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CONSTITUTIVE EQUATIONS AND NUMERICAL APPROACHES IN RATE DEPENDENT MATERIAL FORMULATIONS

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ABSTRACT

The classical Duvaut-Lion and Perzyna formulations for rate dependent constitutive models were recently extended by different proposal to allow a more convenient and efficient numerical treatment in computational simulations of viscoplastic or viscoplastic-damage material proceses. The main goal was the development full consistent formulations so that the well known numerical approches developed for rate independent material models can be still.
This paper focuses on the description of alternatives formulations of rate dependent constitutive equations and on the numerical methods associated with each other. In this regard the fourth order material operators are developed and the features of the performance of diffuse and localized failure indicators are analyzed.

CONSTITUTIVE EQUATIONS FOR PERZYNA VISCOPLASTICITY

In this section the constitutive equations of Perzyna type viscoplastic models are presented. We distinguish between the *classical formulation* and the *continuous formulation* of Perzyna viscoplastic constitutive equations. The second one leads to a constrain condition which plays a fundamental role in the algebraic problem when finite time increments are considered, as we will see in section 5.

The Classical Formulation

Similar to the flow theory of plasticity, the constitutive relations of Perzyna (1966) type elasto–viscoplastic material formulations may be written

$$\dot{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}}_e - \dot{\boldsymbol{\sigma}}_{vp} = \mathbf{E} : (\dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}_{vp}) \tag{1}$$

$$\dot{\boldsymbol{\epsilon}}_{vp} = \mathbf{g}(\psi, F, \boldsymbol{\sigma}) = \frac{1}{\eta}\langle\psi(F)\rangle\mathbf{m} \tag{2}$$

$$\mathbf{m} = \mathbf{A}^{-1} : \mathbf{n} = \mathbf{A}^{-1} : \frac{\partial F}{\partial \boldsymbol{\sigma}} \tag{3}$$

$$\psi(F) = \left[\frac{F(\boldsymbol{\sigma}, \mathbf{q},)}{F_o}\right]^N \tag{4}$$

$$\dot{\mathbf{q}} = \frac{1}{\eta}\langle\psi(F)\rangle\mathbf{H} : \mathbf{m} \tag{5}$$

where $\boldsymbol{\epsilon}_{vp}$ defines the viscoplastic portion of the total strain tensor $\boldsymbol{\epsilon}$, η the viscosity and $\mathbf{q}$ the set of scalar-valued hardening/softening variables. The relations (1) follow the additive decomposition of the total strain rate into an elastic and a viscoplastic part $\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}_e + \dot{\boldsymbol{\epsilon}}_{vp}$, quite similar to the Prandtl-Reuss equations in case of inviscid elasto-plastic constitutive relations. Eqs. (2) and (3) describe a general non-associated flow rule, whereby the direction of the viscoplastic strains $\mathbf{m}$, is obtained by a modification of the gradient tensor $\mathbf{n}$ of the yield surface F by means of the fourth order transformation tensor $\mathbf{A}$. Moreover, $\psi(F)$ is a dimensionless monotonically increasing over–stress function whereby F_o represents a normalizing factor. The Mc Cauley brackets in eq. (2) defines the features of the over–stress function as

$$\langle\psi(F)\rangle > 0 \quad \text{if} \quad F > 0\ ; \qquad \langle\psi(F)\rangle = 0 \quad \text{if} \quad F \leq 0 \tag{6}$$

being $F = F(\boldsymbol{\sigma}, \mathbf{q})$ a convex yield function which defines the limit of the elastic domain.
Finally eq. (5) represents the evolution law of the hardening/softening variables $\mathbf{q}$ by means of a suitable tensor function $\mathbf{H}$ of the state variables.
A consistency condition similar to the flow theory of plasticity can not be obtained in the classical formulation of viscoplastic materials. However, if the viscoplastic problem is treated in a similar way to the elastoplastic one, as we will see in section 4.2, a constrain condition can be obtained which represents a generalization of the inviscid yield condition for viscoplastic materials.
Remark: instantaneous viscoplastic material response do not exhibit deterioration of the elastic properties. Therefore a viscoplastic continuum tangent stiffness tensor $\mathbf{E}_{vp}$ similar to inviscid elastoplastic materials can not be obtained in case of viscoplastic formulations.

The Continuous Formulation

In this formulation the equations (1) to (5) are complemented by a consistency parameter $\dot{\lambda}$, see Ponthot (1995), defined as an increasing function of the over–stress

$$\dot{\lambda} = \frac{1}{\eta}\langle\psi(F)\rangle \tag{7}$$

So that the evolutions equations (2) and (5) take now the classical forms

$$\dot{\boldsymbol{\epsilon}}_{vp} = \dot{\lambda}\,\mathbf{m} \tag{8}$$

$$\dot{\mathbf{q}} = \dot{\lambda}\,\mathbf{H} : \mathbf{m} \tag{9}$$

Thus, from eqs. (2) and (8) follows

$$F = \psi^{-1}\left(\frac{\|\ \dot{\boldsymbol{\epsilon}}_{vp}\ \|}{\|\ \mathbf{m}\ \|}\eta\right) = \psi^{-1}\left(\dot{\lambda}\cdot\eta\right) \tag{10}$$

We may now define for the viscoplastic range, the new constrain condition

$$\bar{F} = F - \psi^{-1}\left(\dot{\lambda}\cdot\eta\right) = 0 \tag{11}$$

which represents a generalization of the inviscid yield condition $F = 0$ for rate–dependent Perzyna viscoplastic materials. The name *continuous formulation* is due to the fact that the condition $\eta = 0$ (no viscosity effect) leads to the elastoplastic yield condition $F = 0$. Moreover, from (7) follows that when $\eta \to 0$ the consistency parameter remains finite and positive since also the over–stress goes to zero. The other extreme case, $\eta \to \infty$, leads to the inequality $\bar{F} < 0$ for every possible stress state, indicating that only elastic response may be activated.
The constrain condition defined before allows a generalization of the Kuhn-Tucker conditions which may be now written as

$$\dot{\lambda}\,\bar{F} = 0\,, \quad \dot{\lambda} \geq 0, \quad \bar{F} \leq 0 \tag{12}$$

Other recent and interesting approach to this problem is due to Wang (see Wang, Sluys and de Borst 1997), which includes the strain rate as state variable into the flow and viscoplastic potential function, i.e.

$$F^{vp} = F^{vp}\,(\boldsymbol{\sigma}, \mathbf{q}, \dot{\boldsymbol{\epsilon}}) \tag{13}$$

this also leads to a rate dependent Kuhn – Tucker conditions as in case of the continuous Perzyna formulation.

CONSISTENT TANGENT STIFFNESS TENSOR

In this section the consistent tangent tensors of both Perzyna viscoplastic material formulations described in previous section are derived. These operators must to be considered for the analysis of diffuse and localized failure predictions of the constitutive rate dependent material formulations.

The lack of a constrain condition in case of the classical formulation of Perzyna viscoplasticity forces the consideration of the stress residual to derive the consistent tangent operator. On the other hand, in the continuous formulation this stiffness tensor follows from the linearization process of the differential form of the generalized consistency condition, similar to the case of the inviscid elastoplastic formulation.

The start point for the derivation of the consistent tangent moduli in both formulations of Perzyna viscoplasticity is the Backward Euler stress equation.

Classical Perzyna Formulation

Integrating eqs. (2) and (5) during the finite time step Δt with the unconditionally stable Backward-Euler (BE) or Closest Point Projection (CPP) algorithm and considering Perzyna formulations of first order, i.e. $N = 1$ in eq. (4), we obtain the algebraic format:

$$\Delta\,\boldsymbol{\sigma}_{n+1} = \mathbf{E} : \Delta\,\boldsymbol{\epsilon}_{n+1} - \Delta t\mathbf{E} : \mathbf{g}_{n+1}; \qquad \Delta\mathbf{q}_{n+1} = \Delta t\mathbf{H}_{n+1} : \mathbf{g}_{n+1} \tag{14}$$

where the Perzyna viscoplastic evolution law is evaluated at $t = t_{n+1}$

$$\mathbf{g}_{n+1} = \frac{1}{\eta}\langle\psi(F)_{n+1}\rangle\mathbf{m}_{n+1} \tag{15}$$

To derive consistent tangent moduli of the Perzyna description we define the stress residual at $t = t_{n+1}$ as

$$\mathbf{R}_{n+1} = \mathbf{E} : \Delta\,\boldsymbol{\epsilon}_{n+1} - \Delta t\,\mathbf{E} : \mathbf{g}_{n+1} - \Delta\,\boldsymbol{\sigma}_{n+1} \tag{16}$$

The root $\mathbf{R}_{n+1} = 0$ of eq. (16) is determined via Newton-Raphson iteration, in the form

$$\mathbf{R}^{k+1}_{n+1} = \mathbf{R}^{k}_{n+1} + \Delta\mathbf{R}^{k+1}_{n+1} = \mathbf{0} \tag{17}$$

where the superscript on the right indicates the current iteration cycle. Linearization of the residual in eq. (17) yields

$$\Delta\mathbf{R}^{k+1}_{n+1} = \frac{\partial\mathbf{R}^{k}_{n+1}}{\partial\,\boldsymbol{\sigma}} : \Delta\,\boldsymbol{\sigma} + \frac{\partial\mathbf{R}^{k}_{n+1}}{\partial\,\boldsymbol{\epsilon}} : \Delta\,\boldsymbol{\epsilon} \tag{18}$$

where the individual terms of the Jacobian involve

$$\frac{\partial\mathbf{R}^{k}_{n+1}}{\partial\,\boldsymbol{\sigma}} = -\mathbf{I} - \Delta t\mathbf{E} : \frac{\partial\mathbf{g}^{k}_{n+1}}{\partial\,\boldsymbol{\sigma}} = -\mathbf{I} - \frac{\Delta t}{\eta}\mathbf{E} : \left[\Psi \otimes \mathbf{m} + \psi(F)\frac{\partial\mathbf{m}}{\partial\,\boldsymbol{\sigma}}\right]_{n+1} \tag{19}$$

$$\frac{\partial\mathbf{R}^{k}_{n+1}}{\partial\,\boldsymbol{\epsilon}} = \mathbf{E} \tag{20}$$

with

$$\Psi = \frac{\partial \psi(F)}{\partial\, \boldsymbol{\sigma}} \tag{21}$$

and **I** the fourth order identity tensor.
Substituting eqs.(19) and (20) into eq. (18) and subsequently into eq. (17) we obtain

$$\frac{d\, \boldsymbol{\epsilon}}{d\, \boldsymbol{\sigma}} = \mathbf{C} : \left[\mathbf{I} + \frac{\Delta t}{\eta} \mathbf{E} : (\Psi \otimes \mathbf{m} + \psi(F)\mathbf{M}) \right] \tag{22}$$

where

$$\mathbf{C} = \mathbf{E}^{-1}, \tag{23}$$

$$\mathbf{M} = \frac{\partial \mathbf{m}}{\partial\, \boldsymbol{\sigma}} = \mathbf{A}^{-1} : \frac{\partial^2 F}{\partial\, \boldsymbol{\sigma} \otimes \partial\, \boldsymbol{\sigma}} \tag{24}$$

Eq. (22) can be alternatively expressed as

$$\frac{d\, \boldsymbol{\epsilon}}{d\, \boldsymbol{\sigma}} = \mathbf{D}^{-1} + \frac{\Delta t}{\eta} \Psi \otimes \mathbf{m} \tag{25}$$

whereby

$$\mathbf{D}^{-1} = \mathbf{C} + \frac{\Delta t}{\eta} \psi(F)\mathbf{M} \tag{26}$$

The final expression of the consistent tangent moduli of classical Perzyna viscoplasticity takes then the form

$$\left[\mathbf{E}^{alg}_{Per}\right]^{class} = \frac{d\, \boldsymbol{\sigma}}{d\, \boldsymbol{\epsilon}} = \mathbf{D} - \frac{\mathbf{D} : \Psi \otimes \mathbf{m} : \mathbf{D}}{\frac{\eta}{\Delta t} + \Psi : \mathbf{D} : \mathbf{m}} \tag{27}$$

Note: the algorithmic tangent operator obtained with the classical Perzyna formulation does not require the determination of the elastoplastic moduli tensor, as in case of Duvaut-Lions (1972) viscoplasticity, see Etse and Willam (1999). From eqs. (22) and (25) follow that the limiting case $\eta \to \infty$ results in instantaneous elasticity $\Delta\, \boldsymbol{\sigma} = \mathbf{E} : \Delta\, \boldsymbol{\epsilon}$ like the Duvaut-Lions viscoplastic material. On the other hand, when $\eta \to 0$ we obtain from eq. (26) $\mathbf{D}^{-1} \to \alpha_t \mathbf{M}$, with $\alpha_t = \frac{\Delta t}{\eta} \psi(F)$ or, alternatively $\mathbf{D} \to \alpha_t^{-1} \mathbf{M}^{-1}$. Thus, from eq. (27), the algorithmic tangent operator of the classical Perzyna formulation approaches

$$\left[\mathbf{E}^{alg}_{Per}\right]^{class} \to \alpha_t^{-1} \left[\mathbf{M}^{-1} - \frac{\mathbf{M}^{-1} : \Psi \otimes \mathbf{m} : \mathbf{M}^{-1}}{\Psi : \mathbf{M}^{-1} : \mathbf{m}} \right] \tag{28}$$

With other words, the limiting case $\eta \to 0$, i.e. $\alpha_t^{-1} \to 0$ in eq.(28), leads to the instantaneous fourth order zero tensor. Thus, the minimum eigenvalue of the underline normalized algorithmic tensor approaches zero indicating perfect viscoplasticity. In spite of this "apparent" regularization capability of the rate-dependent classical Perzyna formulation we will see in section 6 that in this extreme case numerical instability may arise due to the particular form which takes the consistent material moduli.
From eq.(27) follows that, when finite time increments are considered, the eigenvalue of the algorithmic tangent operator normalized with respect to the fourth order tensor **D** (see 26) yields

$$[\lambda_{\min}^{norm}]^{Per} = 1 - \frac{1}{1 - \frac{\frac{\eta}{\Delta t}}{\mathbf{n}:\mathbf{D}:\mathbf{m}}} \tag{29}$$

Thus, the condition for diffuse failure is fulfilled only when $\eta = 0$ (non viscosity effects) as long as $\mathbf{n} : \mathbf{D} : \mathbf{m}$ remains positive. However, due to the particular form of $\mathbf{D}$ in eq. (26), the extreme case $\eta \rightarrow 0$ may lead to quite different values of the bilinear form $\mathbf{n} : \mathbf{D} : \mathbf{m}$

Continuous Perzyna Formulation

Application of the BE or CPP for the integration of the relations (1), (7), (8) and (9) leads to

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}^e_{n+1} - \Delta\lambda\, \mathbf{E} : \mathbf{m}_{n+1} \tag{30}$$
$$\mathbf{q}_{n+1} = \mathbf{q}_n + \Delta\lambda \mathbf{H} : \mathbf{m}_{n+1} \tag{31}$$
$$\boldsymbol{\sigma}^e_{n+1} = \boldsymbol{\sigma}_n + \mathbf{E} : \Delta\, \boldsymbol{\epsilon}_{n+1} \tag{32}$$

with

$$\mathbf{m}_{n+1} = \left[\mathbf{A}^{-1} : (\frac{\partial F}{\partial\, \boldsymbol{\sigma}})\right]_{n+1} \tag{33}$$

The BE enforces the generalized consistency of the continuous formulation of Perzyna viscoplasticity and, from the mathematical point of view, defines the stress projection which is carried out in the Euclidean norm for isotropic elastic and non–associated plastic properties. Therefore, this method is equivalent to the solution of the standard minimization problem

$$minE\{\, \boldsymbol{\sigma}\} \tag{34}$$

with the auxiliary condition $\bar{F}(\, \boldsymbol{\sigma}_{n+1},\, \mathbf{q}_{n+1}) = 0$. $E\{\, \boldsymbol{\sigma}\}$ designates the complementary energy, which for the time step $t = t_{n+1}$ is defined as

$$E\{\, \boldsymbol{\sigma}_{n+1}\} = \frac{1}{2}(\, \boldsymbol{\sigma}^e_{n+1} - \, \boldsymbol{\sigma}_{n+1}) : \mathbf{C}_A : (\, \boldsymbol{\sigma}^e_{n+1} - \, \boldsymbol{\sigma}_{n+1}) \rightarrow \text{Min} \tag{35}$$

whereby

$$\mathbf{C}_A = \mathbf{A} : \mathbf{C} \tag{36}$$

denotes the tensor of elastic compliance moduli that have been transformed by the non-associativity operator $\mathbf{A}$, cf. Weihe (1989).
The algorithmic tangent operator can be formulated from the linearization of the differential form of the generalized consistency condition

$$d\bar{F} = \frac{\partial \bar{F}}{\partial\, \boldsymbol{\sigma}} : d\, \boldsymbol{\sigma} + \frac{\partial \bar{F}}{\partial \mathbf{q}} : d\mathbf{q} + \frac{\partial \psi^{-1}\left(\dot{\lambda}\cdot\eta\right)}{\partial \dot{\lambda}}\ddot{\lambda} = \tag{37}$$

In order to avoid further complications, it's supposed that $\dot{\lambda}$ is accurately approximated by $\dot{\lambda} = \frac{\Delta\lambda}{\Delta t}$, i.e. $\Delta\lambda = \frac{\Delta t}{\eta}\langle\psi(F)\rangle$. This assumption leads to $\dot{\lambda} = \frac{\Delta\lambda}{\Delta t^2}$, then, (37) is rewritten

$$\bar{\mathbf{n}} : d\,\boldsymbol{\sigma} + \bar{\mathbf{r}} : d\mathbf{q} + \frac{\partial\psi^{-1}\left(\dot{\lambda}\cdot\eta\right)}{\partial\dot{\lambda}}\frac{\Delta\lambda}{\Delta t^2} = 0 \tag{38}$$

quite similar to the inviscid elastoplastic case, which is fully recover when $\eta \to 0$ regarding that $\psi(0) = 0$. Moreover, we observe that the gradient tensors

$$\bar{\mathbf{n}} = \frac{\partial\bar{F}}{\partial\,\boldsymbol{\sigma}} = \frac{\partial F}{\partial\,\boldsymbol{\sigma}} + \frac{\partial\psi^{-1}\left(\eta\dot{\lambda}\right)}{\partial\,\boldsymbol{\sigma}} = \mathbf{n} + \hat{\mathbf{n}} = \mathbf{n} \tag{39}$$

where $\frac{\partial\psi^{-1}(\eta\dot{\lambda})}{\partial\,\boldsymbol{\sigma}}$ is a null second order tensor and

$$\bar{\mathbf{r}} = \frac{\partial\bar{F}}{\partial\mathbf{q}} = \frac{\partial F}{\partial\mathbf{q}} = \mathbf{r} \tag{40}$$

Proceeding in a similar form to the algebraic elastoplastic problem, i.e. substituting in eq. (38) the differential changes of the stress tensor and of the state variables evaluated in a consistent form with the BE

$$d\,\boldsymbol{\sigma} = \mathbf{E}^m : (d\,\boldsymbol{\epsilon} - d\Delta\lambda\mathbf{m}) \tag{41}$$

$$d\mathbf{q} = d\Delta\lambda\mathbf{H} : \mathbf{m} + \Delta\lambda\mathbf{H} : \mathbf{m}\,(\mathbf{m} : \mathbf{M} : d\,\boldsymbol{\sigma}) \tag{42}$$

where $[\mathbf{E}^m]^{-1} = \left(\mathbf{E}^{-1} + \Delta\lambda\mathbf{M}\right)$ we obtain the relations $d\,\boldsymbol{\sigma} = \left[\mathbf{E}^{alg}_{Per}\right]^{cont} : d\,\boldsymbol{\epsilon}$, with the algorithmic operator

$$\left[\mathbf{E}^{alg}_{Per}\right]^{cont} = \mathbf{E}^m - \frac{\mathbf{E}^m : \mathbf{m}\otimes\mathbf{n} : \mathbf{E}^m + \Delta\lambda\mathbf{r}\,\|\mathbf{m}\|\,\mathbf{E}^m : \mathbf{m}\otimes\mathbf{m} : \mathbf{M} : \mathbf{E}^m}{\bar{E}^n_m + E^p + \Delta\lambda E^m_m + \frac{\partial\psi^{-1}(\dot{\lambda}\cdot\eta)}{\partial\dot{\lambda}}\cdot\frac{\Delta\lambda}{\Delta t^2}} \tag{43}$$

with the scalar values $\bar{E}^n_m$, E^p and E^m_m defined as

$$\bar{E}^n_m = \mathbf{n} : \mathbf{E}^m : \mathbf{m} \tag{44}$$

$$E^p = -\mathbf{r} : \mathbf{H} : \mathbf{m} \tag{45}$$

$$E^m_m = \mathbf{r} : \mathbf{H} : \mathbf{m}\,(\mathbf{m} : \mathbf{M} : \mathbf{E}^m : \mathbf{m}) \tag{46}$$

The last three equations are completely similar to the elastoplastic case.
Note: the algorithmic tangent operator of the continuous formulation approaches the consistency operator of the rate–independent elastoplastic case when $\eta \to 0$. The other extreme case, when $\eta \to \infty$ leads to the elastic tensor.

With other words, the continuous formulation of Perzyna viscoplastic materials leads to algorithmic tangent tensors which signal a smooth transition between the elastic one and that of the elastoplastic case.

CONCLUSIONS

In this paper two different formulations for Perzyna viscoplasticity were analyzed. Considering the time integration of real viscoplastic material processes within finite time increments, then the algorithmic tangent operator replace the instantaneous one which do not exhibit degradation of the elastic properties. From the consistent linearization process based on the Backward Euler method for time integration of the differential equations, the algorithmic tangent operator of both Perzyna formulations were obtained which exhibit quite different features. This fact is responsible for failure predictions which show considerable disagreement when the viscosity approaches zero. In this extreme case the classical Perzyna model do not reproduce the predictions of the inviscid material. The fourth order algorithmic material tensor approaches zero and the performance of the diffuse and localized failure indicators will exhibit strong oscillations and even discontinuities due to numerical instabilities which arise frome the time integration process.
On the other hand the continuous Perzyna formulation leads to algorithmic material operators which exhibit a smooth transition from the elastic to the elastoplastic tensor according to the assumed value for the viscosity. Therefore, when η approaches zero the same localization predictions as the inviscid material are obtained.

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