Modeling of the metal powder compaction process using the cap model. Part II: Numerical implementation and practical applications

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Abstract

The finite element (FE) simulation method has recently been used as an alternative design tool in powder metallurgy (PM) industry. It allows for the prediction of density and stress distributions in the pressed compact prior to the actual tooling design and manufacturing activity. It thus makes possible the validation of the PM part and associated tooling design. However, the accuracy of FE prediction highly depends on the choice of an appropriate and well calibrated powder material model, as well as on the effectiveness of the computational environment. While the first point was presented in a previous work, the present paper addresses some computational aspects of compaction process modeling approach in the context of industrial production environment.

Hence, this paper presents a discussion of the choice of stress and strain measures used in this large deformation context. It also presents the implementation of the cap constitutive model into ABAQUS FE software using the closest point projection algorithm. Furthermore, an integrated simulation module has been developed and is described herein. This module, designed in order to render the modeling approach practical and industrially attractive to PM engineers, permits an easy definition of the tooling and the powder geometry, as well as the prescription of compaction sequence and all other boundary conditions.

Finally, the simulation of the compaction of an industrial PM part, intended to illustrate the usefulness of the simulation approach in the task of improving the design of PM part and process, is presented. © 2002 Published by Elsevier Science Ltd.

Keywords: Powder metallurgy; Finite element simulation; Constitutive model nonlinearity; Friction; Cap model; Numerical integration; Closest point projection; Algorithmic consistency

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1. Introduction

Due to its numerous technological and economic advantages, powder metallurgy (PM) is a fast evolving manufacturing process (Lenel, 1980). However, due to the complex powder deformation mechanisms occurring during the compaction process, density gradients are often present in pressed parts (Bockstiegel, 1968). These gradients are the main causes of part distortion during the subsequent process of sintering and may even lead to part fracture during its ejection from the compaction die. Thus, part and tooling design is a very delicate task. Except for routine parts, for which PM engineers have developed extensive know-how, this task is traditionally performed through expensive trial and error approach. Thus, more efficient alternatives are still to be settled.

Therefore, the finite element (FE) simulation method has recently been used as such an alternative design tool in PM industry. It allows for the prediction of density and stress distributions in the pressed compact prior to the actual tooling design and manufacturing activity. It thus makes possible the validation of the PM part and associated tooling design (German, 1984). However, the accuracy of FE prediction highly depends on the choice of an appropriate and well calibrated powder material model, as well as on the effectiveness of the computational environment. In fact, in order to correctly model the compaction problem, such an environment should permit a reliable and practical representation of the model boundary conditions and should adequately handle the three involved nonlinearities, i.e.: the geometric nonlinearity associated with the large displacements, the material nonlinearity related to the elastic-plastic behavior of the powder material and finally, the contact nonlinearity related to friction between tools and powder.

In a previous paper (Chtourou et al., 2001), the cap material model, traditionally used for hard and nonductile powder was chosen and adapted for metal powders. The same paper presented an experimental calibration methodology and its application for the case of 316L stainless steel powders, as well as an experimental procedure for the validation of the model simulation results.

The present paper addresses some computational aspects of compaction process modeling approach in the context of industrial production environment. First, we justify the choice of stress and strain measures used in this large deformation context and we succinctly present the basic equations of the cap material model. Then, we present the integration algorithm used to implement the cap model in ABAQUS FE software through the user’s material subroutine. Subsequently, in order to render this modeling approach practical and industrially attractive to PM engineers, an integrated simulation module has been developed and is described herein. This module permits an easy definition of the tooling and the powder geometry, as well as the prescription of compaction sequence and all other boundary conditions. It also handles FE solution and result post-processing. Finally, the simulation of the compaction of an industrial PM part, intended to illustrate the usefulness of the simulation approach in the task of improving the design of PM part and process, is presented.

2. Material modeling

2.1. Strain and stress measures

Let $B \in \mathbb{R}^n$, $n = 2, 3$ and $B_t = \phi_t(B)$ be respectively the reference and the current configuration of the body under consideration and where function $\phi_t$ maps reference points $X$ of $B$ onto current points $x = \phi_t(X) \in B_t$, i.e. $\phi_t$ describes the deformational motion of body $B$. We also introduce a time like interval $[0, T]$ such that $t \in [0, T]$ is to be understood as a monotonically increasing parameter describing the evolution of the deformation process.
To describe the inelastic response in metal plasticity applications, we follow Kröner (1960), Lee and Liu (1967) or Mandel (1971) and introduce the multiplicative split of the deformation gradient, \( F(X) = \frac{\partial \phi_i(X)}{\partial X} \), into elastic part \( F^e \) and plastic part \( F^p \):

\[
F(X, t) = F^e(X, t) F^p(X, t) \tag{1}
\]

An appropriate definition of strain rate is then be introduced by considering the spatial velocity gradient \( l \) which is then expressed as

\[
l = \dot{F} \cdot F^{-1} = \dot{F}^e \cdot F^{-1} + F^e \cdot (\dot{F}^p \cdot F^{-p}) \cdot F^{-1} = F^e + F^e \cdot (F^p) \cdot F^{-1} \tag{2}
\]

Using the polar decomposition of \( F^e \) into the elastic rotation tensor \( R^e \) and the left stretch tensor \( V^e \) (i.e.: \( F^e = V^e \cdot R^e \)) and assuming, as usual for most metals undergoing large deformation, that the elastic strain is negligible compared to the plastic strain, it is then reasonable to consider the elastic stretch tensor \( V^e \) to be given by \( V^e = I + \epsilon^e \) where \( \epsilon^e \) is the infinitesimal elastic strain tensor. Following Lee and Liu (1967), we take \( F^e = V^e \) and by neglecting higher order infinitesimal quantities, one can arrive at the usual approximation of metal plasticity (Eq. (3)), where sym\[ \] denotes the symmetric part of a tensor and where \( d, d^e \) and \( d^p \) denote respectively the total, the elastic and the inelastic strain rate tensors.

\[
sym[l] = d \cong d^e + d^p \tag{3}
\]

As a stress measure, we consider, the Kirchoff stress tensor \( \tau \) which is an energy conjugate stress measure associated with \( d \). Hence, the rate of internal work in the current configuration will be written as: \( \dot{W}_{\text{int}} = \int_B (\tau \cdot d) dV \) (Peric et al., 1992; Simo, 1992; Simo and Ortiz, 1985). However, since the elastic strains are very small, it is common to approximate the Kirchoff stress by the true Cauchy stress since these two tensors are related by: \( \tau = \text{det} |F^e| \sigma \) (HKS, 1995b).

### 2.2. Cap material model

The cap model is a multisurface elastoplasticity permitting the representation of densification, hardening as well as inter-particle friction. It was originally developed for rocks, soils and other geological materials (Chtourou et al., 1995a; Chtourou et al., 1996; Dimaggio and Sandler, 1971). Due to the similarities in behavioral response of geological materials and some hard metal powders, this model was adopted and used to simulate the cold die compaction of tungsten carbide powder (Crawford and Lindskog, 1983; Weber and Brown, 1989). This kind of model was chosen in the present study because of the great flexibility it has shown in modeling all the compaction stages, especially the early ones (Trasorras et al., 1989). Provided some adjustments are performed (Weber and Brown, 1989; Gurson and Posteraro, 1992), this model is suitable for the simulation of the compaction of ductile powders able to attain higher density ranges. Box 1 succinctly presents the main features of the cap model in terms of \( J_1 \), the stress first invariant, and of \( s \), the norm of the stress deviator \( S \) defined by \( S = \sigma - (J_1/3)I \) (Dimaggio and Sandler, 1971; Trasorras et al., 1989; Sandler and Rubin, 1979; Chtourou et al., 1995b; Hofstetter et al. 1993).

Box 1. Summary of the used multisurface plasticity cap model for powder compaction.

1. **Stress–strain relationship (Hyperelastic compressible granular solid):**

\[
\sigma = \mathcal{C} \epsilon^e = \mathcal{C}(\epsilon - \epsilon^p) \quad \text{with} \quad \mathcal{C} = \frac{\partial^2 \psi}{\partial \epsilon^2} = 2G(\rho)I + \left(K(\rho) - \frac{2G(\rho)}{3}\right) \mathbf{1} \otimes \mathbf{1}
\]
where \( \psi \) is an hyperelastic free energy, \( \mathbf{C} \) is the fourth order elasticity tensor, \( \mathbf{I} \) and \( \mathbf{1} \) are respectively the fourth and second order identity tensors, \( G \) and \( K \) are the shear and bulk moduli expressed in terms of the powder relative density \( \rho \).

2. **Multi-yield surface**

(a) Surface tension limit:

\[ f_1(\sigma) = T - J_1 = 0 \quad \text{for} \quad J_1 < -T \]

(b) Shear failure surface:

\[ f_2(\sigma) = s - F_e(J_1) = 0 \quad \text{for} \quad -T \leq J_1 \leq L(k) \]

with:

\[ F_e(J_1) = \alpha - \gamma e^{-\beta J_1} + \theta J_1 \quad \text{and} \quad L(k) = \begin{cases} k & \text{if} \quad k > 0 \\ 0 & \text{if} \quad k \leq 0 \end{cases} \]

(c) Cap hardening surface:

\[ f_3(\sigma, K) = F_e(J_1, s, k) - F_e(k) = 0 \quad \text{for} \quad L(k) \leq J_1 \leq X(k) \]

with:

\[ F_e(J_1, s, K) = \sqrt{s^2 - \frac{1}{R^2} [J_1 - L(k)]^2} \]

and variable aspect ratio:

\[ R(\rho) = \frac{X(k) - k}{F_e(k)} \]

where \( k \) is the internal state variable representing material hardening whereas \( T, \alpha, \beta, \gamma \) and \( \theta \) are material parameters and \( X(k) \) the intersection of the cap and \( J_1 \) axis.

3. **Evolution equations**

(a) Flow rule:

\[ \dot{\varepsilon}^p = \sum_{i=1,3} \dot{\lambda}_i \frac{\partial f_i(\sigma, k)}{\partial \sigma} \]

(b) Hardening law:

\[ \overline{\varepsilon}^p_{\text{v}}(X(k)) = W(1 - e^{-DX(k)}) \quad \text{with} \quad \overline{\varepsilon}^p_{\text{v}} = \begin{cases} \dot{\varepsilon}^p_{\text{v}} & \text{if} \quad \dot{\varepsilon}^p_{\text{v}} \geq 0 \text{ or if} \quad k > 0 \text{ and } k > J_1 \\ 0 & \text{otherwise} \end{cases} \]

(c) Updating of density:

\[ \rho = \rho_0 e^{-\varepsilon^p} \]

where \( \dot{\lambda}_i \) is the plastic consistency parameter associated with the yield surface function \( f_i \), \( W \) and \( D \) are material parameters and \( \rho_0 \) is the initial loose state density.
3. Numerical implementation

3.1. Solution of the nonlinear finite element problem

The compaction process is assumed to be a quasi-static transformation with the final spatial distribution of density \( \rho(x) \) as the driving unknown (Weber and Brown, 1989; Trasorras et al., 1989; Koopman et al., 1992). Every material point undergoes finite strains deformation and elastoplastic transformations take place under the interaction of the powder medium and the tooling components. The corresponding nonlinear structural FE analysis involves integration of the differential elastoplastic equations in time and space. The time integration in the present context is due to the discretization of the loading history, while the spatial integration is normally performed via Gauss quadratures at the FE level and then assembled in terms of the mechanical degrees of freedom.

A nonlinear solver based on the Newton–Raphson method (HKS, 1995b; Dhatt and Touzot, 1984) has been used. This choice is motivated by the presence of strong nonlinearities and the desired quadratic rate of convergence. The used scheme thus required the updating of the consistent tangent stiffness at each iteration and the use of the algorithmic tangent material operator (Simo and Ortiz, 1985). Hence, at the end of each time step, the current stress state satisfies in the weak sense the equilibrium of the mechanical system with the external forces and complies with the full consistency of the elastoplastic material and frictional contact formulation.

3.2. Numerical integration of the cap model

At the core of the nonlinear FE solver resides the constitutive driver for integrating the rate form of the elastoplastic constitutive relations in a finite time step \( \Delta t \) between times \( t_n \) and \( t_{n+1} \). The problem is thus formulated as follows: Given the initial data at an integration point \( (\sigma_n, e^p_n, k_n) \) at time \( t_n \), and assuming that we are also given the total strain increment \( \Delta e_{n+1} \) corresponding to the displacement values \( u_{n+1} \) (best iterative guess at current iteration), one must then obtain the new values of the state variables \( (\sigma_{n+1}, e^p_{n+1}, k_{n+1}) \) satisfying the yield criteria and deduce values of the dependent variables such as stresses \( \tau_{n+1} \) at time \( t_{n+1} \) (Chorin et al., 1978). The incremental integration scheme is then a two-phase process that checks first whether plastic loading takes place by evaluating the yield function at the trial stress state (elastic prediction). In case of plastic loading, the flow direction and the magnitude of the incremental plastic multiplier are subsequently determined using full consistency at \( t_{n+1} \).

The first numerical simulations using the cap model were based on the algorithm proposed by Sandler and Rubin (1979). This algorithm was found to be not fully consistent with the principles of plastic consistency and associativity of the flow rule and was then corrected for these limitations (Simo et al., 1988a). Hofstetter et al. (1993) have then proposed an improved formulation of the cap model yield functions in order to ensure a better numerical stability of the model. They also derived a consistent expression of an algorithmic elastoplastic tangent moduli which is required in order to preserve the quadratic rate of convergence in a Newton–Newton solution technique. An improvement and adaptation of the work of reference Hofstetter et al. (1993) to the case of ductile powder compaction modeling is presented below.

3.2.1. Incremental formulation in the constitutive driver

For a typical finite time step \( \Delta t = t_{n+1} - t_n \), one usually applies the Euler backward algorithm to the evolution equations (Box 1) which then transform into the following general discrete evolution equations (Simo, 1992; Simo et al., 1988b):
\[ e_{n+1} = e_n + \Delta e_{n+1} \]  
\[ \sigma_{n+1}^p = \sigma_n^p + \Delta \sigma_{n+1}^p \]  
\[ k_{n+1} = F(k_n, \Delta e_{n+1}) \]  

with:

\[ \Delta \sigma_{n+1}^p = \sum_{i=1}^3 \Delta \lambda_i \partial \sigma \cdot f_i(\sigma, k) \]  

where \( \Delta \lambda_i \) is the increment of the plastic consistency parameter and where \( \Delta e_{n+1}^p \) is the tensor of plastic strain increment.

The stress tensor \( \sigma_{n+1} \) can then be deduced from the constitutive relation as

\[ \sigma_{n+1} = \mathbf{C} : e_{n+1} \]  

For pressure sensitive yield functions, it is necessary to decompose the involved stress and strain into their spherical and deviatoric parts. For strain increment tensors, we have:

\[ \Delta \sigma_{n+1}^p = \frac{1}{3} (\Delta I_1^p)_{n+1} \mathbf{1} + \Delta e_{n+1}^p \]  
\[ \Delta e_{n+1} = \frac{1}{3} (\Delta I_1)_{n+1} \mathbf{1} + \Delta e_{n+1} \]  

and for the Cauchy stress tensor, this decomposition can be written as

\[ \sigma_{n+1} = \frac{1}{3} f_1 \mathbf{1} + \text{dev}[\sigma] = \frac{1}{3} (J_1)_{n+1} \mathbf{1} + s_{n+1} \]

where \( e = \text{dev}[\varepsilon] \), \( I_1 = \text{tr}[\varepsilon] = 3 \varepsilon \), and \( s = \text{dev}[\sigma] \), \( J_1 = \text{tr}[\sigma] = 3 p \) with \( p \) being the pressure.

The rest of the process comprises the two main phases: an elastic predictor phase followed by a plastic phase when applicable.

3.2.2. Elastic prediction

In this stage, one assumes that the time step increment is totally elastic, or in other words that the plastic flow is frozen during the step and hence set \( \Delta \lambda_{i(n+1)} = 0 \). This results in the so called trial state:

\[ \sigma_{n+1}^{\text{tr}} = \mathbf{C} : (\varepsilon_{n+1} - \varepsilon_n^p) = \mathbf{C} : (\varepsilon_n^p + \Delta \varepsilon_{n+1}) = \sigma_n + \mathbf{C} : \Delta \varepsilon_{n+1} \]

\[ J_{1,n+1}^{\text{tr}} = J_{1,n} + 3 K \Delta e_{n+1} \]

Using constitutive equations (Box 1), we can deduce the trial dependent variables. The so called trial stress is defined by (Eq. (13)) which, in terms of its hydrostatic and deviatoric parts, results in Eqs. (14a) and (14b):

\[ \sigma_{n+1}^{\text{tr}} = \mathbf{C} : (\varepsilon_{n+1} - \varepsilon_n^p) = \mathbf{C} : (\varepsilon_n^p + \Delta \varepsilon_{n+1}) = \sigma_n + \mathbf{C} : \Delta \varepsilon_{n+1} \]

\[ J_{1,n+1}^{\text{tr}} = J_{1,n} + 3 K \Delta e_{n+1} \]

\[ s_{n+1}^{\text{tr}} = s_n + 2G \Delta e_{n+1} \]

If, all of the yield criteria are satisfied for these trial values, i.e. if \( f_i(\sigma_{n+1}^{\text{tr}}, k_{n+1}^{\text{tr}}) \leq 0 \) for all \( i \in \{1, \ldots, 3\} \) with \( (\Delta \lambda_i)_{n+1}^{\text{tr}} = 0 \), the process is elastic; so the trial values of the state variables in (Eq. (12)) can be accepted as the final values at time \( t_{n+1} \). Otherwise, if \( f_i(\sigma_{n+1}^{\text{tr}}, k_{n+1}^{\text{tr}}) > 0 \) for some \( i \in \{1, 2, 3\} \), the process is plastic and we must enforce the plastic consistency condition by determining the active yield function for which \( (\Delta \lambda_i)_{n+1}^{\text{tr}} > 0 \) (Simo et al., 1988b).
3.2.3. Detection of active mode and plastic correction

One of the difficult tasks in multisurface plasticity is the accurate determination of the active mode and the transition from one mode to another (singular cases). At each load increment, only one of six possible modes can be active. The trial stress state is used to evaluate a trial value of the different yield functions. If only one yield surface is active (i.e. if for only one \( \gamma \in (1, 2, 3) \), we have \((\Delta \lambda_\gamma)_{n+1} > 0\), then the condition \( f_\gamma(\sigma_{n+1}, k_{n+1}) > 0 \) does imply that \((\Delta \lambda_\gamma)_{n+1} > 0\) so that the \( \gamma \)-constraint is active.

However, when several yield surfaces are active, condition \( f_\gamma(\sigma_{n+1}, k_{n+1}) \geq 0 \) does not imply that \((\Delta \lambda_\gamma)_{n+1} > 0\) since we may have \( f_\gamma(\sigma_{n+1}, k_{n+1}) \geq 0 \) but \( f_\gamma(\sigma_{n+1}, k_{n+1}) < 0 \). In that case, a corner mode is concerned and involves the intersection of two yield surfaces.

In addition to the elastic mode and to the three modes related to the three yield surfaces, two singular modes thus result from the nonsmooth intersection of these surfaces (Fig. 1). These are the singular compressive mode (4) and the singular tensile mode (2). A general procedure for determining the active yield surfaces is then based on a systematic enforcement of the discrete Kuhn–Tucker conditions. Using the assumption of the convexity of the yield surfaces, it can be shown (Hofstetter et al. 1993, Simo et al., 1988a) that if all of the trial values of the yield functions are negative, the load is totally elastic and the trial stress state corresponds to the real state:

\[
\forall i = (1, 2, 3) \quad \Rightarrow \quad \Delta \lambda_i = 0, \quad \forall i = (1, 2, 3) \quad i = (1, 2, 3)
\]

Instead, if one of the trial values of the yield functions is positive, the loading is elastoplastic and one of the plastic modes is necessarily active. In that case, the elastic stress predictor is larger than the real stress state and a plastic correction must be performed. This is done by a correction procedure, also called return mapping algorithm, done by normally projecting the trial stress to the tension, shear and cap surfaces as shown in (Fig. 2) after evaluating the plastic strain increment required to update the stress state:

\[
\begin{align*}
J_{n+1} &= J_n + 3K \Delta \lambda_{n+1} \\
\sigma_{n+1} &= \sigma_n + 2G(\Delta \lambda_{n+1})
\end{align*}
\]

The stress conditions of each one of the plastic modes is presented in Box 2 together with the corresponding values of the increments of plastic consistency parameters. These values are then used to determine the plastic strain increment (Eq. (7)) and thus the real stress state (Eqs. (14a) and (14b)).

It should be noted that the cap mode is the only one involving strain hardening. Therefore, its numerical treatment is more delicate and will be detailed in the next section.
Box 2. Boundaries and plastic consistency parameters of the plastic modes.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Stress state boundaries</th>
<th>Incremental consistency parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$J_{n+1}^T \leq T$ and $s_{n+1}^T \leq F_c(T)$</td>
<td>$\Delta \lambda_{1n+1} = \frac{T-J_{n+1}^T}{9K}$, $\Delta \lambda_{2n+1} = 0$ and $\Delta \lambda_{3n+1} = 0$</td>
</tr>
<tr>
<td>2</td>
<td>$J_{n+1}^T \leq T$ and $s_{n+1}^T \leq F_c(T)$</td>
<td>$\Delta \lambda_{1n+1} = \frac{s_{n+1}^T-F_c(T)}{2G}$, $\Delta \lambda_{2n+1} = -\frac{T-J_{n+1}^T}{9K} - \frac{dF_c(T)}{dJ} \frac{s_{n+1}^T-F_c(T)}{2G}$, $\Delta \lambda_3 = 0$</td>
</tr>
<tr>
<td>3</td>
<td>$F_c(T) + \frac{T-J_{n+1}^T}{(dF_c(T)/dT)} - s_{n+1}^T$</td>
<td>$\Delta \lambda_1 = 0$, $\Delta \lambda_{2n+1} = \frac{s_{n+1}^T-F_c(J_{n+1})}{2G} [J_{n+1}$ previously obtained by NR solution of the combination of Eqs. (14a) and (14b) and $(f_2(\sigma) = 0)]$ $\Delta \lambda_3 = 0$</td>
</tr>
<tr>
<td>4</td>
<td>$s_{n+1}^T \leq s_{n+1}^T$</td>
<td>$\Delta \lambda_1 = 0$, $\Delta \lambda_{2n+1} = \frac{k_n-J_{n+1}^T}{9K} (dF_c(k_n)/dJ)$, $\Delta \lambda_{3n+1} = \frac{s_{n+1}^T-F_c(k_n)}{2G}$</td>
</tr>
<tr>
<td>5</td>
<td>$L(k_n) &lt; J_{n+1}^T \leq X(k_n)$ or $J_{n+1}^T &gt; X(k_n)$</td>
<td>$\Delta \lambda_1 = 0$, $\Delta \lambda_{2n+1} = \frac{J_{n+1}^T - k_{n+1}}{9K} [J_{n+1}^T - 9K(\Delta \lambda_{3n+1} - 3\Delta \lambda_{n+1})]$ (see details in cap mode treatment)</td>
</tr>
</tbody>
</table>

3.2.4. Cap mode treatment

As for the other modes, the application of the general flow rule to the function $f_3$ of the cap mode allows for the determination of the plastic strain increment:

$$\Delta \epsilon_{p,n+1} = \Delta \lambda_{3n+1} \frac{s_{n+1}}{F_c(s_{n+1},J_{n+1}^T,k_{n+1})}$$  \hspace{1cm} (17a)

$$\Delta \tau_{p,n+1} = 3\Delta \lambda_{3n+1} \frac{J_{n+1}^T - k_{n+1}}{R^2F_c(s_{n+1},J_{n+1}^T,k_{n+1})}$$  \hspace{1cm} (17b)

These quantities are then introduced into the relation between trial and real stress states (Eqs. (14a) and (14b)) together with the plastic consistency condition $(f_{3n+1}(\sigma,k) = 0)$. However, since the yield function undergoes hardening that makes the state variable $k$ attain a new undetermined value $k_{n+1}$, we thus have an additional unknown. Therefore, in order for the problem to be completely defined, a new relation must

Fig. 2. Closest point projection in the different plastic modes.
be introduced. This corresponds to the incremental form of the hardening law obtained by an implicit Euler integration scheme between $t_n$ and $t_{n+1}$:

$$\Delta f_{n+1}^p = W\left( e^{DX(k_n)} - e^{DX(k_{n+1})} \right)$$  \hfill (18)

Thus, the problem is reduced to a single scalar nonlinear equation in $k_{n+1}$ (Eq. (19)) that can be solved by a local Newton–Raphson iterative method. Once this new position of the cap is determined, the plastic strain and the real stress state can be computed (Hofstetter et al. 1993; Simo et al., 1988a).

$$\sqrt{\left[ \frac{\delta^T_{n+1} F_e(k_{n+1})}{F_e(k_{n+1}) + 2G\Delta \lambda_{3,n+1}} \right]^2 + \left[ \frac{J_{n+1}^T - k_{n+1}}{R + \frac{9k_{n+1}\Delta \lambda_{3,n+1}}{RF_e(k_{n+1})}} \right]^2} = F_e(K_{n+1})$$  \hfill (19)

### 3.2.5. Computation of elastoplastic tangent moduli

The last step of the numerical integration of the constitutive evolution equations is concerned with the determination of the algorithmic material contribution of the powder medium to the FE tangent stiffness matrix. This contribution is computed at the integration point level and is called the elastoplastic tangent moduli. In order to preserve a quadratic rate of convergence for the global FE problem, this moduli should be derived from the algorithmic and not from the continuum mechanics formulation (Chtourou et al., 2001; Simo, 1992; Simo and Ortiz, 1985). In fact, this material tangent moduli corresponds to the stress variation caused by an infinitesimal strain variation:

$$H_{\text{ep}} = \left. \frac{d \sigma_{n+1}}{d \varepsilon_{n+1}} \right|_{\text{eq}}$$  \hfill (20)

It is determined by a simple derivation of the stress strain relation (Eq. (21)). This formulation requires the determination of the plastic strain variation. This can be done through (Eq. (22)) if the active mode involves no strain hardening and through (Eq. (23)) if the active mode is the cap mode. Details of this derivation procedure are given in Appendix A whereas the integration algorithm main steps are summarized in Box 3.

$$d \sigma_{n+1} = C : (d \varepsilon_{n+1} - d \varepsilon_{n+1}^p)$$  \hfill (21)

$$d \varepsilon_{n+1}^p = \sum_i \left[ d(\Delta \lambda_i) \frac{\partial f_i}{\partial \sigma} + \Delta \lambda_i \frac{\partial^2 f_i}{\partial \sigma^2} : d \sigma \right]$$  \hfill (22)

$$d \varepsilon_{n+1} = d(\Delta \lambda_2) \frac{\partial f_i}{\partial \sigma} + \Delta \lambda_2 \left( \frac{\partial^2 f_i}{\partial \sigma^2} : d \sigma + \frac{\partial^2 f_i}{\partial \sigma \partial k} : dk \right)$$  \hfill (23)

Box 3. Numerical integration algorithm of the cap model.

**Step 1: Elastic prediction**

Assume plasticity is frozen at the level reached at time $t_n$ and consider the strain increment to be totally elastic, then find a trial stress state: $\sigma_{n+1}^T = \sigma_n + C : \Delta \varepsilon_{n+1}$ using the elasticity tensor $C$.

**Step 2: Finding active mode**

Use the trial stress state to evaluate the different yield functions and find out the active mode among those shown in Fig. 1.
4. Integrated simulation module

4.1. Overview

In order to make the simulation of powder compaction an attractive design tool, an integrated simulation module has been developed for axisymmetric applications. A general 3D version is currently under development. This module is mainly intended to facilitate and to automate some of the tedious modeling related tasks. It is composed of the I-Deas Master Series CAD software (SDRC, 1994), the ABAQUS nonlinear FE solver (HKS, 1995b), the ABAQUS-Post post-processing (HKS, 1995a) software and finally IDEQUS (Chtourou et al., 1995a): an in-house developed pre-processing and interfacing program. The module layout, as well as the main functions of its components, is described in Fig. 3.

4.2. Pre-processing

The pre-processing is first performed through I-Deas in which the component geometries are defined and then meshed with four node quadrilateral axisymmetric elements using a semi-automatic mapped pattern. User defined macro functions, implemented into I-Deas, are then used for the selection and the identification of the special boundary regions of the powder cavity and tooling components. As shown in Fig. 4, this essentially consists in the identification of:

- Sets of nodes at the extremity of tooling components, intended for the prescription of boundary conditions of the imposed displacement type.
- Powder cavity element sets at the boundary with tooling components together with tooling component element sets at the boundary with powder cavity intended for the prescription of contact conditions.

Step 3: Elastic updating (if elastic mode is detected)

- Set the stress state equal to the trial stress state
- Leave the state variable unchanged
- Set the elastoplastic tangent moduli equal to the elasticity tensor
- Go to step 6

Step 4: Plastic correction (if one of the plastic modes is detected)

- Combine the following conditions in a scalar equation that is nonlinear in the plastic consistency parameter $\Delta \lambda_i$ and solve it by a local Newton–Raphson scheme:
- Stress–trial stress relationship $\sigma_n = \sigma_n^{T+1} - C : \Delta \varepsilon_p^{T+1}$
- Plastic flow rule $\Delta \varepsilon_p = \sum_{i=1}^{3} \Delta \lambda_i \partial f_i(\sigma, k) / \partial \sigma$
- Hardening rule $\Delta \varepsilon_p^v = f(k)$ (only for the cap mode)
- Consistency condition: $f_i(\sigma, k) = 0$
- Once $\Delta \lambda_i$ is found, compute and update the consistent plastic strain increment, the stress and all other state variables.

Step 5: Compute the resulting consistent algorithmic elastoplastic tangent moduli

Step 6: Return to the main program