mu \, \partial g_1(-\xi_1) \\ \dot{\delta}_2 \in -\mu \, \partial g_2(\xi_2). \end{cases}
$$

Note that the same symbol  $\hat{c}$  is used to define both the subdifferential of a convex functional and the superdifferential of a concave one.

*Remark* 2.3. For any pair  $(\dot{\delta}, \xi)$  which fulfils the damage flow rule  $\dot{\delta} \in N_G(\xi)$  the following equality holds:

$$
\sqcup_G(\boldsymbol{\xi})+D_d(\boldsymbol{\delta})=D_d(\boldsymbol{\delta})=\prec\boldsymbol{\xi},\boldsymbol{\delta}\succ
$$

being zero the indicator of G since  $\xi$  belongs to the damage domain. Hence, we can give the following expression for  $D_d$ :

$$
D_d(\dot{\boldsymbol{\delta}}) = \sup \{ \langle \boldsymbol{\zeta}, \dot{\boldsymbol{\delta}} \rangle : \boldsymbol{\zeta} \in \mathbb{G} \} = \langle \boldsymbol{\zeta}, \dot{\boldsymbol{\delta}} \rangle.
$$

Thus the functional  $D_d$  has the mechanical meaning of damage dissipation and the equality above represents the *principle oj" the maximum damage dissipation.*

If the origin of the space  $Y_a$  belongs to the interior of G, it can be proved that the dissipation  $D_d$  turns out to be nonnegative following similar argumentations to the one reported in Romano *et al.* (1993a) for the plastic behaviour. •

The damage model developed in this section allows us to consider a tensorial variable

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 $\xi_2$  which can describe anisotropic change of the damage domain G. A fully anisotropic damage model in which  $\delta_1$  is a tensorial variable is the subject of further studies.

It is worth noting that the treatment, and in consequence the computational algorithm, which will be developed in this paper does not depend upon the scalar or tensorial nature of the damage variable  $\xi_2$ . The computational algorithm can thus be specialized in the case of a scalar or tensorial variable  $\xi_2$  as shown in Section 4.

The damage model coupled with plasticity is developed in the next section.

## *2.3. Coupled elastoplastic damage model*

Local stresses for a damaged material are redistributed to the undamaged microbounds so that the stresses effectively acting on the undamaged material turn out to be higher than the nominal stresses. Hence it appears reasonable to assume that the plastic flows occur only in the undamaged part of the material by means of effective stresses  $\hat{\sigma} = M\sigma$  and static internal variables  $\hat{\gamma} = M\gamma$ .

Let us denote by  $\hat{\sigma}$  the effective stress given by:

$$
\hat{\boldsymbol{\sigma}} = (\hat{\sigma}, \chi) = M(\sigma, \chi) = M \boldsymbol{\sigma}.
$$

The yield criterion defines the current yield surface in terms of the effective stresses. Accordingly a convex yield functional  $\hat{f}: \mathscr{S}_a \mapsto \Re \cup \{+\infty\}$  is introduced so that the elastic domain  $\hat{C}$  is provided in terms of the effective stresses  $\hat{\sigma}$  as follows:

$$
\mathbf{\hat{C}} = {\mathbf{\hat{\sigma}} \in \mathscr{S}_a : \hat{f}(\mathbf{\hat{\sigma}}) \leq 0}.
$$

*Remark* 2.4. The presence of the effective stress  $\hat{\sigma}$  in the definition of the elastic domain has the effect of lowering the limit plastic strength of the material. •

2.3.1. *The normality rule.* Assuming a standard behaviour, the plastic flow **p** belongs to the normal cone to the elastic domain  $\tilde{C}$  at the point  $\hat{\sigma}$ :

$$
\dot{\mathbf{p}} \in N_{\mathcal{C}}(\hat{\boldsymbol{\sigma}}) = \partial \Box_{\mathcal{C}}(\hat{\boldsymbol{\sigma}}) \Leftrightarrow \hat{\boldsymbol{\sigma}} \in \partial \hat{D}_p(\dot{\mathbf{p}}),
$$

where  $\hat{D}_p$  is the support functional of the elastic domain expressed in terms of the effective stresses:

$$
\hat{D}_n(\dot{\mathbf{p}}) = \sup \{ \langle \hat{\tau}, \dot{\mathbf{p}} \rangle : \hat{\tau} \in \hat{\mathbf{C}} \} = \langle \hat{\boldsymbol{\sigma}}, \dot{\mathbf{p}} \rangle.
$$

The value of  $\hat{D}_p(\mathbf{p})$  represents the plastic dissipation associated with the flow  $\mathbf{\dot{p}}$ ; the equality above yields the *principle of the maximum plastic dissipation* in the effective stress space.

As in the plastic case, the dissipation  $\hat{D}_p$  turns out to be nonnegative if the null stress belongs to the interior of  $\hat{C}$ .

The associative flow rule above for the coupled elastoplastic damage model is formulated in terms of effective stresses; actually it can be equivalently stated in terms of actual stresses *a.*

In fact we preliminarily note that the yield functional can be written in terms of  $\sigma$  by virtue of the following equalities:

$$
\hat{f}(\hat{\boldsymbol{\sigma}}) = \hat{f}(M\boldsymbol{\sigma}) = (\hat{f} \cdot M)(\boldsymbol{\sigma}) = f(\boldsymbol{\sigma}),
$$

since the effective stress  $\hat{\sigma}$  is related to the actual stress  $\sigma$  by means of the relation  $\hat{\sigma} = M\sigma$ .

Accordingly, effective stresses  $\hat{\sigma}$  which belong to the effective elastic domain  $\hat{C}$  are such that the related actual stresses  $\sigma$  belong to the elastic domain C.

Hence, the normal cone (or equivalently the subdifferential of the indicator) to the elastic domain  $\hat{C}$  at a point  $\hat{\sigma}$  becomes:

$$
N_{\hat{C}}(\hat{\boldsymbol{\sigma}}) = N_{C}(M^{-1}\hat{\boldsymbol{\sigma}}) = \partial_{\square}{}_{C}(M^{-1}\hat{\boldsymbol{\sigma}}) = (M^{-1})'N_{C}(\boldsymbol{\sigma}),
$$

where the second chain rule and the equality between the normal cone and the subdifferential of  $C$  at  $\sigma$ , reported in Appendix A, have been invoked.

The term  $(M^{-1})' = 1 - \delta_1$  turns out to be positive so that the cone  $N_c(\sigma)$  does not change if it is multiplied for  $(1-\delta_1)$ , i.e.,  $(1-\delta_1)N_C(\sigma) = N_C(\sigma)$ . Hence, the flow rule for the elastoplastic damage behaviour can be written in terms of the actual stresses as follows:

$$
\dot{\mathbf{p}} \in N_{\mathcal{C}}(\hat{\boldsymbol{\sigma}}) \Leftrightarrow \dot{\mathbf{p}} \in N_{\mathcal{C}}(\boldsymbol{\sigma}).
$$

Note that this coupled elastoplastic damage model has two dissipation criteria, one for the elastoplastic and the other for the damage behaviour which are expressed by means of the two functionals  $D_p$  and  $D_q$ .

#### *2.4. The free energy*

The Clausius-Duhem inequality can impose conditions on the forms of the constitutive relations for the material of which the body is composed. Following the rules of the thermodynamic of irreversible processes, the forces associated with the kinematic variables can be determined by using the well-known strategy of Coleman and Noll (1963).

In purely mechanical theory, as the one considered in this paper, no internal heat generation sources and heat fluxes are considered. Accordingly the explicit recourse to the thermodynamic of irreversible processes can be avoided in developing the constitutive model.

The static variables can be provided in terms of the derivatives of the free energy with respect to the related dual variables. In particular, stresses  $\sigma$  and static internal variables  $\chi$ can be obtained by deriving the free energy with respect to the elastic strains  $e$  and kinematic internal variables x. Analogously the static damage variables ( $\xi_1, \xi_2$ ) are obtained by deriving the free energy with respect to the pair of kinematic variables  $(\delta_1, \delta_2)$ .

Further, the plastic and damage dissipations  $D<sub>p</sub>$  and  $D<sub>d</sub>$  turn out to be nonnegative by assuming that the null stress  $\sigma$  and the null damage static internal variable  $\xi$  belong, respectively, to the interior of the convex domains C and G at the beginning of the load history. Thus the second law of the thermodynamics is fulfilled.

Let  $\psi : \mathscr{D} \mapsto \mathfrak{R} \cup \{ +\infty \}$  be the convex elastic energy and  $\pi : X \mapsto \mathfrak{R} \cup \{ +\infty \}$  be a convex functional which accounts for the hardening phenomena.

The elastic energy  $\psi$ , the hardening functional  $\pi$  and the damage variable  $\delta_1$  are collected in the functional  $k : \mathfrak{R} \times \mathcal{D} \times X \mapsto \bar{\mathfrak{R}}$  (where  $\bar{\mathfrak{R}} = \{-\infty\} \cup \mathfrak{R} \cup \{+\infty\}$ ) in such a way that it turns out to be convex in  $(e, x)$  and concave in  $\delta_1$ . Moreover, we consider a positive definite damage operator  $A: Y_2 \mapsto Y'_2$ .

The free energy  $\Phi: Y_a \times \mathcal{D}_a \mapsto \bar{\Re}$  is then the saddle (concave-convex) functional given by:

$$
\Phi(\delta_1, \delta_2, e, \alpha) = k(\delta_1, e, \alpha) - \frac{1}{2} \langle A \delta_2, \delta_2 \rangle.
$$

In particular, the free energy  $\Phi$  turns out to be convex in  $\mathbf{e} = (e, \alpha)$  and concave in  $\mathbf{\delta} = (\delta_1, \delta_2)$ .

*Remark* 2.5. In most of the elastoplastic ductile damage models see, e.g., Simo and Ju (1987), Lemaitre and Chaboche (1990), Hansen and Schreyer (1994), the damage variable  $\delta_1$  is associated only with the elastic strain energy  $\psi$ . Experimental evidences show, on the contrary, that plasticity gives a significant contribution to the initiation and growth of microcracks. Accordingly, to couple plasticity and damage, the following expression for the saddle functional *k* is assumed:

$$
k(\delta_1, e, \alpha) = \begin{cases} (1 - \delta_1)[\psi(e) + \pi(\alpha)] & \text{if } \delta_1 \in J \\ -\infty & \text{otherwise} \end{cases}
$$

where  $J = [0, \delta_c]$  and  $\psi$  is the elastic energy for the undamaged material.

The form of the free energy assumes an additive decomposition into a stored elastic and hardening energy term multiplied for a damaging variable and a quadratic form related to the anisotropic change of the damage domain. This formulation is used by others because it is still fairly general to encompass many constitutive models but not so abstract that the computational algorithm becomes overly complicated.

The constitutive relations can thus be obtained by deriving the free energy:

$$
(\xi,\sigma)=d\Phi(\delta,e),
$$

or equivalently:

$$
\begin{cases}\n\boldsymbol{\sigma} = d_e \Phi(\boldsymbol{\delta}, \mathbf{e}) \\
\boldsymbol{\xi} = d_{\boldsymbol{\delta}} \Phi(\boldsymbol{\delta}, \mathbf{e})\n\end{cases}\n\Rightarrow\n\begin{cases}\n\sigma = (1 - \delta_1) d\psi(e) \\
\chi = (1 - \delta_1) d\pi(\alpha) \\
\zeta_1 = -[\psi(e) + \pi(\alpha)] \\
\zeta_2 = -A \delta_2\n\end{cases}
$$

if  $\delta_1$  belongs to the set J.

*Remark* 2.6. The static internal variable  $\xi_1$ , conjugate with the kinematic variable  $\delta_1$ , coincides with the opposite of the sum of the elastic free energy  $\psi$  and the hardening functional  $\pi$ . Hence plasticity and damage are directly coupled.

The expressions of the constitutive potentials are left purposely unspecified. Accordingly the solution algorithm can be developed in a general form which can be applied to a wide class of elastoplastic damage theories by suitably specifying the potentials for the problem at hand. The specialization of the proposed algorithm to the one developed by Ju (1989) is provided at the end of Section 3.

It is worth noting that most of the damage theories have phenomenological origin and are based either on the principle of *equiralenf strains* (Lemaitre and Chaboche, 1990) or on the principle of *equiralenf elasfie energy* (Cordebois and Sidoroff. 1979).

On the contrary. neither the principle of equivalent strains nor the principle of equivalent elastic energy are explicitly imposed at the very beginning of this model as an additional hypothesis.

*Remark* 2.7. The expression of the stress  $\sigma$  derived from the previously defined free energy  $\Phi$  coincides with the stress obtained by postulating the principle of the equivalent strains.

In fact the undamaged elastic energy for a linear clastic behaviour is given by the quadratic form  $\psi(e) = 1/2 \langle E_e e, e \rangle$  so that the actual stress  $\sigma$  turns out to be:

$$
\sigma = (1 - \delta_1) E_o e = E e
$$

where  $E = (1 - \delta_1)E_0$  is the damaged elastic stiffness.

Hence the assumed form of the free energy provides the expressions of the stress  $\sigma$  and of the damaged elastic stiffness  $E$  which coincide with the relevant ones derived from the principle of the equivalent strains. •

*Remark* 2.8. Assuming a different expression of the saddle functional *k.* we can provide a model in which the damage elastic stiffness E coincides with the one derived according to

thc principle of the equivalent elastic energy. Accordingly the following expression *k* has to be considered:

$$
k(\delta_1, e, \alpha) = \begin{cases} (1 - \delta_1)^2 [\psi(e) + \pi(\alpha)] & \text{if } \delta_1 \in J \\ +\infty & \text{otherwise.} \end{cases}
$$

Provided that the elastic energy  $\psi$  and the hardening potential  $\pi$  are nonnegative, the functional *k* is convex in  $(\delta_1, e, \alpha)$ .

For a linear elastic behaviour, if  $\delta_1 \in J$ , the actual stress  $\sigma$  turns out to be:

$$
\sigma = d_e k(\delta_1, e, \alpha) = (1 - \delta_1)^2 E_e e = E e
$$

where  $E = (1 - \delta_1)^2 E_0$  is the damaged elastic stiffness.

It is then immediate to prove that the elastic energy expressed in terms of the effective stress  $\hat{\sigma}$  and of the undamaged elastic stiffness  $E_{\sigma}$  coincides with the elastic energy expressed in terms of the actual stress  $\sigma$  and of the damaged elastic stiffness E (principle of the equivalent elastic energy),

Further, in this case, the static internal variable  $\xi_1$  is given by:

$$
\xi_1 = d_{\delta_1} k(\delta_1, e, \alpha) = -2(1 - \delta_1)[\psi(e) + \pi(\alpha)]
$$

and the damage variable  $\zeta_1$  depends on the kinematic internal variable  $\delta_1$ , the elastic free energy  $\psi$  and the hardening functional  $\pi$ .

For sake of clearness we report hereafter both the principles of the equivalence of the strain and of the elastic energy.

*2.4.1. Principle olequiwlent strains.* The principle of the equivalent strains was introduced by Lemaitre, see Lemaitre and Chaboche (1990). This principle states that the strain associated with a damaged state under the applied stress is equivalent to the strain associated with its undamaged state under the effective stress.

In essence, it requires that the effective material behaviour is represented in the effectivestress space and in the actual-strain space. Accordingly, the expressions of  $\hat{\sigma}$  in terms of  $\epsilon$ and of the damage elastic operator *E* are:

$$
\hat{\sigma} = E_o e \qquad E = M^{-1} E_o
$$

where  $E<sub>o</sub>$  denotes the elastic operator in the undamaged state.

For the isotropic damage model the damage elastic operator is :

$$
E = (1 - \delta_1) E_a.
$$

*2.4.2. Principle ole(juivalent elastic energy.* The principle of equivalent elastic energy was introduced by Cordebois and Sidoroff (1979) and states that the complementary elastic energy of the damaged material is the same as that of an undamaged material except that the stress is replaced by the effective stress.

The complementary elastic energy  $\varphi^*$  can then be written as follows:

$$
\varphi^*(\sigma) = \frac{1}{2} \langle \hat{\sigma}, E_{\sigma}^{-1} \hat{\sigma} \rangle = \frac{1}{2} \langle \sigma, E^{-1} \sigma \rangle.
$$

Hence, recalling that  $\hat{\sigma} = M\sigma$ , the expression of the damage elastic operator *E* is:

$$
E = M^{-1} E_{\sigma} M^{\prime -1}.
$$

and, in the scalar case, it becomes:

$$
E = (1 - \delta_1)^2 E_o.
$$

Note that the effective stress derived according to the principle of equivalent strains turns out to be higher than the relevant effective stress derived from the principle of equivalent elastic energy (Hansen and Schreyer, 1994).

## 3. VARIATIONAL PRINCIPLES

The evolutive constitutive model is reported in the following box:

$\varepsilon = \mathbf{e} + \mathbf{p}$	additivity of strains
$\dot{\mathbf{p}} \in N_C(\boldsymbol{\sigma})$	plastic flow rule
$\dot{\delta} \in N_G(\xi)$	damage flow rule
$\sigma = d_{\rho} \Phi(\delta, e)$	elastic relation
$\xi = d_{\delta} \Phi(\delta, \mathbf{e})$	damage relation

Box I. The evolutive constitutive model

The evolutive analysis of a non-linear elastoplastic constitutive problem with damage can be performed by solving a sequence of problems in which the strain increment is applied and updating the state variables at the end of each increment (Simo *et al.,* 1989, Reddy and Martin, 1991).

Attention is focused on a single step of the procedure for which the strain increment is given. Accordingly we need to evaluate the finite increments of the unknown variables corresponding to the increment of strain when their values are assigned at the beginning of the step. Let  $(\cdot)$  denote the known quantities  $(\cdot)$  as the beginning of each step.

Adopting a fully implicit time integration scheme (Euler backward difference), the finite-step formulation of the elastoplastic constitutive model with damage is achieved by enforcing the relations of the model. The plastic and damage flow rules are enforced at the end of the step in the form:

$$
\mathbf{p} - \mathbf{p}_o \in N_C(\boldsymbol{\sigma}), \quad \delta - \delta_o \in N_G(\boldsymbol{\xi})
$$

where the time derivative  $\dot{\rho}$  and  $\dot{\delta}$  have been replaced by the relevant finite increment ratios and the time increment has been neglected being  $N<sub>C</sub>$  and  $N<sub>G</sub>$  convex cones.

In view of the variational formulation of the constitutive model. the plastic flow rule is more conveniently expressed in terms of the dissipation  $D_p$  in the form:

$$
\sigma\in \partial D_p(\mathbf{p}-\mathbf{p}_o).
$$

Hence the finite-step constitutive model with damage and plasticity is summarized in the next box:

$\varepsilon = e + p$	additivity of strains
$\sigma \in \partial D_{p}(\mathbf{p}-\mathbf{p}_{o})$	plastic rule
$\delta \in \delta_o + \partial \Box_G(\xi)$	damage rule
$\sigma = d_{\rho}\Phi(\delta, e)$	elastic relation
$\xi = d_{\delta}\Phi(\delta, \mathbf{e})$	damage relation

Box 2. The finite-step constitutive model

To derive the variational formulations for the elastoplastic constitutive model above the related operator form has to be built up. Defining the product space  $2 = \mathcal{S}_a$ 

 $x \mathscr{D}_a x \mathscr{D}_a x Y_a \times Y'_a$  and its dual  $\mathscr{Q}' = \mathscr{D}_a x \mathscr{S}_a x \mathscr{S}_a x Y'_a \times Y'_a$ , the operator form of the constitutive problem, for a given total strain *e,* is:

 $0 \in \mathbf{A}(q) + \hat{q}$ 

where  $q, \hat{q} \in \mathcal{Q}$  and  $\mathbf{A} : \mathcal{Q} \mapsto \mathcal{Q}'$  is the multivalued constitutive operator. Explicitly it is written as follows:



The conservativity of  $A$  can be proved by noting that  $A$  is built up by a linear symmetric and hence conservative operator, by the derivative  $d\Phi$ , by the multi-valued operators  $\partial D_n$ and  $\partial_{\Box G}$  which are conservative according to the integral theorem presented in Romano *et al.* (1993d). The potentials of  $\partial D_p$  and  $\partial \Box_G$  are given by  $D_p$  and  $\Box_G$ , respectively.

The potential of the multivalued finite-step constitutive model of box 2 can be given by a direct integration of **A** along a straight line in the space 2 and turns out to be:

$$
\Sigma(\sigma, \mathbf{p}, \delta, \mathbf{e}, \xi) = \Phi(\delta, \mathbf{e}) + D_n(\mathbf{p} - \mathbf{p}_n) + \bigsqcup_G (\xi) - \langle \sigma, \mathbf{e} + \mathbf{p} \rangle + \langle \sigma, \mathbf{e} \rangle - \langle \xi, \delta - \delta_n \rangle
$$

which is convex in  $(e, p, \xi)$ , concave in  $\delta$  and linear in  $\sigma$ . The potential  $\Sigma$  assumes finite values if the damage variable  $\delta$  belongs to the set  $V = [0, \delta_c] \times Y_2$ .

Hence it is:

*Proposition* 1. For a given  $\varepsilon$ , a vector  $(\sigma, \rho, \delta, e, \xi)$  is a solution of the elastoplastic damage constitutive model reported in box 2 if and only if it is a saddle point of the potential  $\Sigma$ .

From the computational standpoint it is useful to derive a variational principle in  $(\sigma, \delta)$  since it provides the variational basis to perform the elasto-plastic-damage return mapping.

## 3.1. *The variational principle in*  $(\sigma, \mathbf{p}, \delta, \xi)$

Let us first derive an intermediate potential in the four state variables ( $\sigma$ ,  $\rho$ ,  $\delta$ ,  $\xi$ ). The starting point is the potential  $\Sigma$  in which the elastic strain e has to be eliminated from the set of independent state variables.

To this end the elastic relation:

$$
\boldsymbol{\sigma} = d_e \boldsymbol{\Phi}(\boldsymbol{\delta}, \mathbf{e})
$$

must be written in terms of a unique relation involving the free energy  $\Phi$ , its associated convex functional  $\Xi: Y_a \times \mathcal{S}_a \mapsto \Re \cup \{+\infty\}$  and the virtual work between the dual variables  $(e, \sigma)$ .

The equivalence (ii) reported in the box A.2 of Appendix B involving the partial subdifferential of a saddle functional can thus be rewritten in terms of  $\Phi$  and  $\Xi$  as follows:

$$
\sigma = d_{\rho} \Phi(\delta, \mathbf{e}) \Leftrightarrow \Xi(\delta, \sigma) + \Phi(\delta, \mathbf{e}) = \langle \sigma, \mathbf{e} \rangle,
$$

for any  $\delta_1 \in J$ .

Substituting the equality above in the expression of the potential  $\Sigma$  it results:

$$
\Sigma_1(\pmb\sigma,\mathbf{p},\pmb\delta,\xi)=-\Xi(\pmb\delta,\pmb\sigma)+D_p(\mathbf{p}\!-\!\mathbf{p}_o)+\sqcup_G(\xi)\!-\!\prec\!\pmb\sigma,\mathbf{p}\!\succ\!+\!\prec\!\pmb\sigma,\varepsilon\!\succ\!-\!\prec\!\xi,\pmb\delta\!-\!\pmb\delta_o\!\!>
$$

which is concave in the pair  $(\sigma, \delta)$  and convex in  $(p, \xi)$ . Accordingly it can be stated:

*Proposition* 2. For a given  $\varepsilon$ , a vector  $(\sigma, \rho, \delta, \xi)$  is a solution of the elastoplastic damage constitutive model reported in the box 2 if and only if it is a saddle point of the potential  $\Sigma_1$ .

To explicitly prove that the stationary condition of the saddle functional  $\Sigma_1$  yields back the constitutive model reported in box 2, let us assume that a quartet  $(\sigma, \mathbf{p}, \delta, \xi)$  be a stationary point of  $\Sigma_1$ , i.e.,

$$
(0,0,0,0) \in \widehat{c} \Sigma_1(\sigma, p, \delta, \xi).
$$

The stationary condition above can then be rewritten as follows:

$$
\begin{cases}\n(\mathbf{0},\mathbf{0}) = d_{(\delta,\sigma)}\Sigma_1(\sigma,\mathbf{p},\delta,\xi) \Leftrightarrow \begin{bmatrix} -\xi \\ \varepsilon-\mathbf{p} \end{bmatrix} = d\Xi(\delta,\sigma) \\
(\mathbf{0},\mathbf{0}) \in \partial_{(\rho,\xi)}\Sigma_1(\sigma,\mathbf{p},\delta,\xi) \Leftrightarrow \begin{cases} \sigma \in \partial D_p(\mathbf{p}-\mathbf{p}_o) \\
\delta - \delta_o \in \partial_{\Box(\sigma)}(\xi)\n\end{cases}\n\end{cases}
$$

Hence, there exists an elastic strain  $\mathbf{e} = \mathbf{\varepsilon} - \mathbf{p}$  such that:

$$
(-\xi, \mathbf{e}) = d\Xi(\delta, \sigma).
$$

This condition is equivalent to the elastic and damage relations in terms of the free energy  $\Phi$ ; in fact the equivalence between the relations (a) and (c) of the box A.1 in the Appendix B allows us to write:

$$
(-\xi, \mathbf{e}) = d\Xi(\delta, \sigma) \Leftrightarrow (\xi, \sigma) = d\Phi(\delta, \mathbf{e}).
$$

Further, the stationary condition with respect to the pair ( $\mathbf{p}, \xi$ ) yields the plastic flow rule, expressed in terms of the plastic dissipation  $D<sub>p</sub>$ , and the damage flow rule.

The converse implication follows by reverting the steps above.

*Remark* 3.9. The expression of the jointly convex functional  $\Xi$  associated with the saddle free energy  $\Phi$  can be derived in accordance with the results established in Appendix B.

Then the functional  $\Xi$  is given by (see Appendix C for the proof):

 $\Xi(\delta, \sigma) = \sup_{e} {\{<\sigma, e>- \Phi(\delta, e)\}}$ 

$$
= \begin{cases} \frac{1}{2} \langle A\delta_2, \delta_2 \rangle + (1 - \delta_1) \left[ \psi^* \left( \frac{\sigma}{1 - \delta_1} \right) + \pi^* \left( \frac{\chi}{1 - \delta_1} \right) \right] & \text{if } \delta_1 \in J \\ +\infty & \text{otherwise} \end{cases}
$$

•

*Remark* 3.10. The derivative of  $\Xi$  with respect to  $\delta$  and  $\sigma$  can now be explicitly performed in order to obtain the relation between the pairs of state variables ( $-\xi$ , e) and  $(\delta, \sigma)$ .

The derivative of  $\Xi$  with respect to  $\delta_1$ , if  $\delta_1 \in J$ , is:

$$
d_{\delta_1} \Xi(\delta_1, \delta_2, \sigma, \chi) = -\left[\psi^*\left(\frac{\sigma}{1-\delta_1}\right) + \pi^*\left(\frac{\chi}{1-\delta_1}\right)\right] + (1-\delta_1)\left[\left\langle d_{\delta_1} \frac{\sigma}{1-\delta_1}, d\psi^*\left(\frac{\sigma}{1-\delta_1}\right)\right\rangle + \left\langle d_{\delta_1} \frac{\chi}{1-\delta_1}, d\pi^*\left(\frac{\chi}{1-\delta_1}\right)\right\rangle\right] = -\left[\psi^*\left(\frac{\sigma}{1-\delta_1}\right) + \pi^*\left(\frac{\chi}{1-\delta_1}\right)\right] + \left\langle \frac{\sigma}{1-\delta_1}, d\psi^*\left(\frac{\sigma}{1-\delta_1}\right)\right\rangle + \left\langle \frac{\chi}{1-\delta_1}, d\pi^*\left(\frac{\chi}{1-\delta_1}\right)\right\rangle.
$$

Note that the symbol *d* without any subscript means the derivative with respect to the argument of the functional which it is applied to.

At this point the constitutive model derived in Section 2.4 shows that the elastic energy  $\psi$  and the hardening functional  $\pi$  link together the pairs  $\{e, \sigma/(1 - \delta_1)\}$  and  $\{\alpha, \chi/(1 - \delta_1)\}.$ Hence, the following Fenchel's equivalences hold:

$$
\sigma = (1 - \delta_1)d\psi(e) \Leftrightarrow e = d\psi^* \left(\frac{\sigma}{1 - \delta_1}\right) \qquad \chi = (1 - \delta_1)d\pi(\alpha) \Leftrightarrow \alpha = d\pi^* \left(\frac{\chi}{1 - \delta_1}\right)
$$

which yields the Fenchel's equalities:

$$
\psi(e) + \psi^* \left( \frac{\sigma}{1 - \delta_1} \right) = \left\langle \frac{\sigma}{1 - \delta_1}, e \right\rangle \qquad \pi(\alpha) + \pi^* \left( \frac{\chi}{1 - \delta_1} \right) = \left\langle \frac{\chi}{1 - \delta_1}, \alpha \right\rangle
$$

so that the expression of  $d_{\delta_1} \Xi$  becomes:

$$
d_{\delta_1} \Xi(\delta_1, \delta_2, \sigma, \chi) = -\psi^* \left( \frac{\sigma}{1-\delta_1} \right) - \pi^* \left( \frac{\chi}{1-\delta_1} \right) + \left\langle \frac{\sigma}{1-\delta_1}, e \right\rangle + \left\langle \frac{\chi}{1-\delta_1}, \chi \right\rangle = \psi(e) + \pi(\chi).
$$

The derivative of  $\Xi$  with respect to  $\delta_2$ , if  $\delta_1 \in J$ , is:

$$
d_{\delta_2} \Xi(\delta_1, \delta_2, \sigma, \chi) = A \, \delta_2,
$$

and the derivatives of  $\Xi$  with respect to  $\sigma$  and  $\chi$ , if  $\delta_1 \in J$ , are:

$$
d_{\sigma}\Xi(\delta_1,\delta_2,\sigma,\chi)=d\psi^*\left(\frac{\sigma}{1-\delta_1}\right)\ d_{\chi}\Xi(\delta_1,\delta_2,\sigma,\chi)=d\pi^*\left(\frac{\chi}{1-\delta_1}\right).
$$

Hence it results:

$$
(-\xi, \mathbf{e}) = d\Xi(\delta, \sigma) \Leftrightarrow \begin{bmatrix} -\xi_1 \\ -\xi_2 \\ e \\ \alpha \end{bmatrix} = \begin{bmatrix} \psi(e) + \pi(\alpha) \\ A\delta_2 \\ d\psi^* \left( \frac{\sigma}{1 - \delta_1} \right) \\ d\pi^* \left( \frac{\chi}{1 - \delta_1} \right) \end{bmatrix}
$$

and the constitutive relations of the elastoplastic model with damage are recovered. •

# 3.2. *The variational principle in*  $(\sigma, \delta, \xi)$

In order to derive from the potential  $\Sigma_1$  the saddle potential  $\Sigma_2$  which depends on the state variables  $(\sigma, \delta, \xi)$ , it is necessary to enforce the plastic flow rule in terms of Fenchel's equality:

$$
\sigma\!\in\!\hat{c}D_p(\mathbf{p}\!-\!\mathbf{p}_o)\Leftrightarrow D_p(\mathbf{p}\!-\!\mathbf{p}_o)\!+\!\sqcup_{\substack{c}}(\sigma)=\prec\!\sigma,\mathbf{p}\!-\!\mathbf{p}_o\!\succ.
$$

Substituting the equality at the right hand side above in the expression of the potential  $\Sigma_1$ , we have the following:

*Proposition* 3. For a given  $\varepsilon$ , a vector  $(\sigma, \delta, \xi)$  is a solution of the following saddle problem

$$
\min_{\xi} \max_{(\sigma,\delta)} \Sigma_2(\sigma,\delta,\xi)
$$

with:

$$
\Sigma_2(\boldsymbol{\sigma},\boldsymbol{\delta},\boldsymbol{\xi})=-\Xi(\boldsymbol{\delta},\boldsymbol{\sigma})-\sqcup_{C}(\boldsymbol{\sigma})+\sqcup_{G}(\boldsymbol{\xi})-\prec\boldsymbol{\sigma},\mathbf{p}_o\rangle+\prec\boldsymbol{\sigma},\boldsymbol{\epsilon}\rangle-\prec\boldsymbol{\xi},\boldsymbol{\delta}-\boldsymbol{\delta}_o\rangle
$$

if and only if it is a solution of the elastoplastic damage constitutive model reported in box  $\Box$ 2.  $\Box$ 

The constitutive model associated with a saddle point of the potential  $\Sigma_2$  can be obtained by enforcing the condition:

$$
\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \in \partial \Sigma_2 (\sigma, \delta, \xi) \Leftrightarrow \begin{cases} \begin{bmatrix} 0 \\ 0 \end{bmatrix} \in -d \Xi(\delta, \sigma) + \begin{bmatrix} -\xi \\ -\partial \Box_C(\sigma) - \mathbf{p}_o + \varepsilon \end{bmatrix} \\ 0 \in \partial \Box_G(\xi) + (\delta - \delta_o) \end{cases}
$$

Explicitly it can be written:

$$
\begin{cases} \boldsymbol{\xi} = -d_{\delta} \boldsymbol{\Xi}(\boldsymbol{\delta}, \boldsymbol{\sigma}) \\ \varepsilon - \mathbf{p}_{\sigma} - d_{\sigma} \boldsymbol{\Xi}(\boldsymbol{\delta}, \boldsymbol{\sigma}) \in \widehat{c}_{\square C}(\boldsymbol{\sigma}) \\ \boldsymbol{\delta} - \boldsymbol{\delta}_{\sigma} \in \widehat{c}_{\square C}(\boldsymbol{\xi}). \end{cases}
$$

The relations above show that the static damage internal variable  $\xi$  can be dropped from the constitutive model by substituting the argument of the indicator of  **with the** expression of  $\xi$  provided by the first relation.

The related variational formulation can be derived starting from the potential  $\Sigma_2$  and is shown hereafter.

#### 3.3. The *rariational principle in*  $(\sigma, \delta)$

The static damage internal variable can be eliminated from the set of independent variables by assuming that the static damage internal variable  $\xi$  and the increment of the kinematic damage internal variable  $\delta - \delta_o$  fulfils the damage relation:

$$
(\boldsymbol{\delta}-\boldsymbol{\delta}_{o})\in\hat{c}\bigsqcup_{G}(\boldsymbol{\xi})\Leftrightarrow\bigsqcup_{G}(\boldsymbol{\xi})+D_{d}(\boldsymbol{\delta}-\boldsymbol{\delta}_{o})=\langle\boldsymbol{\xi},\boldsymbol{\delta}-\boldsymbol{\delta}_{o}\rangle.
$$

Introducing the r.h.s. of the equivalence above in the expression of the potential  $\Sigma_2$  we have the following:

*Proposition* 4. For a given  $\varepsilon$ , a vector  $(\sigma, \delta)$  is a solution of the following concave problem

$$
\max_{(\sigma,\delta)}\Sigma_3(\pmb{\sigma},\pmb{\delta})
$$

with:

$$
\Sigma_3(\boldsymbol{\sigma},\boldsymbol{\delta})=-\Xi(\boldsymbol{\delta},\boldsymbol{\sigma})-\textstyle{\bigsqcup_{\mathcal{C}}}\boldsymbol{\sigma}-D_d(\boldsymbol{\delta}-\boldsymbol{\delta}_a)-\textstyle{\prec \sigma, \mathbf{p}_a \succ+\textstyle{\prec \sigma, \epsilon}}>
$$

if and only if it is a solution of the elastoplastic damage constitutive model reported in box 2.

*Remark* 3.11. The functional  $\Sigma$ <sub>3</sub> is the generalization to the elastoplastic damage constitutive model of the finite-step counterpart of the Prager-Hodge principle limited to its constitutive part (Koiter, 1960). **In** fact in the absence of damage it turns out to be:

$$
\Sigma_{31}(\pmb{\sigma}) = -\Phi_{c}^{*}(\pmb{\sigma}) - \bigsqcup_{\mathcal{C}} (\pmb{\sigma}) - \text{diag}_{c} \pmb{\sigma}, \pmb{\mu}_{c} \text{diag}_{c} + \text{diag}_{c} \pmb{\sigma}
$$

where  $\Phi_e^*(\sigma) = \Xi(0,\sigma) = \psi^*(\sigma) + \pi^*(\chi)$ .

Moreover, assuming an elastic behaviour. no internal variables are necessary so that it results:

$$
\Sigma_{32}(\sigma) = -\psi^*(\sigma) + \langle \sigma, \varepsilon \rangle
$$

which is the well-known complementary elastic potential limited to the constitutive model.

The constitutive model associated with a maximum point of the potential  $\Sigma_3$  can be obtained by enforcing the stationarity condition:

$$
(\mathbf{0},\mathbf{0})\in\widehat{c}\Sigma_{\beta}(\delta,\sigma)\Leftrightarrow\begin{bmatrix}\mathbf{0}\\\mathbf{0}\end{bmatrix}=-d\Xi(\delta,\sigma)+\begin{bmatrix}-\widehat{c}D_{d}(\delta-\delta_{\sigma})\\-\widehat{c}\sqcup_{\widehat{c}}(\sigma)-\mathbf{p}_{\sigma}+\varepsilon\end{bmatrix}
$$

and explicitly it becomes:

$$
\begin{cases} \mathbf{\varepsilon} - \mathbf{p}_o - d_o \Xi(\boldsymbol{\delta}, \boldsymbol{\sigma}) \in \hat{c} \sqcup_{\mathcal{C}} (\boldsymbol{\sigma}) \\ - d_o \Xi(\boldsymbol{\delta}, \boldsymbol{\sigma}) \in \hat{c} D_d (\boldsymbol{\delta} - \boldsymbol{\delta}_o) \end{cases}
$$

Box 3. Constitutive relations associated with the potential  $\Sigma_3$ 

The former relation of the box 3 above shows that there exists an elastic strain:

$$
\mathbf{e} = d_{\sigma} \Xi(\boldsymbol{\delta}, \boldsymbol{\sigma}) \Leftrightarrow \boldsymbol{\sigma} = d_{c} \Phi(\boldsymbol{\delta}, \mathbf{e})
$$

such that the plastic strain  $p = \varepsilon - e$  fulfils the discrete counterpart of the plastic flow rule:

$$
\mathbf{p} - \mathbf{p}_o \in \widehat{c} \sqcup_{C}(\boldsymbol{\sigma}).
$$

The latter condition of the box 3 provides the static damage internal variable  $\xi$ :

$$
\boldsymbol{\xi} = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = -d_{\delta} \boldsymbol{\Xi}(\boldsymbol{\delta}, \boldsymbol{\sigma}) = \begin{bmatrix} -\psi(e) - \pi(\boldsymbol{\alpha}) \\ -A \delta_2 \end{bmatrix}
$$

such that the discrete counterpart of the flow rule is fulfilled:

$$
\xi \in \partial D_d(\delta - \delta_o) \Leftrightarrow \delta - \delta_o \in \partial \Box_G(\xi).
$$

#### 4. SOLUTION OF THE ELASTOPLASTIC DAMAGE MODEL

The result established in the proposition 4 provides the variational basis to exploit the *elastic predictor-plastic corrector-damage corrector* for the numerical solution of the elastoplastic damage finite-step problem. The algorithm presented hereafter turns out to be

a generalization of the one proposed by Simo and Ju (1987), Ju (1989) and is consistently derived from a variational principle.

The solution of the incremental model of box 2 for a given history of strain  $\epsilon$  over a sequence of time steps  $[t_n, t_{n+1}]$  amounts to updating the state variables in a fashion which is consistent with the constitutive model once the state variables are known at the beginning of the step.

Let us consider the time step  $[t_n, t_{n+1}]$  and let  $\Delta \varepsilon_{n+1} = \varepsilon_{n+1} - \varepsilon_n$  be the given increment of the total strain.

A maximum point  $(\delta, \sigma)$  of the potential  $\Sigma_3$  is a solution of the constitutive model reported in box 2 and can be found as follows.

The functional  $\Sigma_3$  is first maximized with respect to  $\sigma$  under the assumption that the kinematic damage internal variable  $\delta$  is held constant to its initial value  $\delta_{w}$ .

The relevant stationary condition of  $\Sigma_3$  then yields the former relation of box 3 which can be rewritten as follows:

$$
\begin{bmatrix} \varepsilon_{n+1} - p_n - \mathrm{d} \psi^*(\hat{\sigma}) \\ \alpha_n - \mathrm{d} \pi^*(\hat{\chi}) \end{bmatrix} \in \hat{\mathcal{C}} \sqcup \hat{\mathcal{C}}(\hat{\sigma}),
$$

where the normality rule of  $\Delta p$  with respect to the domain C has been substituted with the equivalent expression in terms of the effective domain  $\hat{C}$ .

Hence the minimization of  $\Sigma_3$  with respect to  $\sigma$  amounts to finding a stress  $\hat{\sigma}_{n-1}$  so that there exists an elastic strain:

$$
\mathbf{e}_{n+1} = \begin{bmatrix} \mathrm{d}\psi^*(\hat{\sigma}_{n+1}) \\ \mathrm{d}\pi^*(\hat{\chi}_{n+1}) \end{bmatrix}
$$

such that the incremental plastic strain  $\mathbf{p}_{n+1}-\mathbf{p}_n = \mathbf{\varepsilon}_{n+1}-\mathbf{p}_n-\mathbf{e}_{n+1}$  fulfils the discrete flow rule:

$$
\mathbf{p}_{n+1}-\mathbf{p}_n\in\widehat{c}\_\widehat{c}(\widehat{\boldsymbol{\sigma}}_{n-1})=N_{\widehat{c}}(\widehat{\boldsymbol{\sigma}}_{n+1}).
$$

*Remark* 4.12. By virtue of the expression of the free energy and. hence, of the convex functional  $\Xi$  reported in Remark 3.9, the stationary condition of  $\Sigma_3$  with respect to  $\sigma$  for a given increment  $\Delta \varepsilon_{n-1}$  of the total strain is thus equivalent to solve an elastoplastic problem in the effective stresses and in the actual strain. •

The next step consists in evaluating the stationarity of the potential  $\Sigma_3$  with respect to the kinematic damage internal variable  $\delta$  assuming  $\hat{\sigma} = \hat{\sigma}_{n-1}$ . The stationary condition yields the latter relation of box 3 :

$$
\begin{bmatrix} -\psi(e)-\pi(\alpha) \\ -A\delta_2 \end{bmatrix} \in \hat{c} D_d(\delta_1-\delta_{1n},\delta_2-\delta_{2n}).
$$

The maximization of  $\Sigma_3$  with respect to  $\delta$  amounts to finding a static damage internal variable  $\xi_{n+1}$ :

$$
\xi_{n+1} = \begin{bmatrix} -\psi(e_{n+1}) - \pi(\alpha_{n+1}) \\ -A \, \delta_{2,n+1} \end{bmatrix}
$$

and a kinematic internal variable  $\delta_{n+1}$  such that the discrete damage flow rule is fulfilled:

$$
\boldsymbol{\delta}_{n+1} - \boldsymbol{\delta}_n \in N_G(\boldsymbol{\xi}_{n+1}).
$$

*Remark* 4.13. For a given stress  $\hat{\sigma}_{n-1}$ , the maximization condition of  $\Sigma_3$  with respect

to  $\delta$  is equivalent to solve a damage problem in which the elastoplastic part of the model is *.li·ozen. •*

*Remark* 4.14. The use of the variational principle involving the variables  $\delta$  and  $\sigma$ provides two equations which can be solved in sequence. Although plasticity and damage are coupled, no alternate fulfilment of the two relations is needed to solve the elastoplastic model with damage.

In fact the strain  $e_{n+1} = (e_{n+1}, a_{n+1})$  derived from the elastoplastic problem with the damage variables frozen yields the value of the damage variable  $\xi_{1,n+1} = -\psi(e_{n+1}) - \pi(\alpha_{n+1}).$ 

If  $\xi_{n+1,n} = (\xi_{1,n+1}, \xi_{2,n})$  belongs to the interior of G, the subdifferential of the indicator of the domain **G** at the point  $\xi_{n+1,n}$  is zero and hence:

$$
\xi_{2,n+1}=\xi_{2,n}-\pmb\delta_{n+1}=\pmb\delta_n
$$

that is the damage variables  $\xi_2$  and  $\delta$  do not change.

On the other hand, if  $\xi_{n+1,n}$  does not belong to the interior of G, the new damage internal variables  $\delta_{n+1} = (\delta_{1,n+1}, \delta_{2,n+2})$  and  $\xi_{2,n+1}$  are evaluated according to the expressions:

$$
\delta_{n+1} - \delta_n \in N_G(\xi_{n+1}) \Leftrightarrow \begin{cases} \delta_{1,n+1} - \delta_{1,n} = \mu \, dg_1(-\xi_{1,n+1}) \\ \delta_{2,n+1} - \delta_{2,n} = -\mu \, dg_2(\xi_{2,n+1}) \end{cases}
$$

under the loading/unloading damage conditions:

$$
\mu \geq 0
$$
  $g(\xi_{1,n+1}, \xi_{2,n+1}) \leq 0$   $\mu g(\xi_{1,n+1}, \xi_{2,n+1}) = 0.$ 

Consequently, the updated actual stress is given by:

$$
\sigma_{n+1} = (1 - \delta_{1,n+1})\hat{\sigma}_{n+1}
$$

#### *4.1. Solution algorithm*

The solution algorithm for the resolution of the elastoplastic model with damage derives from the results presented in the previous sections. In fact, the solution scheme consists of the following steps:

(i) Strain update. Given the incremental strain  $\Delta \varepsilon_{n+1}$  go to the next step.

(ii) Elastoplastic problem. The damage variables  $\delta$  and  $\xi$  are fixed to their initial values  $\delta_n$  and  $\xi_n$  and the elastoplastic problem for a given increment of the total strain  $\Delta \varepsilon_{n-1}$ is solved in terms of the effective stresses.

Ifthe material is not damaged this step is similar to a classical strain driven elastoplastic problem and the elastic predictor-plastic corrector algorithm can be adopted. In the case of an elastoplastic behaviour see Simo and Taylor (1985), Simo *et al.* (1988, 1989), Lubliner (1990), Crisfield (1991), Reddy and Martin (1991), Auricchio *et al.* (1992). Note that the elastic-predictor. plastic-corrector algorithm can be obtained starting from the variational principle which derives from the potential  $\Sigma_{31}$  reported in Marotti de Sciarra (1994).

In the present elastoplastic damage context the elastic predictor-plastic corrector algorithm is performed in terms of the effective stresses and the essential steps are reported hereafter:

(a) Elastic trial stress. The trial stress  $\hat{\sigma}_{n+1}^*$  is evaluated assuming that the behaviour of the body is elastic:

$$
\hat{\sigma}_{n+1}^* = \hat{\sigma}_n + d\psi(\Delta \varepsilon_{n+1})
$$

where  $\hat{\sigma}_n$  is the effective stress at the beginning of the step.

The plastic strain and the damage variables are kept unchanged. Then go to the next step.

(b) Plastic check. The plastic condition is first checked. If  $\hat{f}(\hat{\sigma}_{n+1}^{*}) \leq 0$  then the behaviour is elastic and no plastic return is necessary. In the other case, that is  $\hat{f}(\hat{\sigma}_{n+1}^{*}) > 0$ , go to the next step.

(c) Plastic return mapping. The plastic return consists in projecting the trial stress  $\hat{\sigma}_{n+1}^*$ onto the elastic domain in order to obtain the updated strains  $e_{n+1}$ ,  $p_{n+1}$  and stress  $\hat{\sigma}_{n+1}$ which fulfil the elastoplastic problem.

The step (ii) provides the solution of the former relation of box 3, that is the solution of the elastoplastic model for the given increment of the total strain  $\Delta \varepsilon_{n+1}$  with frozen damage variables.

Once this problem is solved we have the following set of state variables  $\{\hat{\sigma}_{n+1}, \mathbf{e}_{n+1}, \mathbf{p}_{n+1}\}\$  and the static damage variable  $\xi_{1,n+1}$  since it results:

$$
\xi_{1,n+1} = -\psi(e_{n+1}) - \pi(\alpha_{n+1}).
$$

(iii) Damage corrector. If  $\xi_{n+1,n} = (\xi_{1,n+1}, \xi_{2,n})$  does not belong to the interior of **G**, the increment of the damage parameter  $\Delta \mu = \mu_{n+1} - \mu_n$  in the time step  $[t_n, t_{n+1}]$  has to be evaluated.

The increment  $\Delta \mu = \mu_{n+1} - \mu_n$  is given by the condition:

$$
g[\xi_1,\xi_2(\Delta\mu)]=0.
$$

where  $\xi_1$  is fixed.

The increment of the damage parameter can be obtained by directly solving the condition:

$$
g_2[\xi_2(\Delta \mu)] = g_1(-\xi_1),
$$

or by a Newton-Raphson scheme:

$$
g_1(-\xi_{1,n+1}) - g_2(\xi_{2,n}) - \langle dg_2(\xi_{2,n}), d\xi_2(\Delta\mu) \rangle_{|\Delta\mu=0} \Delta\mu = 0
$$

Accordingly the updated value of the kinematic damage variable  $\delta_{1,n+1}$  is given by:

$$
\delta_{1,n+1} = \delta_{1,n} + \Delta \mu \, dg_1(-\xi_{1,n-1})
$$

and the damage updated threshold  $\xi_{2,n+1}$  is:

$$
\xi_{2,n+1} = -A\,\delta_{2,n+1} = \xi_{2,n} + \Delta\mu A\,\mathrm{d}g_2(\xi_{2,n}).
$$

Finally the updated actual stress  $\sigma$  is obtained:

$$
\sigma=(1-\delta_{1,n+1})\hat{\sigma}.
$$

#### *4.2. Speciali::atioll of the algorithm*

No iteration are required for the damage part of the problem if the damage threshold function  $g_2$  is the identity function  $g_2(\xi_2) = \xi_2$  or an exponential function such as  $g_2(\xi_2) = 1/m\xi_2^m$  where  $\xi_2$  is a scalar variable.

Assume that the damage threshold has the expression  $g(\xi_2) = \xi_2$ . The operator A becomes a scalar parameter and the increment of the damage multiplier  $\Delta \mu$  can be directly obtained by means of the formula:

$$
\Delta \mu = \frac{1}{A} [g_1(-\xi_{1,n+1}) - \xi_{2,n}]
$$

The updated value of the kinematic damage variable  $\delta_{1,n+1}$  is then given by:

$$
\delta_{1,n+1} = \delta_{1,n} + \frac{1}{A} [g_1(-\xi_{1,n+1}) - \xi_{2,n}] dg_1(-\xi_{1,n+1}).
$$

The updated value of the static damage internal variable  $\xi_{2,n+1}$  is given by:

$$
\xi_{2,n+1} = \xi_{2,n} + g_1(-\xi_{1,n+1}) - \xi_{2,n} = g_1(-\xi_{1,n+1})
$$

and turns out to be equal to the value of the damage mode  $g_1$  at the updated value of the damage energy release rate due to the peculiar expression of the damage threshold. The updated values of the stress can thus be derived from the formula  $\sigma = (1 - \delta_{1,n+1})\hat{\sigma}$ .

Moreover, setting  $A = 1$ , the above expressions coincide with the one reported in the computational algorithm for the elastoplastic damage model presented in Ju (1989).

Let us now assume that the force  $\xi_2$  conjugate to the damage evolution is a tensor and let the damage threshold be expressed in the form  $g_2(\xi_2) = ||\xi_2||$ .

The scalar product between tensors is denoted by the symbol "." and is defined as  $A \cdot B = \text{tr}(A'B)$  where "tr" represents the trace operator and A' is the transpose of A. The norm of a tensor is denoted by  $\|\bullet\|$ .

The damage multiplier  $\Delta \mu$  is now obtained from a Newton-Raphson scheme and the updated value  $\Delta \mu_{n+1}$  is provided by the formula:

$$
\Delta \mu_{n+1} = \frac{g_1(-\xi_{1,n+1}) - ||\xi_{2,n}||}{\frac{\xi_{2,n}}{||\xi_{2,n}||} \cdot \frac{A \xi_{2,n}||}{||\xi_{2,n}||}}
$$

The updated values of  $\delta_{1,n+1}$  and  $\xi_{2,n+1}$  are accordingly obtained and are given by:

$$
\delta_{1,n+1} = \delta_{1,n} + \Delta \mu_{n+1} \, dg_1(-\xi_{1,n+1})
$$

and

$$
\xi_{2,n+1} = \xi_{2,n} + \Delta \mu_{n+1} \frac{A \xi_{2,n}}{\|\xi_{2,n}\|}.
$$

The damage condition  $g(\xi_{1,n+1}, \xi_{2,n+1}) = 0$  is checked and if it is not fulfilled we set  $n = n + 1$ , a new value of  $\Delta \mu_{n+1}$  is computed and the iteration is repeated. If the damage condition is fulfilled the updated actual stress  $\sigma$  is then evaluated.

## 5. ELASTOPLASTIC DAMAGE TANGENT OPERATOR

The expression of the tangent elastoplastic modulus *consistent* with the Euler backward scheme (Ortiz and Simo. 1986) has been obtained for a general elastoplastic model with hardening in Marotti de Sciarra and Rosati (1995).

In this section the expression of the tangent modulus for the damage elastoplastic model is derived.

The elastic trial of the elastoplastic algorithm is performed in the effective stress space so that it appears reasonable to derive a tangent elastoplastic modulus in the effective stress space and in the actual strain space.

Hence we first set  $\Psi(\mathbf{e}) = \psi(e) + \pi(\alpha)$ . To obtain the derivative of the effective stress with respect to the total strain we evaluate the derivative of the effective stress  $\hat{\sigma}$  with respect to the parameter time and invoke the additivity of the strains:

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$$
d\hat{\sigma} = d^2 \Psi(\mathbf{e}) d\mathbf{e} = d^2 \Psi(\mathbf{e}) (d\mathbf{e} - d\mathbf{p}).
$$

The expression of the discrete flow rule yields the relation:

$$
d\mathbf{p} = d\lambda \, d\hat{f}(\hat{\boldsymbol{\sigma}}) + \lambda \, d^2 \hat{f}(\hat{\boldsymbol{\sigma}}) \, d\hat{\boldsymbol{\sigma}},
$$

so that:

$$
d\hat{\sigma} = d^2 \Psi(\mathbf{e}) \left[ d\mathbf{\varepsilon} - d\lambda \, d\hat{f}(\hat{\sigma}) - \lambda \, d^2 \hat{f}(\hat{\sigma}) \, d\hat{\sigma} \right].
$$

Denoting by  $\mathcal I$  the identity operator in the stress space  $\mathcal S_{\alpha}$ , the expression above becomes:

$$
d\hat{\sigma} = [\mathcal{I} + \lambda d^2 \Psi(\mathbf{e}) d^2 \hat{f}(\hat{\sigma})]^{-1} d^2 \Psi(\mathbf{e}) [d\mathbf{e} - d\lambda d\hat{f}(\hat{\sigma})]
$$
  
= 
$$
[d^2 \Psi(\mathbf{e})^{-1} (\mathcal{I} + \lambda d^2 \Psi(\mathbf{e}) d^2 \hat{f}(\hat{\sigma}))]^{-1} [d\mathbf{e} - d\lambda d\hat{f}(\hat{\sigma})]
$$
  
= 
$$
\mathbf{P}[d\mathbf{e} - d\lambda d\hat{f}(\hat{\sigma})],
$$

where:

$$
\mathbf{P} = [d^2 \Psi(\mathbf{e})^{-1} (\mathscr{I} + \lambda d^2 \Psi(\mathbf{e}) d^2 \hat{f}(\hat{\boldsymbol{\sigma}}))]^{-1} = [d^2 \Psi(\mathbf{e})^{-1} + \lambda d^2 \hat{f}(\hat{\boldsymbol{\sigma}})]^{-1}.
$$

The operator P turns out to be symmetric and positive definite and hence invertible. Actually, it is the sum of the tangent elastic compliance  $d^2\Psi(e)^{-1}$ , which is symmetric and positive definite, and of the symmetric and positive semidefinite operator  $d^2f(\hat{\sigma})$ .

The plastic parameter  $\lambda$  can be derived by enforcing the Prager's consistency condition for plasticity which yields the condition:

$$
\langle d\hat{f}(\hat{\boldsymbol{\sigma}}), d\hat{\boldsymbol{\sigma}} \rangle = \langle d\hat{f}(\hat{\boldsymbol{\sigma}}), P[dk - d\lambda] d\hat{f}(\hat{\boldsymbol{\sigma}})] \rangle = 0.
$$

so that the differential of the plastic multiplier is given by:

$$
d\lambda = \frac{\prec df(\hat{\boldsymbol{\sigma}}), \mathbf{P} \, d\mathbf{e} \succ}{\prec d\hat{f}(\hat{\boldsymbol{\sigma}}), \mathbf{P} \, d\hat{f}(\hat{\boldsymbol{\sigma}}) \succ} = \beta^{-1} \prec d\hat{f}(\hat{\boldsymbol{\sigma}}), \mathbf{P} \, d\mathbf{e} \succ,
$$

where the parameter  $\beta$  is:

$$
\beta = \langle df(\hat{\boldsymbol{\sigma}}), P\, df(\hat{\boldsymbol{\sigma}}) \rangle.
$$

The *algorithmic* tangent elastoplastic modulus can thus be obtained by substituting the relation above in the expression of  $d\hat{\sigma}$ :

$$
d\hat{\sigma} = \mathbf{P}[d\epsilon - \beta^{-1} < d\hat{f}(\hat{\sigma}), \mathbf{P} d\epsilon > d\hat{f}(\hat{\sigma})]
$$
  
=  $[\mathbf{P}d\epsilon - \beta^{-1} < d\hat{f}(\hat{\sigma}), \mathbf{P} d\epsilon > \mathbf{P} d\hat{f}(\hat{\sigma})]$   
=  $[\mathbf{P} - \beta^{-1} (\mathbf{P} d\hat{f}(\hat{\sigma})) \otimes (\mathbf{P} d\hat{f}(\hat{\sigma}))] d\epsilon.$ 

where the symbol  $\otimes$  denotes the tensorial product.

Setting  $N = P df(\hat{\sigma})$ , the expression of the tangent elastoplastic modulus consistent with the Euler backward time integration scheme becomes:

$$
\mathbf{D}^{op} = \mathbf{P} - \beta^{-1} \mathbf{N} \otimes \mathbf{N}
$$

The symmetry of  $\mathbf{D}^{op}$  is apparent.

#### 6. APPLICATIONS

The ductile damage model developed in this paper allows us to compare the behaviour of an elastoplastic material with hardening when different expressions of the damage domain are provided. For now, assume that the material data are correct for a representative volume element.

A one-dimensional model is considered. The elastic domain  $\tilde{C}$  is given by:

$$
|\hat{\sigma} - \hat{\chi}_1| - \hat{\chi}_2 \leq 0.
$$

where  $\hat{\chi}_1$  accounts for the kinematic hardening behaviour and  $\hat{\chi}_2$  is the static internal variable associated with the isotropic hardening.

The damage domain  $G$  has five different shapes according to the following five different expressions of the damage function  $q_1$  and damage threshold function  $q_2$ :

> case 1a  $g_1(\xi_1) = |\xi_1|$   $g_2(\xi_2) = \xi_2$  $1b$   $g_1(\xi_1) = \frac{1}{2}\xi_1^2$ case 1b  $g_1(\xi_1) = \frac{1}{2}\xi_1^2 - g_2(\xi_2) = \xi_2$ case 2a  $g_1(\xi_1) = |\xi_1|$   $g_2(\xi_2) = \frac{\xi_2^m}{m^2}$ case 2b  $g_1(\xi_1) = \frac{1}{2}\xi_1^2 - g_2(\xi_2) = \frac{1}{m}\xi_2^m$ case 3  $q_1(\xi_1) = |\xi_1| - q_2(\xi_2) = |\xi_2|$ .

Note that in the functional form 3, the variable  $\xi_2$  is a square two by two matrix.

The elastic energy  $\psi$  and the hardening potential  $\pi$  are given by:

$$
\psi(e) = \frac{1}{2} E_o e^2 - \pi(\alpha_1, \alpha_2) = \frac{1}{2} H_{kin} \alpha_1^2 + \frac{1}{2} H_{iso} \alpha_2^2 + \sigma_v \alpha_2.
$$

where  $\sigma_r$  is the initial yield threshold,  $H_{kin}$  and  $H_{iso}$  are the kinematic and isotropic moduli. Accordingly, the free energy  $\Phi$  is then written in the form:

$$
\Phi(e, \alpha_1, \alpha_2, \delta_1, \delta_2) = (1 - \delta_1)[\psi(e) + \pi(\alpha_1, \alpha_2)] - \frac{1}{2}A \delta_2 \cdot \delta_2.
$$

if  $\delta_1 \in [0, \delta_c]$ . The last term above is a scalar product in the case 3 since  $\delta_2$  is a square matrix; in all the other four cases  $\delta$ , is a scalar variable.

The set of parameters adopted in the present application is deduced from Hansen and Schreyer (1994) for a 2024-T3 aluminum alloy at a room temperature and is listed hereafter: undamaged elastic modulus  $E_0 = 74500$  MPa, initial yield strength  $\sigma<sub>x</sub> = 250$  MPa, linear isotropic hardening modulus  $H_{iso} = 200 \text{ MPa}$ , isotropic hardening exponent  $m = 0.4$ , linear kinematic hardening modulus  $H_{kin} = 0$  MPa. damage threshold  $\xi_{1,y} = 1.9$  MPa and linear damage parameter  $A = 15$  MPa.

A monotonically increasing strain  $\varepsilon = 0.6*10^{-2}t^{2/3}$  from 0 to 3, 79 $*10^{-2}$  is considered and the strain increment is assumed to be  $0.246*10^{-3}$  (154 strain steps). In Fig. 2 the stressstrain relations for the expressions  $1 = \text{case } 2b$ ,  $2 = \text{case } 1b$ ,  $3 = \text{case } 2a$  and  $4 = \text{case } 1a$ of the damage domain are reported.

In Fig. 3 the evolution of the clastic modulus in terms of the axial strain is sketched. Each of the four curves in the Figs 2 and 3 is obtained by assuming a different expression of the damage functional  $g_1$  and damage threshold  $g_2$ . It is possible to note that the maximum strain corresponding to the complete damage, i.e.,  $\delta = 1$ , is quite different for the different expression of G and that the condition  $\delta = 1$  is achieved before the strain path is completed.

In Fig. 4 it is reported the evolution of the elastic domain and of the damage domain (amplified by the factor 10) in terms of the axial strain when the case la is considered.



Fig. 4. The evolution of the damage G and elastic C domains for the case Ia.







**In** Fig. 5 the stress-strain relations are pictured when the damage parameter A changes in the set  $\{15, 20, 30, 45\}$  and the damage domain is expressed by means of the functions reported in the case Ia).

If  $A = \{15, 20\}$ , the figure shows that the complete damage, i.e.,  $\delta = 1$ , is achieved before the maximum strain is reached. If the damage parameter increases  $A = \{30, 45\}$  the stress-strain curve is more rigid and the maximum strain is reached.

Let us now consider a cyclic strain history  $\varepsilon = 0.6* 10^{-2} \sin t$  where *t* ranges from 0 to  $5\pi$ .

**In** Figs 6. 7 and 8 the stress-strain relations are reported when the damage parameter A varies in the set  $\{15, 30, 45\}$ . The isotropic modulus  $H_{\text{iso}}$  is now set equal to 600 MPa and the damage domain is that of the case Ia.



Fig. 7. Stress-strain relation for a cyclic strain history with  $A = 30$  MPa





Moreover, the correlation between the elastic damaged modulus and the axial strain is shown in Fig. 9.

In Figs 10. II and 12 the stress-strain relations for the abovementioned cyclic strain are reported when the hardening parameter  $H_{kin}$  changes in the set {400,800, 1200},  $H_{iso}$  = 600 MPa,  $A = 15$  MPa and the damage domain is that of the case 1a. The evolution of the elastic and damage domain and the correlation between the elastic damaged modulus and the axial strain are reported in Figs 13 and 14.

The stress-strain relations for the functional form 3 of the damage domain G are reported in Figs 15 and 16. The kinematic hardening parameter  $H_{kin}$  is 1200 MPa, the isotropic hardening modulus  $H_{i\omega}$  is 800 MPa. The damage parameter *A* is 7 MPa in the former figure and 15 MPa in the latter one. The degradation of the elastic modulus vs strains is painted in the Figs 17 and 18.



Fig. 9. The damage elastic modulus vs strains for a cyclic strain history with  $A = 45 \text{ MPa}$ .













 $\bar{\mathcal{A}}$ 



Fig. 13. The evolution of the damage and elastic domain for case 1a and  $H_{kin} = 1200 \text{ MPa}$ .





Fig. 15. Stress-strain relation for a cyclic strain history with  $H_{kin} = 1200$  MPa,  $H_{iso} = 800$  MPa *A* = 7 MPa and case 3 of damage domain.



Fig. 16. Stress-strain relation for a cyclic strain history with  $H_{km} = 1200$  MPa,  $H_{tot} = 800$  MPa  $A = 15$  MPa and case 3 of damage domain.



Fig. 17. The damage elastic modulus vs strain related to the stress-strain diagram for Fig. 15.



Fig. IX. The damage elastic modulus vs strain related to the stress-strain diagram for Fig. 16.

## 7. CONCLUSION

An energy based continuous model coupling plasticity and damage has been presented. The model can exhibit a damage threshold governed by a scalar or tensorial variable  $\xi_2$ .

The treatment presented in this paper provides a unified framework to encompass constitutive elastoplastic models with hardening and damage phenomena.

The yield and damage functionals are assumed to be convex and the damage threshold has been chosen to be monotone, nonnegative and concave thus generalizing previous formulations.

The convexity of the damage and elastic domains led to the definition of the damage and plastic dissipation which turn out to be nonnegative provided that the origin of the space belongs to the interior of the relevant convex domain.

The free energy is given in a form such that the damage force associated with the elastoplastic microcrack evolution turns out to be the opposite of the sum of the elastic strain energy and hardening functional. The principle of equivalent strain naturally follows from the assumed form of the free energy.

The expression of the elastoplastic damage tangent modulus consistent with the Euler backward scheme is provided following a general procedure.

The elastoplastic damage model with hardening is then cast in a consistent variational framework and the general variational principle is provided.

Different variational formulations in a reduced number of state variables are derived. The variational principle in  $\delta$  and  $\sigma$  provides the consistent variational basis to solve the elastoplastic damage problem in a straightforward manner.

The elastic predictor-plastic corrector followed by the solution of the damage problem has been implemented for different expressions of the damage mode and damage threshold. The results have been compared for a monotonically increasing strain history and for different cyclic strain histories with different damage and hardening parameters.

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# APPENDIX A-A BACKGROUND OF CONVEX ANALYSIS

Some notations of convex analysis used in the paper are reported for sake of clearness; for more details see Hiriart-Hurruty and Lemarechal (1993).

Let  $(X, X')$  be a pair of locally convex topological vector spaces placed in separating duality by a bilinear form  $\langle \cdot, \cdot \rangle$ . Let us set  $\overline{\mathfrak{R}} = \{-\infty\} \cup \mathfrak{R} \cup \{+\infty\}$ 

Convex sets-A subset *K* of *X* is said to be convex if

$$
\lambda x_1 + (1 - \lambda)x_2 \in K
$$
 whenever  $x_1 \in K$ ,  $x_2 \in K$ ,  $\lambda \in [0, 1]$ .

Convex cone—A set *K* contained in *X* is a cone if  $\lambda x \in K$  for every  $\lambda \ge 0$  and  $x \in K$ . A convex cone is a cone which is also a convex set.

Normal cone-The normal cone to a convex set  $K$  at a point x is defined as follows:

$$
N_K(x) = \begin{cases} \{x^* \in X' : \langle x^*, y - x \rangle \le 0 & \forall y \in X\}, & \text{if } x \in K \\ \varnothing & \text{otherwise.} \end{cases}
$$

Convex functional  $-A$  functional *f*:  $X \mapsto \mathfrak{R} \cup \{+\infty\}$  is convex if:

$$
f[\lambda x_1 + (1 - \lambda)x_2] \le \lambda f(x_1) + (1 - \lambda)f(x_2)
$$

for any  $x_1 \in \text{dom } f$ ,  $x_2 \in \text{dom } f$  and  $\lambda \in [0, 1]$  where dom f denotes the domain of f. The functional f is strictly convex if the inequality above is strict.

Proper functional—A functional  $f: X \mapsto \overline{\mathfrak{R}}$  is proper if it is never  $-\infty$  and  $f(x) < +\infty$  for at least one *x*. Sublinear functional-- A functional  $f: X \mapsto \mathfrak{R} \cup \{+ \infty\}$  turns out to be sublinear if it is positively homogeneous and subadditive :

$$
\begin{cases}\nf(xx) = \alpha f(x) & \forall x \ge 0 \quad \text{(positive homogeneity)} \\
f(x_1) + f(x_2) \ge f(x_1 + x_2) & \forall x_1, x_2 \in X \quad \text{(subadditivity)}.\n\end{cases}
$$

Lower semicontinuous functional—A functional  $f: X \mapsto \mathcal{R} \cup \{+\infty\}$  is said to be lower semicontinuous if:

$$
\liminf_{z \to x} f(z) = f(x) \quad \forall z \in X.
$$

A lower semicontinuous functional  $f$  has a closed epigraph. i.e.,  $f$  is closed. Young function--A Young function  $Y: \mathbb{R} \to \mathbb{R} \cup \{+ \infty\}$  is an extended real-valued function on  $\mathbb{R}$  which is monotone, l.s.c., convex and nonnegative with  $Y(0) = 0$ .

Conjugate functional - The conjugate of a convex functional  $f: X \mapsto \mathfrak{R} \cup \{+\infty\}$  is the convex functional  $f^*$ :  $X \mapsto \mathfrak{R} \cup \{ +\infty \}$  defined by :

$$
f^*(x^*) = \sup_{y \in X} \left\{ \langle x^*, y \rangle - f(y) \right\}.
$$

Note that  $f^*$  is convex and closed; further if f is closed we have  $f^{**} = f$ . Indicator functional--- Given a set *K* contained in *X*, the indicator of *K* at a point  $x \in X$  is defined as follows:

$$
\bigsqcup_{K}(x) = \begin{cases} 0 & \text{if } x \in K \\ -x & \text{otherwise} \end{cases}
$$

Support functional Given a set K contained in X, the support functional of K at a point  $x^* \in X'$  is defined as follows:

$$
D(x^*) = \sup_{x \in K} \langle x^*, x \rangle.
$$

Note that the support and the indicator functionals of a convex set  $K$  are conjugate. Subdifferential- The subdifferential of a convex functional  $f: X \rightarrow \mathfrak{R} \cup \{+ \infty\}$ , having a nonempty domain, is the set  $\partial f(x) \subseteq X'$  such that:

$$
x^* \in \partial f(x) \Leftrightarrow f(y) - f(x) \ge \langle x^*, y - x \rangle \quad \forall y \in X.
$$

In particular, if the functional f is differentiable at  $x \in X$ , the subdifferential is a singleton and coincides with the usual differential.

Note that the subdifferential of the indicator functional of a convex set *K* at a point  $x \in K$  coincides with the normal cone to  $K$  at  $x$ :

$$
\partial \Box_K(x) = N_K(x).
$$

Fenchel's equality  $-G$ iven two convex conjugate functional  $f$  and  $f^*$ , the Fenchel's inequality holds:

$$
f(x) + f^*(x^*) \ge \langle x^*, x \rangle \quad \forall x \in X, \quad \forall x^* \in X'.
$$

The elements  $\{x, x^*\}$  for which Fenchel's inequality holds as an equality are said to be conjugate and the following relations are equivalent when  $f$  is closed:

$$
f(x) + f^*(x^*) = \langle x^*, x \rangle, \quad x^* \in \partial f(x), \quad x \in \partial f^*(x^*).
$$

Subdifferential rules-The following rules usually hold for subdifferentiability:

• Chain-rule. Given a monotone convex function  $m: \mathfrak{R} \mapsto \mathfrak{R} \cup \{+\infty\}$  and a continuous convex functional  $f: X \mapsto \mathfrak{R} \cup \{+\infty\}$ , the functional (*mf*) is convex and its subdifferential at a point  $x \in X$ , which is not a minimum for  $f$ , is given by (Romano, 1995):

$$
\hat{c}(m-f)(x) = \hat{c}m[f(x)]\hat{c}f(x).
$$

• A second chain-rule. Given a differentiable operator  $A: X \mapsto Y$  and a continuous convex functional  $f: Y \mapsto \mathfrak{R} \cup \{+\infty\}$  which is subdifferentiable at  $y = A(x)$  we have:

$$
\partial(f \mid A)(x) = [dA(x)]' \partial f[A(x)],
$$

where  $dA(x)$  is the derivative of the operator A at x and  $\left[ dA(x) \right]$ ' is the dual operator. • Additivity. Given two convex functionals  $f_1: X \mapsto \mathbb{R} \cup \{+\infty\}$  and  $f_2: X \mapsto \mathbb{R} \cup \{+\infty\}$  which are subdifferentiable at  $x \in X$ , it turns out to be:

$$
\hat{c}(f_1+f_2)(x)=\hat{c}f_1(x)+\hat{c}f_2(x).
$$

Analogous results hold for concave functionals by interchanging the role of  $-\infty$ ,  $\ge$  and "sup" with those of  $-\infty$ ,  $\leq$  and "inf"; the prefix "sub" used in the convex case has now to be replaced by "super".

#### APPENDIX B-SADDLE FUNCTIONALS

We report here the main results concerning with the saddle functionals which have been used in the paper. The proofs and a complete analysis of the subject can be found in Rockafellar (1970).

Given a function  $f: X \times Y \mapsto \mathfrak{R} \cup \{+ \infty\}$ , jointly convex in *X* and *Y*, its conjugate  $f^*: X \times Y \mapsto \mathfrak{R} \cup \{+ \infty\}$ is given by:

$$
f^*(x^*, y^*) = \sup_{(y,z)} \left\{ \langle x^*, x \rangle + \langle y^*, y \rangle - f(x, y) \right\}.
$$

and turns out to be closed and convex in  $X' \times Y'$ .

A saddle functional  $k: X \times Y \mapsto \Re(\Re) = \{-\infty\} \cup \cup \{+\infty\}$ , concave in X and convex in Y', is said to be fully closed if both the concave and the convex closure of *k* coincide with *k* itself. that is:

$$
\begin{cases}\n\text{concave closure} & \text{cl}_1 k(x, y^*) = k(x, y^*) \\
\text{convex closure} & \text{cl}_2 k(x, y^*) = k(x, y^*) \\
\end{cases} \quad \forall (x, y^*) \in X \times Y'.
$$

It can be proved that a fully closed saddle functional  $k: X \times Y \mapsto \overline{M}$  can be associated with a unique closed convex functional  $f: X \times Y \mapsto \mathfrak{R} \cup \{+\infty\}$  and with the conjugate  $f^*: X \times Y \mapsto \mathfrak{R} \cup \{+\infty\}$  of f as follows:

$$
k(x, y^*) = \sup_{x} \{ \langle y^*, y \rangle - f(x, y) \} \quad k(x, y^*) = \inf_{x \in \{x^*, x\}} \langle x^*, x \rangle + f^*(-x^*, y^*) \}
$$

The former equality shows that *k* is the partial conjugate of the convex functional  $f(x, \cdot)$  for a fixed x at the point  $y^*$ ; the latter one shows that *k* coincides with the partial conjugate of the concave functional  $(-f^*)(\cdot, y^*)$ for a given  $y^*$  at the point  $(-x)$ .

To explicitly prove that the functional  $k$  is saddle, we report the following:

*Theorem A.* I. The functional  $k: X \times Y \mapsto \overline{\mathfrak{R}}$  is concave in the space *X* and is convex in the space *Y'*.

*Proof.* The functional *k* turns out to be convex since it is the conjugate of the convex functional  $f(x, \cdot)$ . To prove that  $k(x, \cdot)$  is concave. let us introduce the projector  $P_1: X \times Y \mapsto X$  given by:

$$
P_1(x, y) = x \quad \forall (x, y) \in X \times Y.
$$

Defining, for any  $v^* \in Y'$ , the convex functional in the space  $X \times Y$ :

$$
h(x, y; y^*) = f(x, y) - \langle y^*, y \rangle.
$$

the expression of *k* becomes:

$$
k(x, y^*) = -\inf_{y} \{f(x, \bar{y}) - \langle y^*, \bar{y} \rangle\} = -\inf_{y} h(x, \bar{y}; y^*) = -\inf_{y \in \bar{y}} \{h(\bar{x}, \bar{y}; y^*) : P_1(\bar{x}, \bar{y}) = x\}.
$$

Hence, a theorem of convex analysis (Rockafellar, 1970. theorem 16.3) allows us to rewrite the "inf" above in the form:

$$
k(x, y^*) = -(P_1' - h^*)^*(x; y^*).
$$

where  $P'_1$  is the dual of  $P_1$ .

Being the functional  $(P_1 \mid h^*)^*$  convex in *x* for any  $y^*$ , it follows that  $k(x, \cdot)$  is concave.

Conversely the functionals  $f$  and  $f^*$  can be expressed in terms of the saddle functional  $k$  according to the following expressions:

$$
f(x, y) = \sup_{x^*} {\{\langle y^*, y \rangle - k(x, y^*)\}}, \quad - f^*(-x^*, y^*) = \inf_{y} {\{\langle x^*, x \rangle - k(x, y^*)\}}.
$$

Analogous results hold for the concave functionals by interchanging the role of  $+\infty$ ,  $\geq$  and "sup" with those of  $-\infty$ ,  $\le$  and "inf".

Hence let us now consider the closed concave functional  $(-f): X \times Y \mapsto \mathfrak{R} \cup [-x]$  and its conjugate  $(-f)^*: X \times Y \mapsto \mathfrak{R} \cup (-\infty)$ . Note that the relation between  $(-f)^*$  and  $(-f^*)$  is given by :

$$
-f^*(x^*, y^*) = (-f)^*(-x^*, -y^*).
$$

A fully closed saddle functional  $k^*: X \times Y \mapsto \overline{\mathfrak{R}}$ , concave in *X'* and convex in *Y*, is associated with the closed concave functional  $(-f)$  and with its conjugate  $(-f)^*$  as follows:

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$$
k^*(x^*, y) = \inf_{y} \{ \langle x^*, x \rangle + f(x, y) \}, \quad k^*(x^*, y) = \sup_{y^*} \{ \langle y^*, y \rangle - f^*(-x^*, y^*) \}
$$

The functionals ( $-f$ ) and ( $-f^*$ ) can be equivalently expressed in terms of  $k^*$  in the form:

$$
-f(x, y) = \inf \{ \langle x^*, x \rangle - k^*(x^*, y) \} \quad f^*(-x^*, y^*) = \sup \{ \langle y^*, y \rangle - k^*(x^*, y) \}
$$

It is easy to prove that the conjugate saddle functionals *k* and *k\** are linked together by the equalities:

 $k^*(x^*, y) = \inf \sup \{ \langle x^*, x \rangle + \langle y^*, y \rangle - k(x, y^*) \} = \sup \inf \{ \langle x^*, x \rangle + \langle y^*, y \rangle - k(x, y^*) \}$ 

so that the saddle functional  $k^*$  is said to be the *conjugate* of the saddle functional  $k$ . For sake of completeness we also report the expressions of *k* in terms of its conjugate:

$$
k(x, y) = \sup_{x} \inf_{x} \left[ \langle x^*, x \rangle + \langle y^*, y \rangle - k^*(x^*, y) \right] = \inf_{x} \sup_{x} \left[ \langle x^*, x \rangle + \langle y^*, y \rangle - k^*(x^*, y) \right].
$$

Given any saddle functional *k*, we define by  $\partial_k k(x, y^*)$  the superdifferential of the concave functional  $k(\cdot, y^*)$ at x and by  $\hat{c}_i \cdot k(x, y^*)$  the subdifferential of the convex functional  $k(x, \cdot)$  at  $y^*$ 

Note that the same symbol  $\partial$  is used to define both the subdifferential of a convex functional and the superdifferential of a concave one.

The subdifferential of the saddle functional k at the point  $(x, y^*)$  is defined as follows:

$$
\hat{c}k(x, y^*) \stackrel{\text{def}}{=} \hat{c}, k(x, y^*) \times \hat{c} * k(x, y^*).
$$

It can be proved that given a closed convex functional *f*, its conjugate *f*<sup>\*</sup> and the associated closed saddle<br>tionals *k* and *k*<sup>\*</sup>, the following relations are equivalent:<br>a)  $(x^*, y^*) \in \partial f(x, y)$ <br>b)  $(x, y) \in \partial f^*(x^*, y^*)$ functionals  $k$  and  $k^*$ , the following relations are equivalent:



The equivalence between c) and d) allows us to generalize Fenchel's equality in the following form:

 $(i)$  =  $x^* \in \partial_x k(x, y^*) \Leftrightarrow -f^*(x^*, y^*) + k(x, y^*) = -\langle x^*, x \rangle$ (ii)  $y \in \hat{C}_1, k(x, y^*) \Leftrightarrow f(x, y) + k(x, y^*) = \langle y^*, y \rangle$ (iii)  $x \in \hat{\epsilon}_x, k^*(-x^*, y) \Leftrightarrow -f(x, y)+k^*(-x^*, y) = -\langle x^*, x \rangle$ (iv)  $y^* \in \partial_1 k^*(-x^*, y) \Leftrightarrow f^*(x^*, y^*) + k^*(-x^*, y) = \langle y^*, y \rangle$ 

Box A.2. Generalized Fenchel's equalities

#### APPENDIX C

The expression of the convex functional  $\Xi$  associated with the saddle free energy  $\Phi$  is given by:

$$
\begin{aligned} \Xi(\delta, \sigma) &= \sup_{e} \{ \langle \sigma, e \rangle - \Phi(\delta, e) \} \\ &= \sup_{t \in \mathbb{R}^3} \{ \langle \sigma, e \rangle + \langle \chi, \chi \rangle - k(\delta_1, e, \chi) \} + \frac{1}{2} \langle A \delta_2, \delta_2 \rangle \\ &= \frac{1}{2} \langle A \delta_2, \delta_2 \rangle + \sup_{t \in \mathbb{R}^3} \{ \langle \sigma, e \rangle + \langle \chi, \chi \rangle - (1 - \delta_1) [\psi(e) + \pi(\chi)] \} \quad \text{if } \delta_1 \in J \\ &= \frac{1}{2} \langle A \delta_2, \delta_2 \rangle + \sup_{t \in \mathbb{R}^3} \{ \langle \sigma, e \rangle + \langle \chi, \chi \rangle - (1 - \delta_1) [\psi(e) + \pi(\chi)] \} \quad \text{if } \delta_1 \in J \end{aligned}
$$

In the case in which  $\delta_1$  does not belong to the set J this "sup" is + x. Hence. assuming  $\delta_1 \in J$ , the "sup" above can be performed by evaluating separately the one acting on the state variable *e* from the other on  $x$  to get:

$$
\sup_{\epsilon x} \left\{ \langle \sigma, e \rangle + \langle \chi, \alpha \rangle - (1 - \delta_1) [\psi(\epsilon) + \pi(\alpha)] \right\}
$$
  
=  $(1 - \delta_1) \sup_{\epsilon} \left\{ \left\langle \frac{\sigma}{1 - \delta_1}, e \right\rangle - \psi(\epsilon) \right\} + (1 - \delta_1) \sup_{\alpha} \left\{ \left\langle \frac{\chi}{1 - \delta_1}, \alpha \right\rangle - \pi(\alpha) \right\}$   
=  $(1 - \delta_1) \left[ \psi^* \left( \frac{\sigma}{1 - \delta_1} \right) + \pi^* \left( \frac{\chi}{1 - \delta_1} \right) \right].$ 

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