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Smooth finite strain plasticity with non-local pressure support

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SUMMARY

The aim of this work is to introduce an alternative framework to solve problems of finite strain elasto-plasticity including anisotropy and kinematic hardening coupled with any isotropic hyperelastic law. After deriving the constitutive equations and inequalities without any of the customary simplifications, we arrive at a new general elasto-plastic system. We integrate the elasto-plastic algebraico-differential system and replace the loading–unloading condition by a Chen–Mangasarian smooth function to obtain a non-linear system solved by a trust region method. Despite being non-standard, this approach is advantageous, since quadratic convergence is always obtained by the non-linear solver and very large steps can be used with negligible effect in the results. Discretized equilibrium is, in contrast with traditional approaches, smooth and well behaved. In addition, since no return mapping algorithm is used, there is no need to use a predictor. The work follows our previous studies of element technology and highly non-linear visco-elasticity. From a general framework, with exact linearization, systematic particularization is made to prototype constitutive models shown as examples. Our element with non-local pressure support is used. Examples illustrating the generality of the method are presented with excellent results. Copyright © 2009 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Association of the return-mapping technique [1–3] and well-founded mixed formulations [4, 5] led to a standardization of elasto-plastic modeling with finite elements (see the treatise by Belytschko and co-workers [6]). However, the return-mapping algorithm still poses challenges to systematization: the predictor in the presence of damage may give a false indication and there is an implied inequality for the plastic multiplier. Another problem for implicit return mapping occurs when the

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hardening law depends on the plastic strain rate and temperature, such as in the Johnson–Cook model and certain Nemat-Nasser models [7]: the predictor can also give a false indication, since typically the plastic strain rate may raise the yield stress and produce spurious results. Empirical integration methods have been devised for each case (see, e.g. [8]).

Besides the problems with the predictor, the convergence radius is often not satisfactory (Crisfield and Norris [9] show dense clouds of points due to step halving). Here, we introduce a new finite strain elasto-plastic algorithm able to include, in the same underlying framework, kinematic hardening, anisotropy, damage, etc. This differs from our recent application to non-linear viscoelasticity [10], where the constitutive system was smooth.

Few, if any, attempts have been made to integrate the general finite strain elasto-plastic constitutive system. Typically, strong assumptions and simplifications are made, which substantially reduce the true complexity of the problem (small elastic strains and/or isotropic plasticity and coaxiality are often assumed). For the continuum case, a notable exception has been the work of Nemat-Nasser [3], which showed the complete system in continuum form. However, to our knowledge, no attempt to implicitly integrate it has been made.

As for the finite element part, recent experiments with the inf–sup (IS) test (e.g. [5]) led to a simple element with non-local pressure support (see also [10]).

Concerning certain simplified (small strain or coaxial) constitutive models, solutions based on the dual formulation are now strongly established both with predictor/corrector [1] and Shur-based methodologies [11]. We propose here an alternative that consists of smoothing the loading/unloading condition (also called complementarity condition, see Han and Reddy [12, p. 60, Equation 3.37] and solving monolithically the resulting system. That system can therefore be solved by classical Newton-based root finders. Accuracy of the solution depends on the smoothing parameter, which measures the distance to the origin of the complementarity graph. Mathematical foundations of this method were established by Chen and Mangasarian [13].

Numerous works have shown the advantages of ordinary differential equation (ODE) integration and correct calculation of the derivatives in loading for elasto-plastic problems. This is often called ‘consistent linearization’ and was introduced for smooth constitutive calculations context by Hughes and Taylor [14] and for non-smooth problems by Simo and co-workers (see the monograph [2]). The linearization consists of an application of the chain rule and, in the finite strain case, use of Lie group theory.

For elastoplasticity, however, the overall problem remains non-smooth [12, 15, 16]. For a sequence of global iterations, a given quadrature point can have successive loading/unloading or reloading/unloading states. Because derivatives are not continuous, erratic behavior is often observed.

The primal version of the FEM in small strains has a relatively straightforward weak form with a differential inclusion. For finite strains, because the elastic part of the deformation gradient depends implicitly on the stress, this simplicity cannot be retained. The dual form is advantageous from the implementation point of view. Numerous papers have dealt with $J_2$ [17–20] plasticity in finite strains including kinematic hardening. Cost-effective algorithms are then adopted for von-Mises plasticity, based on radial-return technique (parallel trial elastic strain and final deviatoric stress [1]) that reduces the constitutive solution to one algebraic equation. In that case, for finite strains the additional condition of coaxiality of the strain measures and the Kirchhoff stress is either verified or imposed. This started with the paper by Weber and Anand [21]. Semi-implicit methods, which freeze the flow vector in the solution, hence retaining the attractiveness of the Key and Krieg approach for more complex cases, have been disseminated by Moran and co-workers.
Other yield functions require the direct use of Lee’s decomposition [23] and monolithic integration. This has been done for a similar case by Hartmann et al. [24] and it was applied to the von-Mises yield criterion. The lack of smoothness of the problem is still not tackled consistently for this case. We first enumerate our requirements to clarify the options:

- Use of isotropic hyperelastic law: $T_t \equiv T_t(V^e)$, where $V^e$ is the left elastic stretch tensor and $T_t$ is the Kirchhoff stress measure (see [25, p.142] for the isotropy limitation).
- Unique framework for viscoelasticity, viscoplasticity and elastoplasticity with no restrictions in the form either of the flow law or the yield function.
- Use of any kinematic hardening model (including multi-surface models) as an additional equations to the system.
- Element-independence: specific properties of the elements, such as mixed or hybrid techniques should not be used to simplify the constitutive calculations.

For moderate elastic strains (often the case for metals), simplified methods are often used, such as the ‘rotated configuration’ by Areias and Belytschko [26]. With the previous work [10], topics covered are:

- Quantified evaluation of absence of locking and spurious modes in the nearly incompressible regime.
- Integration of the constitutive ODE and incompressibility preservation.
- Objectivity and monotonicity of the back-stress treatment.
- Smoothing the loading/unloading condition or use of a non-smooth solver.

The first two themes were treated in our previous work. In the essence, the behavior of an element with constraints introduced by the material it represents is indicated by the inspection of the IS value with mesh refinement. We evaluated this behavior [10] and it confirms, for the specific conditions shown here, that the stability and convergence are satisfied.

2. FORMULATION OF THE COUPLED EQUILIBRIUM/CONSTITUTIVE PROBLEM

2.1. Governing equations

A given open set $\Omega_0 \subset \mathbb{R}^3$ is the reference configuration of a given body: each point $X$ is associated by a bijective map to its position in that configuration: $X \rightarrow x \in \Omega_0$. See Figure 1 for a clarification of this notation. In the absence of discontinuities of maps defined in $\Omega_0$, a unique deformation map $\phi(X) \in \mathcal{H}^{-1}(\Omega_0)^{n_{sd}}$ exists such that any position besides the reference one is determined $x = \phi(X)$ with the difference being $u = x - X$. We use the standard notation $n_{sd}$ as the number of space dimensions. The deformation gradient is obtained as $F = \nabla_0 \phi(X)$, where $\nabla_0$ represents the gradient with respect to $X$. The Jacobian of the deformation map is given by $J = \det F$ and represents the local volume ratio.

The deformation gradient is decomposed into elastic ($e$) and plastic ($p$) parts, using Lee’s decomposition [23]: $F = F^e F^p$ where $F^e$ includes the lattice rotation, in the sense of Nemat-Nasser (see [3, p. 250]), but with a redefinition of $F^e$

$$F = V^e Q U^p$$ (1)
with $V^e$ being the left elastic stretch tensor, $Q$ the orthogonal rotation tensor (such that $F^e = V^eQ$, a variant of [3] valid for isotropic elastic laws) and $U^p = FP$ the right plastic stretch tensor. Since there is no danger of mixing $V^e$ and $U^p$ with their total counterparts we drop the superscripts from this point on. From the elastic part we extract the elastic left Cauchy–Green tensor $V^2 = F^eF^eT$ and from the plastic part the right Cauchy–Green tensor $C = U^2$ is obtained (we also omit the superscripts $e$ and $p$ for $V$ and $C$, respectively). The first Piola–Kirchhoff stress $P$ is related to the body forces $B_0(X) \in L^2(\Omega_0)$ by the equilibrium equation. Cauchy stresses (required for the elasto-plastic model) are obtained as $\sigma = (1/J)PF^T$. Body forces are assumed to be defined in the reference configuration.

The outer boundary of $\Omega_0$ is partitioned into two sets: the Neumann set, $\Gamma_{\partial \Omega}$ where some stress components are known and the Dirichlet set, $\Gamma_{\partial \Omega}$ where some components of displacement are known. Also used is the Kirchhoff stress, $T_i = J\sigma$ that depends on $V$, which indeed restricts the elastic law to be isotropic [25]. Since for metals, elastomers and other materials often $J \approx 1$ then we can write $\sigma \approx T_i$.

After introducing a yield function, $\phi$, we can calculate the flow vector $N$, which is the gradient with respect to its tensorial argument. This is convenient to remove one term in the linearization operation. When writing the back stresses $B$, it is assumed that these are Kirchhoff back stresses.

The strong form of the governing equations is first shown. The system consists of equilibrium equations, essential and natural boundary conditions and the constitutive laws for both stress, plastic rate and rate of back stresses. In addition, there is the loading/unloading condition (also known as the complementarity condition [12]), a switch between purely hyperelastic and hyperelastic/plastic behavior. After regularization of the governing equations, we introduce a smooth version of the

Figure 1. Problem description: finite strain elastoplasticity with non-local pressure.
complementarity condition and perform a semi-discretization of the partial differential equation (PDE) part of the equations followed by a backward time-stepping method.

For isotropic elasticity and symmetric flow vector, the problem can be written as:

Find $u(X, t), U(X, t), \dot{\gamma}(X, t)$ and $B(X, t)$ such that

\[
\nabla_0 \cdot P^T + B_0 = 0 \quad \text{in } \Omega_0
\]

\[
u = \overline{u} \quad \text{on } \Gamma_\nu
\]

\[
t = \overline{t} \quad \text{on } \Gamma_\nu
\]

\[
T = T(FU^{-1})
\]

\[
P = \pi F^{-T} + T F^{-T}
\]

\[
N = N(T, B, \gamma)
\]

\[
\dot{U} = \text{arg}((FU^{-1} \dot{U}_t F^{-1})_{\text{symm.}} - \gamma N = 0]
\]

\[
\begin{aligned}
\dot{\circ}B &= \dot{\gamma} g(T, B, \gamma) \\
\phi(T, B, \gamma) &\leq 0 \\
\dot{\gamma} &\geq 0 \\
\phi(T, B, \gamma) \dot{\gamma} = 0
\end{aligned}
\]

where $(\bullet)_{\text{symm.}}$ indicates the symmetric part of $\bullet$.

The system consists of a second-order PDE (2) with boundary conditions (3)–(4), three algebraic equations (5)–(7), two first-order ODEs (8)–(9) and the complementarity condition (10)–(12). The latter can be replaced by a first-order non-smooth ODE

\[
c_d \dot{\gamma} - [c_d \dot{\gamma} + \phi(T, B, \gamma)]_+ = 0
\]

where $[x]_+ = \max(0, x)$ for $x \in \mathbb{R}$ and $c_d \in \mathbb{R}^+$ is a dimensional parameter ensuring dimensional consistency. In (8) $\dot{U}_t$ is unknown.

Frequently, authors fail to recognize the intricate form of the flow law (8) and provide ill-explained explicit approximations to it. However, authoritative works in the subject clearly advertise this fact (see, e.g. Equation 4.9.27 in [3] and the derivations in [27]). Note that a closed-form solution of (8) exists and is used here, perhaps for the first time. Using Voigt notation (identified by a subscript $v$) we can write Equation (8) as

\[
\dot{U}_v = \dot{\gamma} \Phi^{-1} N_v
\]

with $\Phi^{-1}$ being calculated by Mathematica [28] with the AceGen add-on.

In Equation (9) we use the Lie derivative with respect to the elastic velocity gradient. As stated by Johansson et al. [20] the material derivative is not objective, the fact that being overlooked by many authors, even in recent papers.

The constitutive pressure, $\tilde{\pi}$, is completely defined given $J$, by means of a constitutive equation [29]. In contrast, the equilibrium pressure, $\pi$, which is used in the equilibrium system, is
obtained indirectly from $\tilde{\pi}$ by an inhomogeneous Helmholtz equation which is added to the global system. The constitutive pressure, $\tilde{\pi}$, is obtained using a convex bulk strain energy density and reads

$$\tilde{\pi} \equiv g(J) = \kappa [J^2 - J + \ln(J)] \quad (15)$$

and the equilibrium pressure, $\pi$, is obtained from the solution of the following inhomogeneous Helmholtz equation [30]:

$$\pi - c_0 \nabla^2_0 \pi - \tilde{\pi} = 0 \quad (16)$$

where $\nabla^2_0$ is the Laplace operator with respect to the material coordinates. The parameter $c_0$ controls the non-locality of the pressure field. After imposing a zero flux in the boundaries, $\nabla_0 \pi \cdot \mathbf{N}_0 = 0$ for $\mathbf{X} \in \Gamma_0$ (this was introduced by Lasry and Belytschko [31]) we can write a weak form of (16)

$$\int_{\Omega_0} [\pi^A(\pi - \pi) + c_0 \nabla_0 \pi^A \cdot \nabla_0 \pi] dV_0 = 0 \quad (17)$$

for all admissible variations $\pi^A \in [H^1(\Omega_0)]^1$ with $[H^1(\Omega_0)]^{n_{sd}}$ denoting the Sobolev space of square-integrable functions with weak derivatives up to order one with range in $\mathbb{R}^{n_{sd}}$. The stabilizing effect of (17) in the solution is illustrated in the diagram of Figure 2. In this diagram, we show the effect of $\sqrt{c_0}$ and the distribution of $\tilde{\pi}$ in the response $\pi$. We can observe that $c_0$ has a strong effect in the width and height of the equilibrium pressure and that spikes in pressure are filtered.

2.2. Smoothing of the complementarity condition

Owing to the presence of the plus function in (13), the constitutive system is non-smooth. Although specific solvers have been developed to solve this type of problems, (e.g. [32]) smoothing methods have also been very successful (the paper by Areias and Rabczuk [33] shows an example). By using the Chen and Mangasarian [13] smoothing method, we can use a smooth root finder. The ‘plus’ function $[x]_+$ is replaced by the smooth ramp function $S(x) : [x]_+ \equiv S(x)$.

This function is given by

$$S(x) = x + \frac{1}{\beta} \ln(1 + e^{-\beta x}) \quad (18)$$

where $\beta$ is a parameter controlling the accuracy of reproduction of the original function. The parameter $\beta$ is obtained as a fraction of the initial yield stress $\sigma_{0y}$ as

$$\beta = \frac{0.693147}{\text{tol} \sigma_{0y}} \quad (19)$$

where tol is a new constitutive property. This value of $\beta$ is obtained by solving:

$$\min_x \left\{ x^2 + \left[ \frac{\ln(1 + e^{-\beta x})}{\beta} \right]^2 \right\} \quad (20)$$
Figure 2. Effect of $c_0$ and the spatial distribution of $\tilde{\pi}$. We use the conditions $\pi'(x=0)=0$ and $\lim_{x\to \infty} \pi'=0$. Smearing of $\tilde{\pi}$ occurs and this allows an artificial support for the pressure. The equation $\pi - c_0 \pi'' - \tilde{\pi} = 0$ is solved in $x \in ]0, +\infty[$ and $\tilde{\pi} = 1$ for $x \leq a$.

After performing the necessary substitutions, the graph of $c_d \dot{\gamma} - S[c_d \dot{\gamma} + \phi] = 0$ for normalized $\phi$ is shown in Figure 3 for several values of tol. We can see that tol corresponds to the maximum difference in the yield function near the tip of the complementarity condition, i.e. $\dot{\gamma} \phi = 0$. It converges to the exact result as tol is decreased, since

$$\lim_{\beta \to +\infty} [S(x) - [x]_+] = 0 \quad \forall x \in \mathbb{R}$$

(21)

can be proved.
2.3. Time integration, constitutive solution and linearization

Time integration provides constitutive quantities at time step \( t \) given all quantities in \( t_0 < t \) and \( F \) at time step \( t \); \( F \) is provided by the equilibrium iteration. To calculate the remaining constitutive quantities, we introduce a general integration procedure, prone to exact linearization of most particular elasto-plastic laws. Specific laws will be casted into this framework.

To simplify the notation we introduce the following auxiliary quantities:

\[
Z = (U^{-1})_v
\]

\[
vZ_0 = (U_0^{-1})_v
\]

with the subscript \( v \) being the Voigt form of the corresponding argument, which must be a symmetric tensor. In general, using the Voigt matrix \( v \),

\[
v = \begin{bmatrix}
1 & 4 & 5 \\
4 & 2 & 6 \\
5 & 6 & 3
\end{bmatrix}
\]

we obtain \( Z_{ij} = [U^{-1}]_{ij}, i, j = 1, 2, 3 \); the matrix form of \( Z \) being denoted as \( Z \). The notation \( (\bullet)' = \partial \bullet / \partial \Delta y \) is also used for conciseness.

To clarify the notation, blackboard style is used for the Voigt form of full minor-symmetric fourth-order tensors, calligraphic style is used for the Voigt form of fourth-order tensors with
minor symmetry in the first two indices only; sans-serif notation is reserved for the Voigt form of second-order tensors.

Using this notation, the smoothed complementarity condition is integrated implicitly as

\[ \mu \Delta \gamma - S \{ \mu \Delta \gamma + \phi [T(Z), B, \Delta \gamma] \} = 0 \]  

and the integrated flow law is given by

\[ \mathbb{P} \mathbb{Z} = \{ I - \Delta \gamma N [T(Z), B, \Delta \gamma] \} \]  

with \( \mathbb{L} = (1 1 1 0 0 0)^T \). The fourth-order symmetric tensor \( \mathbb{P} \) is calculated using Mathematica 6.0 [28] as the derivative of the left-hand side with respect to \( Z \).

Back stresses are integrated using the approximation \( \mathbb{B} = \mathbb{B} + \Delta \gamma \mathbb{g} [T(Z), B, \Delta \gamma] \)

with \( \mathbb{B} \) being also calculated as a derivative of the corresponding Truesdell rate with respect to \( B \).

Linearization of Equations (25)–(27) is required both for the constitutive solution and the application of the equilibrium Newton–Raphson method. When solving the constitutive system, unknowns are \( \Delta \gamma, Z, \text{ and } B \). For the equilibrium Newton–Raphson method, the derivative of \( T \) with respect to \( F \) is required:

\[ \mathbf{\varepsilon} = \frac{\partial T}{\partial F} \]  

The non-linear constitutive system consists of finding the roots of the following equations:

\[ R_1 = \mu \Delta \gamma - S \{ \mu \Delta \gamma + \phi [T(Z), B, \Delta \gamma] \} \]  

\[ R_2 = \mathbb{P} \mathbb{Z} - I + \Delta \gamma N [T(Z), B, \Delta \gamma] \]  

\[ R_3 = B - B_0 - \mathbb{B} - \Delta \gamma \mathbb{g} [T(Z), B, \Delta \gamma] \]

with zero left-hand sides.

The Jacobian of this system is concisely written as

\[ \mathbf{J} = \begin{bmatrix} J_{11} & J_{12}^T & J_{13}^T \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix} \]  

where

\[ J_{11} = \mu - S' (\mu + \phi') \]  

\[ J_{12} = -S' N_1\mathbb{M} \]  

\[ J_{13} = S' N_2 \]  

\[ J_{21} = N \]
\[ J_{22} = P + \Delta \gamma UM \]  
(37)  
\[ J_{23} = -\Delta \gamma U \]  
(38)  
\[ J_{31} = -g - \Delta \gamma g' \]  
(39)  
\[ J_{32} = -\Delta \gamma GM \]  
(40)  
\[ J_{33} = I - B - \Delta \gamma \]  
(41)  

and

\[ N_2 = \frac{\partial \phi}{\partial \mathbf{T}} \]  
(42)  
\[ \mathbb{M} = \frac{\partial \mathbf{T}}{\partial \mathbf{Z}} = \left( \frac{\partial \mathbf{T}}{\partial \mathbf{F}^t} \right)_v \]  
(43)  
\[ \mathbb{U} = \frac{\partial \mathbf{N}}{\partial \mathbf{T}} \]  
(44)  
\[ \mathbb{G} = \frac{\partial g}{\partial T} \]  
(45)  
\[ \mathbb{H} = \frac{\partial g}{\partial B} \]  
(46)

Note that \( N \neq N_2 \) since, in the latter, the Voigt form of \( \mathbf{T} \) is used. We can write

\[ N_2 = l_6 N \]  
(47)

where \( l_6 \) is obtained from the \( 6 \times 6 \) identity matrix by replacing 1 by 2 in the \((4, 4), (5, 5)\) and \((6, 6)\) components.

It can be observed that the deformation gradient is present in \( \mathbb{P}, \mathbb{B} \) and \( \mathbf{T} \); the infinitesimal variation of \( \mathbf{T} \) with \( \mathbf{F} \) is simply given as a differential form as

\[ d\mathbf{T} = \mathcal{D} : d\mathbf{F} = \mathbb{M} : d\mathbf{Z} + \mathcal{N} : d\mathbf{F} \]  
(48)

where

\[ \mathcal{N} = \frac{d\mathbf{T}}{d\mathbf{F}^c} : \mathbf{Z} \]  
(49)

The remaining non-trivial derivatives are

\[ \mathcal{D} = \left[ \frac{d}{d\mathbf{F}} (\mathbf{F} \mathbf{Z} \mathbf{Z}^{-1} \mathbf{F}^{-1})_{\text{symm.}} \right]_v \]  
(50)

\[ \mathcal{B} = \frac{d}{d\mathbf{F}} (\mathbf{B} \mathbf{B}) \]  
(51)

which we calculate using Mathematica 6.0 [28] with the AceGen add-on.
Linearization follows directly from the solution of the modified linear system (whose coefficient matrix is still $J$)

$$
\begin{align*}
\mathbf{J} \left\{ \begin{array}{l}
\frac{d\gamma}{dt} \\
\frac{d\mathbf{Z}}{dt} \\
\frac{dB}{dt}
\end{array} \right\} &= - \left\{ \begin{array}{l}
\mathbf{J}_1 \mathbf{F} : \frac{d\mathbf{F}}{dt} \\
\mathbf{J}_2 \mathbf{F} : \frac{d\mathbf{F}}{dt} \\
\mathbf{J}_3 \mathbf{F} : \frac{d\mathbf{F}}{dt}
\end{array} \right\}
\end{align*}
$$

(52)

where:

$$
\begin{align*}
\mathbf{J}_1 &= - \mathbf{S}^T \mathbf{N}_2 \mathbf{N} \\
\mathbf{J}_2 &= \mathbf{D} + \Delta \gamma \mathbf{U} \\
\mathbf{J}_3 &= - \mathbf{B} - \Delta \gamma \mathbf{G} \\
\end{align*}
$$

(53, 54, 55)

Of course, only the second equation in (52) is relevant, which can be re-written as

$$
\frac{d\mathbf{Z}}{dt} = - \left( \mathbf{J} \mathbf{F} : \frac{d\mathbf{F}}{dt} \right)_{21} \otimes \mathbf{J}_1 \mathbf{F} + \left( \mathbf{J} \mathbf{F} : \frac{d\mathbf{F}}{dt} \right)_{22} \mathbf{J}_2 \mathbf{F} + \left( \mathbf{J} \mathbf{F} : \frac{d\mathbf{F}}{dt} \right)_{23} \mathbf{J}_3 \mathbf{F}
$$

(56)

resulting in the sum of an elastic and an elasto-plastic tangent:

$$
\mathbf{\sigma} = \mathbf{\mathcal{N}} + \mathbf{M} \mathbf{\mathcal{T}}_{ZF}
$$

(57)

Accuracy of this approach can be assessed for the plane-stress case (imposed by zeroing the $T_{33}$ stress by modifying $F_{33}$). Iso-error maps for $tol = 1 \times 10^{-2}$ and plane stress are shown in Figure 4. Note that these are finite strain error maps and, in addition to the constitutive integration error, kinematical approximations (such as the velocity gradient $\mathbf{L}$) also contribute for the error.

### 2.4. Specific constitutive equations

Prototype models are used for the testing purposes. Both von-Mises and Hill yield criteria are used, and both isotropic and combined isotropic/kinematic hardening laws are inspected. The yield function $\phi(T, B, \Delta \gamma)$ is decomposed as (Table I)

$$
\phi(T, B, \Delta \gamma) = y(T - B) - \sigma_y(\Delta \gamma)
$$

(58)

where $y$ is called the equivalent stress and $\sigma_y$ is the hardening function. More complex models (see [37]) do not require large modifications.

### 2.5. Weak form—equilibrium and first variation

The Galerkin method is used to obtain a weak form of equilibrium. This was performed before for the equilibrium pressure in (17). The test functions for the equilibrium equation are now vector fields, which we denote by $\mathbf{x}^A \in \mathcal{H}^{-1}(\Omega_0)^3$. After writing the weak form, a symmetric discretization is employed to obtain an algebraic system.

To simplify the notation, we introduce the notation $\mathbf{T} = \mathbf{T}_i - g(J)\mathbf{I}$, resulting in:

$$
W^A = \int_{\Omega_0} \left\{ \mathbf{T} : \nabla \mathbf{x}^A + c_0 \nabla_0 \pi \cdot \nabla_0 \pi^A - g(J)\pi^A + \pi \mathbf{I} : \nabla \mathbf{x}^A + \pi \pi^A + \mathbf{B}_0 \cdot \mathbf{x}^A \right\} = 0
$$

(59)
Neo-Hookean material von-Mises yield criterion

\[ y = 300 \]

\[ \varepsilon = \frac{(\mathbf{T} - \mathbf{T}^\ast):(\mathbf{T} - \mathbf{T}^\ast)}{\sqrt{\mathbf{T}^\ast:\mathbf{T}^\ast}} \]

Plane stress \([T_{33}(F_{33}) = 0]\)

Figure 4. Finite strain iso-error maps \((\text{tol}=1 \times 10^{-2})\) for plane stress.

Table I. Back-stress laws in Voigt form.

<table>
<thead>
<tr>
<th>Back-stress law</th>
<th>(g(\mathbf{T}, \mathbf{B}, \dot{\gamma}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>0</td>
</tr>
<tr>
<td>Tsakmakis and Willuweit [34]</td>
<td>((c\mathbf{N} - b\mathbf{B}))</td>
</tr>
<tr>
<td>Burlet–Cailletaud [36]</td>
<td>([c\mathbf{N} - b\mathbf{B}]_{\mathbf{N}\otimes\mathbf{N}}:\mathbf{B})</td>
</tr>
</tbody>
</table>

A Newton–Raphson-based solver is used, and therefore exact derivatives of all quantities in (59) are required. The time derivative of \(\mathbf{T}\) is given by

\[ \dot{\mathbf{T}} = \nabla \mathbf{x} \mathbf{T} + \mathbf{T} \nabla \dot{\mathbf{x}}^T + \mathbf{D} : \nabla \dot{\mathbf{x}} \]  

(60)
where $\mathbb{D}$ can be calculated from $\mathcal{E}$ as

$$
\mathbb{D}((q)n)(k)p = \mathcal{E}((q)n)k_j F_{pj} - T_{(q)p}\delta_{(nk)} - T_{(p)n}\delta_{(kq)}
$$

(61)

where the parenthesis in the index notation point out the Voigt grouping.

This useful relation (61) between moduli is obtained by re-deriving the work of Truesdell and Noll ([38, pp. 131–133]). Despite being more direct than the often used push-back/linearize/push-forward procedure, the authors could not find this relation in the bibliography. The reader can note that no deviatoric projection is required (as in, e.g. [2]).

Time derivative of $\mathbf{T}:\nabla \mathbf{x}$ is given by the well-known (cf. [39]) relation:

$$
(\mathbf{T} : \dot{\nabla} \mathbf{x}) = \dot{\nabla} \mathbf{x} : \mathbb{D} : \dot{\nabla} \mathbf{x} + (\dot{\nabla} \mathbf{x}^T \nabla \mathbf{x} + \nabla \mathbf{x}^T \dot{\nabla} \mathbf{x}) : \mathbf{T}
$$

(62)

The linearized form of the equations is easily obtained with this relation, and the final partitioned result is shown

$$
\dot{\mathbf{W}} = \int_{\Omega_0} \left\{ \nabla \mathbf{x}^\Lambda : \mathbb{D} : \nabla \mathbf{x} + (\nabla \mathbf{x}^T \nabla \mathbf{x}^\Lambda + \nabla \mathbf{x}^\Lambda) : \mathbf{T} \right. \\
\left. - \pi^\Lambda \mathbf{J} g'(\mathbf{J}) \mathbf{I} : \nabla \mathbf{x} + \mathbf{\dot{\pi}} \mathbf{I} : \nabla \mathbf{x}^\Lambda + c_0 \nabla_0 \pi^\Lambda \cdot \nabla_0 \mathbf{\dot{\pi}} + \pi^\Lambda \mathbf{\dot{\pi}} \right\} d\Omega_0
$$

(63)

$$
(64)
$$

where, for the formulation in use, $\nabla \mathbf{x}^\Lambda = \mathbf{0}$.

2.6. Discretization

The discretization is performed for the nodal unknowns $\{\mathbf{x}_K, \pi_K\}$ as

$$
\mathbf{x}_h = \sum_{K=1}^{4} N_K \mathbf{x}_K
$$

(65)

$$
\pi_h = \sum_{K=1}^{4} N_K \pi_K
$$

(66)

where $K$ represents a local node number.

A symmetric discretization is employed for the test functions:

$$
\mathbf{x}_h^\Lambda = \sum_{K=1}^{4} N_K \mathbf{x}_K^\Lambda
$$

(67)

$$
\pi_h^\Lambda = \sum_{K=1}^{4} N_K \pi_K^\Lambda
$$

(68)

The gradients are calculated using the shape function derivative tables $\mathbf{N}_n$ and $\mathbf{N}_{n0}$ from

$$
\nabla \mathbf{x}_h^T = \mathbf{N}_n \mathbf{x}_n
$$

(69)

$$
\nabla_0 \pi_h = \mathbf{N}_{n0} \pi_n
$$

(70)

$$
\nabla \mathbf{v}_h^T = \mathbf{N}_n \mathbf{v}_n
$$

(71)

$$
\nabla_0 \xi_h = \mathbf{N}_{n0} \xi_n
$$

(72)

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DOI: 10.1002/nme
where

\[
N_n = \begin{bmatrix}
\frac{dN_1}{dx_1} & \frac{dN_2}{dx_1} & \frac{dN_3}{dx_1} & \frac{dN_4}{dx_1} \\
\frac{dN_1}{dx_2} & \frac{dN_2}{dx_2} & \frac{dN_3}{dx_2} & \frac{dN_4}{dx_2} \\
\frac{dN_1}{dx_3} & \frac{dN_2}{dx_3} & \frac{dN_3}{dx_3} & \frac{dN_4}{dx_3}
\end{bmatrix}
\] (73)

and

\[
N_{n0} = \begin{bmatrix}
\frac{dX_1}{dx_1} & \frac{dX_2}{dx_1} & \frac{dX_3}{dx_1} & \frac{dX_4}{dx_1} \\
\frac{dX_1}{dx_2} & \frac{dX_2}{dx_2} & \frac{dX_3}{dx_2} & \frac{dX_4}{dx_2} \\
\frac{dX_1}{dx_3} & \frac{dX_2}{dx_3} & \frac{dX_3}{dx_3} & \frac{dX_4}{dx_3}
\end{bmatrix}
\] (74)

Unknowns and nodal test parameters are grouped as:

\[
x_n = \begin{bmatrix}
x_1^T \\
x_2^T \\
x_3^T \\
x_4^T
\end{bmatrix}
\] (75)

\[
\pi_n = \begin{bmatrix}
\pi_1 \\
\pi_2 \\
\pi_3 \\
\pi_4
\end{bmatrix}
\] (76)

\[
x_n^\Lambda = \begin{bmatrix}
x_1^{\Lambda T} \\
x_2^{\Lambda T} \\
x_3^{\Lambda T} \\
x_4^{\Lambda T}
\end{bmatrix}
\] (77)

\[
\pi_n^\Lambda = \begin{bmatrix}
\pi_1^\Lambda \\
\pi_2^\Lambda \\
\pi_3^\Lambda \\
\pi_4^\Lambda
\end{bmatrix}
\] (78)
The deformation gradient is calculated as
\[ \mathbf{F}_h = \mathbf{x}_h^T \mathbf{N}_n^T \]
from which the table of the updated shape function derivatives is obtained:
\[ \mathbf{N}_n = \mathbf{F}_h^T \mathbf{N}_n^0 \]
A specific quadrature scheme is used. Terms involving the deviatoric Kirchhoff stress \( \mathbf{T} \) use one Gauss point and the remaining terms use four Gauss points to correctly sample the pressure terms.

The element forces and stiffness matrices (note that \( N_{ijK}^n \) are uniform for 4-node tetrahedra) are given by
\[
\begin{align*}
  f_{Ki}^+ &= \frac{V_0}{4} \left\{ 4 T_{ij} N_{iK}^n + \sum_{l=1}^{4} \left( N_{iK} (\xi_l) B_{0i} + N_{iL}^n (\xi_l) \pi_L \right) \right\} \\
  f_{Ki}^- &= c_0 V_0 N_{iK}^0 N_{iL}^0 \pi_L + \frac{V_0}{4} \sum_{l=1}^{4} \left( N_{iK} (\xi_l) (N_{iL}^n (\xi_l) \pi_L - g_J (\xi_l)) \right)
\end{align*}
\]
Figure 6. Effect of the number of steps for a five cycle loading with \( \text{tol} = 1 \times 10^{-4} \) and \( b = 1.35 \) (strain control): (a) Armstrong-Frederick and (b) Burlet-Cailletaud.

\[
K^{\lambda_{1}}_{KiLm} = \frac{V_{0}}{4} \left[ 4N_{jK}^{m}N_{nL}^{m}J_{(i)mn} - N_{mK}^{n}N_{iL}^{n} \sum_{l=1}^{4} N_{M}^{l}(\xi_{l})\pi_{M} \right] \tag{83}
\]

\[
K^{\lambda_{2}}_{KiL} = \frac{V_{0}N_{iK}^{m}}{4} \sum_{l=1}^{4} N_{L}(\xi_{l}) \tag{84}
\]

\[
K^{\lambda_{3}}_{KL} = c_{0}V_{0}N_{iK}^{0}N_{iL}^{0} + \frac{V_{0}}{4} \sum_{l=1}^{4} N_{K}(\xi_{l})N_{L}(\xi_{l}) \tag{85}
\]

\[
K^{\lambda_{4}}_{KLl} = -\frac{V_{0}N_{iL}^{m}}{4} \sum_{l=1}^{4} \left\{ N_{K}(\xi_{l})J(\xi_{l})g'\left[J(\xi_{l})\right]\right\} \tag{86}
\]
where $V_0$ is the tetrahedron volume

$$V_0 = \frac{1}{6} \det \begin{bmatrix} X_{11} - X_{31} & X_{21} - X_{31} & X_{41} - X_{31} \\ X_{12} - X_{32} & X_{22} - X_{32} & X_{42} - X_{32} \\ X_{13} - X_{33} & X_{23} - X_{33} & X_{43} - X_{33} \end{bmatrix}$$

(87)

with the notation $X_{Ki}; K = 1, \ldots, 4, i = 1, \ldots, 3$. The often costly constitutive update is performed at one Gauss point only, whereas the less expensive pressure terms are evaluated at four Gauss points (summation with index I). This decoupling is first proposed here.

The reader can note that, in Equation (83), the modulus $G$ was used, which is the spatial tangent modulus used for the strong ellipticity condition (see [38, Equations 45.6 and 45.14] where the notation $B$ is used):

$$G_{ijkl} = D_{ijkl} + \delta_{ik} T_{jl}$$

(88)

The ellipticity indicator is obtained as follows:

$$e = \min_{x_1, x_2} \arg \min_{\hat{\lambda}} \{ \hat{\lambda} \mid \det[n_i(x_1, x_2)n_k(x_1, x_2)G_{ijkl} - \hat{\lambda} \delta_{jl}] = 0 \}$$

(89)
Figure 10. Stress control: ellipticity indicator (both Armstrong–Frederick and Burlet–Cailletaud are shown): (a) Armstrong-Frederick and (b) Burlet-Cailletaud.

with \( \mathbf{n} \) being a unit vector, function of two angles \( \alpha_1, \alpha_2 \):

\[
\mathbf{n} = \begin{bmatrix} 
\sin \alpha_1 \cos \alpha_2 \\
\sin \alpha_1 \sin \alpha_2 \\
\cos \alpha_1 
\end{bmatrix}
\]  

(90)

Therefore, all quantities required for a constitutive analysis are readily available from the finite element implementation. Equation (89) involves a large number of eigenvalue evaluations and will be used in the next section.

2.7. Armstrong–Frederick/Burlet–Cailletaud hardening

With the purpose of also verifying the patch-test satisfaction, we use a cube of irregular elements as shown in Figure 5 where the relevant data are presented. The Armstrong–Frederick [35] and Burlet–Cailletaud [36] kinematic hardening models are tested. The relevant data are shown in Figure 5: both strain and stress control are used. For strain control, the effect of the number of time steps is shown in Figure 6. Large steps can be used, with no signs of convergence problems and with only slight result differences.
For strain control, the evolution of the Kirchhoff stress is shown in Figure 7 and compared with the results of Dettmer and Reese [19] (their model A). This comparison shows a difference, explained by the use of a different elastic model and kinematic part of the flow law. The ellipticity indicator (δ) shows loss of ellipticity for large stretch values, as seen in Figure 8.

For stress control, results are shown in Figures 9 and 10. It is noticeable that, for the Burlet–Cailletaud model, strong ellipticity is lost in several occasions, as shown in the latter figure. These losses are not unforeseen due to the presence of the stress tensor in the tangent modulus G, the yield-limited tangent G and the shift in the yield surface origin. This means that a crack may occur when kinematic hardening is present even if the slope in the hardening law is positive.

3. TENSION TEST OF A TRUNCATED CONE: COMPARISON OF VON-MISES AND HILL CRITERIA

A truncated cone built out of ASTM A-533 steel is subject to an imposed displacement at its larger base. This geometry is used to induce necking and has been adopted in the past in finite element
Table II. Tension test: constitutive properties (consistent units).

<p>| | |</p>
<table>
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<tr>
<td>$E$</td>
<td>206.9</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.29</td>
</tr>
<tr>
<td>$c_{0\text{small}}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$c_{0\text{big}}$</td>
<td>2</td>
</tr>
<tr>
<td>$t_{0\text{small}}$</td>
<td>$1 \times 10^{-6}$</td>
</tr>
<tr>
<td>$t_{0\text{big}}$</td>
<td>$1 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sigma_y$</td>
<td>$0.45 + (0.715 - 0.45)(1 - e^{-16.93\varepsilon_p}) + 0.12929\varepsilon_p$</td>
</tr>
</tbody>
</table>

Simulations [17]. The test data were obtained by Norris et al. [40] who, besides having performed the experimental test, successfully used a 2D finite difference code to perform a simulation. For our test, we use the properties of their specimen 2499R with the hardening law fitted by Simo [17].

An extension to this validation test is made with an anisotropic variant.

In finite element simulations with the radial-return algorithm, convergence problems are known to occur after the limit point is reached (see [41, pp. 358–359], and in the past hybrid solution techniques (BFGS followed by Newton iterations) were employed to efficiently solve the problem. This indicates the inability of Newton method (where the exact derivative is used) to deal with a non-smooth problem.

The geometry, boundary conditions and material properties are summarized in Figure 11. Two yield criteria are used:

von-Mises:

$$\gamma_{VM} = \frac{1}{\sqrt{2}} \sqrt{\left(T_{11} - T_{22}\right)^2 + \left(T_{22} - T_{33}\right)^2 + \left(T_{11} - T_{33}\right)^2 + 3(T_{12}^2 + T_{13}^2 + T_{23}^2)}$$  (91)

and Hill (with specific parameters):

$$\gamma_H = \frac{1}{\sqrt{2}} \sqrt{4T_{11}^2 - T_{11}T_{33} + T_{33}^2 - 7T_{11}T_{22} - 7T_{22}T_{33} + 4T_{22}^2 + 6T_{12}^2 + 6T_{13}^2 + 6T_{23}^2}$$  (92)

The effects of both the tolerance $t_{0}$ and the parameter $c_{0}$ are inspected, as well as the mesh. (Table II)

Two meshes are employed: a uniform mesh containing 7817 elements and a finer mesh with a localized refinement in the region indicated in Figure 11 containing 40271 elements of which 20867 are placed in the zone of mesh refinement (see Figure 11). For the purpose of stress convergence, a third mesh with 24436 elements is also inspected. Only $\frac{1}{8}$th of the specimen geometry is meshed, since three planes of symmetry exist. The reason for this refinement is the same that led Norris et al. [40] to introduce points in that region during their finite difference simulation: large elements in the necking region tend to deform into high aspect ratio tetrahedra and resolution worsens.

It was also found in [40] that a teardrop region adjacent to the necking region is in the state of compression, forcing the outer annulus to withstand the tension (this is particularly acute at a certain distance from the specimen’s center). We plot the longitudinal stress along the axisymmetric axis in Figure 13 for $u_y = 7$. The shift to the left of the curve is apparent when the fine mesh is used. The reason for this is that the finer mesh captures more of the necking in terms of...
Figure 12. Load versus longitudinal displacement results for the present model compared with the return-mapping algorithm. 14, 28 and 70 uniform displacement steps are used with $\text{tol} = 1 \times 10^{-6}$ and $c_0 = 10$ consistent units (von-Mises law). Return mapping makes use of finite strain Simo’s algorithm [17]. The energy residual and the effect of $\text{tol}$ are also shown.
stress distribution, and hence elements further away from the high stress gradient region are not so stretched.

To inspect the robustness of our method, we fix each longitudinal displacement increment, \( \Delta \mathbf{u} = (0.5, 0.25, 0.1) \) corresponding, respectively, to 14, 28 and 70 uniform displacement steps and observe the effect in the load/displacement results for the coarse mesh. With only 14 steps, the results used are sufficiently accurate. We tested Simo’s [17] radial-return mapping in principal directions and show the results in Figure 12. It is clear that the proposed method allows very large steps in comparison with the return-mapping technique that makes 112 non-uniform steps. This results from step halving that occurs when, for a certain step, convergence fails. A large number of steps were also pointed out in [41] and Crisfield and Norris [9] for the 2D case. Very dense clouds of points due to step-cutting were also shown in the latter paper. Note that we use a trust region solution method which is typically more robust than the standard Newton method (the residual...
Figure 15. Tension test: necking displacement comparison.

norm is shown in Figure 12). We are not aware of other authors solving this problem with 14 uniform steps.

The value of tol has some effect on the convergence response, as the study in the same figure shows. This is despite the fact that the load-deflection results are nearly unchanged for reasonable values, as illustrated in Figure 12.

An acceptable load–displacement result is obtained with the coarse mesh. However, stress values and necking shape are better reproduced with finer meshes (Figure 13 shows the longitudinal stress for three mesh densities). In Figure 14, results are compared with the mixed $Q_1-P_0$ hexahedron, the numerical results by Simo [17] (with their finer mesh) and Norris et al. [40]. The experimental results from the same reference [40] are also shown.

Our results are within the experimental envelope obtained by Norris et al. [40] and more pronounced softening is obtained by the proposed method than with other methods. The hexahedron $Q_1-P_0$ used the radial-return algorithm (with the finer mesh) and produced results close to the ones by Simo [17]. Overall, there is some spreading in these results, since the methods are also different. The response of the Hill criterion is slightly stiffer, and this is expected.

The necking behavior is also important, since it explains the softening response (with strain hardening) and shows how good the element performance is. Numerical results are shown in Figure 15 and compared with the upper and lower experiments by Norris et al. [40]. With the exception of the radial-return results, both meshes are within the experimental envelope.

For the von-Mises criterion, the deformed mesh, the effective plastic strain and longitudinal stress contour plots are presented in Figure 16. We note that near the necking region, the outer ring is supporting the specimen while the specimen core is in compression, as observed by Norris et al. Results are smooth and relatively unaffected by the mesh aspect ratio in the necking region. A run was made with a more refined mesh but the results are indistinguishable.

Although the load-deflection results obtained using Hill criterion are close to the ones obtained with von-Mises criterion, the deformed mesh is obviously not (see Figure 17).
The imposed displacement can reach very high values without any mesh distortion problems, see Figure 18 where the cross section for the Hill criterion is shown.

4. CONCLUSIONS

A general framework for finite strain plasticity with anisotropy and kinematic hardening was presented. Despite being restricted to elastic isotropy, the resulting model is much more general than the previous proposals. At the continuum level, Nemat-Nasser presented a closely related approach (see [3]). Smoothing by use of the Mangasarian functions replaced the exact complementarity condition, so that the return-mapping algorithm was avoided. Examples included kinematic
hardening and plastic anisotropy; the ellipticity indicator was obtained for kinematic hardening, showing loss of strong ellipticity under strain control and, for the Burlet–Cailletaud model, under stress control.

The overall scheme is also computationally simpler than previous integration schemes. It was found that computational costs are higher than classical $J_2$ neo–Hookean-based or Hencky-based approaches, but arbitrary isotropic elastic laws, anisotropic flow laws, yield functions and hardening functions can be adopted. For example, to model feature–full viscoelasto-plastic elastomers (see [10]) and solid propellants this can be very important [42]. In addition, since no return mapping is required, nor a particular solution method for plasticity, we can include more complex behavior.
Figure 18. Cross-section evolution, Hill criterion.

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