The new numerically-analytic method for integrating the multiscale thermo elastoviscoplasticity equations with internal variables

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Abstract. Integration of the constitutive equations of ductile fracture models is analyzed in this paper. The splitting method is applied to the Gurson’s and Kukudzhanov’s models. The analysis of validity of this method is done. It was shown that Kukudzhanov’s model describes a large variety of materials since it involves residual stress and viscosity.

1. Introduction
Finite strain problems, such as metal forming, where plastic strains are by two to three orders of magnitude larger than elastic strains, involve both the problems: choosing of the appropriate material model and integration scheme. In this paper we consider a material model for void-containing ductile solids that has been developed by Gurson [3], and micromechanical model of fracture that was suggested by Kukudzhanov [4, 6]. A brief description of these models is given in Section 2. The distinctive feature of the constitutive equations of the plasticity theory is that in addition to differential relations, these equations involve also a finite relation that constrains the stress tensor invariants. Owing to this, various mathematical methods can be used. Here we use the splitting method, proposed by Kukudzhanov [5]. This method is based on splitting of the constitutive relations with respect to physical processes. In the paper a numerical example of a uni-axial tension test on a square element is considered to illustrate the basic model features.

2. Elastoviscoplastic constitutive relations
2.1. General formulation of the elastoviscoplastic constitutive relations
We assume the strain-rate additivity

\[ \dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{pl}, \]

(1)

For the case of linear elasticity

\[ \sigma = D : \dot{\varepsilon}^{el}, \]

(2)

where \( D \) is the fourth-order elasticity tensor. In the following, we assume linear isotropic elasticity, so that

\[ D_{ijkl} = 2G \delta_{ik} \delta_{jl} + \left( K - \frac{2}{3}G \right) \delta_{ij} \delta_{kl}, \]

where \( \delta \) is the Kronecker delta.
where $G$ and $K$ are the elastic shear and bulk moduli respectively, and $\delta_{ij}$ is the Kronecker delta.

The yield function involves the first and second invariants of the stress tensor and is given by

$$\Phi(p, q, H) = 0,$$

where $p = -\frac{1}{3} \sigma : I$ is the hydrostatic stress, $q = \left(\frac{3}{2} s : s \right)^{1/2}$ is the equivalent stress and $H_i$, $i = 1, 2, \ldots, n$, is a set of internal state variables, $I$ is the second order identity tensor and $s$ is the stress deviator. The function $\Phi$ is defined such that when $\Phi < 0$, the response is purely elastic. The flow rule is written as

$$\dot{\varepsilon}^{pl} = \lambda \frac{d\Phi}{d\sigma},$$

where $\lambda$ is a positive scalar. Using (3), the flow rule becomes

$$\dot{\varepsilon}^{pl} = \lambda \left( -\frac{1}{3} \frac{\partial \Phi}{\partial p} I + \frac{\partial \Phi}{\partial q} n \right),$$

where $n = \frac{3}{2q} s$. According to [1] $n$ can be determined as

$$n = \frac{3}{2q^2} s^{ijkl}.$$

Using this notation, the stress tensor can be written as

$$\sigma = -p I + \frac{2}{3} q n.$$

The plasticity model is completed by describing the evolution of the state variables

$$H_i = h_i(\dot{\varepsilon}, \sigma, H_j).$$

### 2.2. Gurson’s plasticity model

We briefly discuss the material model for void-containing ductile solids. Based on a rigid-plastic upper-bound solution for spherically symmetric deformations around a single spherical void, Gurson [3] proposed the yield condition

$$\Phi = \left( \frac{q}{\sigma_y} \right)^2 + 2q_1 f \cosh \left( -\frac{3q_2 p}{2 \sigma_y} \right), - (1 + q_3 f^2)$$

where $\sigma_y$ is the equivalent tensile flow stress representing the actual microscopic stress state in the matrix material, and $f$ is the current void volume fraction. The parameters $q_1$, $q_2$ and $q_3$ were introduced by Tvergaard [7] to make the predictions of Gurson’s equations agree with numerical studies of the materials containing periodically distributed circular cylindrical voids. The yield surface given by Equation (8) becomes that of von Mises (which is assumed in Gurson’s model to hold for the matrix material) when $f = 0$.

In Gurson’s model the microscopic equivalent plastic strain $\bar{\varepsilon}_{pl}^{m}$, to vary is assumed according to the equivalent plastic work expression

$$(1 - f) \sigma_y d\bar{\varepsilon}_{pl}^{m} = \sigma : d\varepsilon^{pl}.$$

The change in void volume fraction during an increment of deformation is partly due to the growth of existing voids and partly due to the nucleation of new voids

$$df = df_{nuc} + df_{gr}.$$
The matrix is assumed to satisfy the plastic incompressibility condition but, because of the existence of voids, the macroscopic response does not. The change of the void volume fraction due to growth is related to the change of the total volume as

\[ df_{gr} = (1 - f) d\varepsilon_{pl} : I. \]  

In this model, voids nucleation is considered to be controlled by plastic strain

\[ df_{nuc} = A d\varepsilon_{pl}^m. \]  

As suggested by Chu and Needleman [2] the parameter \( A \) is chosen so that the nucleation strain follows a normal distribution with mean value \( \varepsilon_N \) and standard deviation \( s_N \):

\[ A = A(\varepsilon_{pl}^m) = \frac{f_N}{s_N\sqrt{2\pi}} \exp \left( -\frac{1}{2} \left( \frac{\varepsilon_{pl}^m - \varepsilon_N}{s_N} \right)^2 \right), \]  

where \( f_N \) is the volume fraction of void nucleating particles.

2.3. Micromechanical model of damage and fracture

We briefly discuss the micromechanical model of ductile fracture, as suggested by Kukudzhanov [4, 6]. The model is based on the phenomenological theory of dislocations and micro-defect development. According to this model, the plastic deformation and damage is a single process caused by the motion of dislocations and also by generation and development of microdefects. The deformation process is assumed to consist of two stages.

In the first stage, the material is subjected to plastic deformation due to the motion of dislocations in crystal grains of the material. Part of these dislocations that have accumulated at the grain boundaries, leads to residual microstresses (it is assumed that the deviatoric components of the residual stress tensor are proportional to the tensor of accumulated flux of dislocations). On the macrolevel, it leads to an elastoviscoplastic flow with simultaneous hardening of the material. The stress tensor consists of active and residual parts

\[ \sigma = \sigma^a + \sigma^r. \]  

Active stress is determined by using the associated flow rule

\[ \dot{\varepsilon}_{pl} = \lambda \frac{d\Phi}{d\sigma^a} \]  

and the von Mises type flow condition for elastoviscoplastic material with kinematic and isotropic hardening

\[ \Phi = q^a - \sigma_y = 0, \]  

\[ \sigma_y = \left( 1 + 3\mu_1 \varepsilon_{pl} \right)^N + \psi(\tau_1 \dot{\varepsilon}_{pl}), \]  

where \( q^a = \sqrt{\frac{3}{2}} s^a : s^a \) is the equivalent active stress; \( \varepsilon_{pl} = \sqrt{\frac{2}{3} \varepsilon_{pl}^d : \varepsilon_{pl}^d} \) is the equivalent plastic strain; \( \psi \) function determines the influence of strain rate on the yield stress, \( \psi(0) = 0 \). For residual stress we have the well-known law of kinematic hardening

\[ \sigma^r = 2\alpha \varepsilon_{pl}. \]
The second stage begins after the intensity of the dislocation flux accumulated at the boundaries of grains attains a critical level, beyond which the process of annihilation of dislocations begins (it is assumed that the flux of annihilation of dislocations is proportional to the amount of dislocations accumulated at the inclusions). This process is accompanied by disclinations of grains with the formation of voids between them. On the macrolevel, this process leads to relaxation of the internal stresses and softening of the material. The appearance of voids changes the behavior of the material essentially. In this case the material consists of the matrix and the voids, i.e., it is a two-phase material with the flow condition for active stress

$$\Phi = \left( \frac{q^n}{\sigma_y} \right) + 2q_1 f \cosh \left( \frac{3 q_2 p^n}{2 \sigma_y} \right) - (1 + q_3 f^2) = 0. \tag{18}$$

Voids nucleates once the equivalent residual stress $q^r$ achieves the critical value $q^r_c$. The volume of nucleated voids is considered to be a small disturbance. The relaxation of residual stress is described by equation

$$\dot{s}^r + 2\mu_2 Q (q^r - q^r_c) \tau_2 s^r = 2\alpha \dot{e}^{pl}, \tag{19}$$

function $Q$, that characterizes the relaxation, is supposed to be a linear function of its argument, $\tau_2$ is relaxation time of residual stresses ($\tau_2 \gg \tau_1$).

3. Splitting method

Splitting method for the integration of equations governing the behavior of elastoviscoplastic media was proposed by Kukudzhanov [5]. The idea of this method is based on the fact that an additive operator can be replaced by a multiplicative operator on a small time interval.

It was shown that for the classical elastoplastic medium independent of the time scale, the splitting leads to an algebraic powerlaw equation for the correction coefficient of the elastic solution. For elastoviscoplastic media, the splitting leads to a differential equation for the correction coefficients, which in this case are functions of time. The general scheme of splitting looks as follows. We decompose the equation

$$\dot{\sigma} = D : (\dot{\varepsilon} - \dot{\varepsilon}^{pl}). \tag{20}$$

The predictor is taken at $\dot{\varepsilon}^{pl} = 0$, which corresponds to the elastic material. In this case, for each step $\Delta t$, one should solve the elastic problem

$$\dot{\sigma} = D : \dot{\varepsilon} \tag{21}$$

subjected to the initial conditions obtained at the previous step for the complete elastoplastic problem.

The corrector is taken at $\dot{\varepsilon} = 0$ in equation (20). Using equation (4), equations (20) and (7) becomes

$$\dot{\sigma} = -\lambda D \frac{\partial \Phi}{\partial \sigma}, \quad \dot{H}_i = \tilde{h}_i (-\lambda \frac{\partial \Phi}{\partial \sigma}, \sigma, H_j). \tag{22}$$

The second relation in (22) provides the evolutionary equations for the internal parameters that characterize the structure of the material, hardening, damage, porosity and other properties.

For the classical (equilibrium) elastoplastic medium, the properties of which are independent of the change in the time scale, one can eliminate the time $t$ from equations (22) and proceed to the variable $\lambda$, to obtain

$$d\sigma = -d\lambda D \frac{\partial \Phi}{\partial \sigma}, \quad dH_i = \tilde{h}_i (-d\lambda \frac{\partial \Phi}{\partial \sigma}, \sigma, H_j). \tag{23}$$
Solving equations (23) subjected to the initial conditions resulting from the solution of the elastic problem $\sigma(\lambda_0) = \sigma^{el}$, $H_i(\lambda^n) = H^n_i$, we find the variables $\sigma^{n+1}$ and $H^{n+1}_i$ as functions of $\lambda$, $\sigma^{el}$, $H^{el}_i$

$$\sigma = \sigma(\lambda, \sigma^{el}, H^{el}_i), \quad H_i = H_i(\lambda, \sigma^{el}, H_j) \quad \text{for} \quad \lambda = \lambda^{n+1}. \quad (24)$$

Substituting these relations into the plasticity condition (3), we obtain the equation

$$\Phi(p(\lambda), q(\lambda), H_i(\lambda), \lambda) = 0. \quad (25)$$

Solving this equation and substituting the resulting $\lambda$ into (24) we obtain the final solution of the problem.

For the elastoviscoplastic medium, the plasticity condition is of differential type. In this case, equation (3) for $\lambda$ leads to the differential equation

$$\Phi(p(\lambda), q(\lambda), H_i(\lambda), \lambda, \dot{\lambda}) = 0. \quad (26)$$

This splitting scheme is stable, if the predictor scheme for the solution of the elastic problem is stable and there exist solutions of equations (25) and (26).

4. Integration of the constitutive relations of GTN model by the splitting method

For simplicity we assume that there is no nucleation of voids, i.e. $df_{nuc} = 0$, and that the yield stress is constant, $\sigma_y = \sigma_{y0} = const$. During the constitutive calculations, where stresses and state variables are updated, the total strain $e$ is known. The aim of this integration is to find stresses and state variables at the end of the time increment $t + \Delta t$.

At the predictor step one has to solve the elastic problem.

$$\dot{p}^{el} = -K \dot{\varepsilon} : \textbf{I}, \quad \dot{q}^{el} = 2G \dot{\varepsilon} : \textbf{n}. \quad (27)$$

We integrate these equations taking the solutions at the previous step $t$ as the initial conditions. The result can be written as

$$p^{el} = p_t + \Delta p^{el}, \quad q^{el} = q_t + \Delta q^{el}, \quad (28)$$

At the correction step, the first equation in can be written as

$$\frac{d\sigma}{d\lambda} = -K \frac{\partial \Phi}{\partial p} \textbf{I} - 2G \frac{\partial \Phi}{\partial q} \textbf{n}. \quad (29)$$

Projecting this equation onto $\textbf{I}$ and $\textbf{n}$, and using equation (6), we find

$$\frac{dp}{d\lambda} = -K \frac{\partial \Phi}{\partial p}, \quad \frac{dq}{d\lambda} = -6Gq, \quad \frac{df}{d\lambda} = -(1 - f) \frac{d\Phi}{dp}. \quad (30)$$

Initial conditions for equations (30) are taken from the solution of the elastic problem at the predictor step: $p(\lambda_0) = p_0 = p^{el}$, $q(\lambda_0) = q_0 = q^{el}$, $f(\lambda_0) = f_0 = f_t$.

Integrating this equation with initial conditions, we find

$$dp = \frac{K}{(1 - f)} df, \quad f = 1 - (1 - f_0) \exp \left( -\frac{p - p_0}{K} \right). \quad (31)$$

Eliminating $d\lambda$ from equations (30), we find

$$\frac{dp}{dq} = \frac{K}{6Gq} \frac{\partial \Phi(p, q)}{\partial p} \quad \text{for} \quad \Phi(p, q) = \varphi(p)\psi(q). \quad (32)$$
The problem of integrating the elastoplastic equations reduces to the solution of one differential equation and one non-linear algebraic equation

\[
\frac{dp}{dq} = \alpha \frac{1}{q} \psi(p), \quad p(q_0) = p_0,
\]

(33)

\[
\Phi(p, q) = q^2 + \phi(p) = 0,
\]

(34)

where \( \alpha = K_6 \frac{G}{6} \), \( \psi(p) = \frac{\partial \Phi}{\partial p} \), \( \phi(p) = 2q_1 f(p) \cosh \left( \frac{3}{2} q_2 p \right) - (1 + q_3 f^2(p)) \).

Writing this equation in the incremental form, we obtain a non-linear algebraic equation. Thus, the problem reduces to the solution of the set of two non-linear equations.

The computational advantages of the splitting method, as compared with standard methods, are achieved due to at the correction step some equations can be integrated analytically.

5. Integration of the constitutive relations of the micromechanical model

We use the splitting method to integrate the constitutive equations of plasticity by Mises with kinematical hardening.

Relaxation equations (15) and (16) give

\[
\dot{\varepsilon}^{pl} = \dot{\lambda} \left( \frac{3}{2q^3} \right)^{\alpha} \dot{s}^{\alpha} = \dot{\Lambda}^{\alpha}, \quad \dot{\lambda} = \frac{3}{2q^3} \dot{\lambda},
\]

(35)

Equation (23) for stresses relaxation can be written as

\[
ds^{\alpha} = -2Gs^{\alpha} d\Lambda.
\]

(36)

Integrating this equation with initial condition \( \Lambda = \Lambda_0, s^{\alpha}(\Lambda_0) = s^{el} \), we find

\[
s^{\alpha} = s^{el} X, q^{\alpha} = q^{el} X,
\]

(37)

where \( X = \exp(-2G(\Lambda - \Lambda_0)) \) is the correction coefficient of the elastic solution.

Using equations (35) and (37), and taking into account that \( \dot{\varepsilon}^{pl} = \dot{\varepsilon}^{pl} \) one can find

\[
\dot{\varepsilon}^{pl} = \sqrt{\frac{2}{3} \varepsilon^{pl}}, \quad \dot{\varepsilon}^{pl} = \frac{2}{3} \dot{\lambda} q^{el} l^{-2G(\Lambda - \Lambda_0)} = -\frac{1}{3G} q^{el} X.
\]

(38)

Integrating this equation we obtain

\[
\varepsilon^{pl} = \dot{\varepsilon}^{pl} - \frac{1}{3G} q^{el} (X - 1),
\]

(39)

Substituting the values \( \varepsilon^{pl} \) and \( \dot{\varepsilon}^{pl} \) in the matrix flow condition (16), we have

\[
\Phi = q^{el} X - \left[ 1 + 3 \mu_1 \left( \varepsilon_i^{pl} - \frac{1}{3G} q^{el} (X - 1) \right) \right] \psi \left( -\frac{1}{3G} q^{el} \tau_1 X \right) = 0,
\]

(40)

where \( \psi(x) = \alpha \tanh(x) \).

To solve this differential equation we approximate \( \dot{X} = \frac{X - 1}{\Delta t} \) and obtain a non-linear equation for \( X \) which is solved by means of Newton’s method. Using equation (17), we find the equivalent residual stress

\[
q^r = 3\alpha \varepsilon^{pl}.
\]

(41)

In the first stage of deformation, the stress tensor can be written as

\[
\sigma = -p^0 I + \frac{2}{3} (q^{\alpha} + q^r) n,
\]

(42)
where $p^\alpha = -K(\varepsilon : I)$ is the elastic pressure.

To integrate the constitutive relations at the second stage of deformation, after nucleation of voids, we generalized the numerical method [1] for the rate-dependent plasticity.

Flow rule (15) in the incremental form at the end of the increment is written

$$
\Delta \varepsilon^{pl} = \frac{1}{3} \Delta \varepsilon_p I + \Delta \varepsilon_q n, \quad \Delta \varepsilon_p = -\Delta \lambda \frac{\partial \Phi}{\partial p^\alpha}, \quad \Delta \varepsilon_q = -\Delta \lambda \frac{\partial \Phi}{\partial q^\alpha}. \tag{43}
$$

$$
\Delta \varepsilon_p \frac{\partial \Phi}{\partial q^\alpha} + \Delta \varepsilon_q \frac{\partial \Phi}{\partial p^\alpha} = 0. \tag{44}
$$

We can rewrite equation (2) in incremental form

$$
\sigma^\alpha = \sigma^{el} - K \Delta \varepsilon_p I - 2G \Delta \varepsilon_q n. \tag{45}
$$

Projecting the elasticity equation (45) onto $I$ and $n$, and using equation (6), we find

$$
p^\alpha = p^{el} + K \Delta \varepsilon_p, \quad q^\alpha = q^{el} - 3G \Delta \varepsilon_q. \tag{46}
$$

where $p^{el} = p_t + \Delta p^{el}$, $q^{el} = q_t + \Delta q^{el}$.

Taking into account that $f = f_t + \Delta f$, we can write the expression for porosity

$$
f = f_t + \Delta \varepsilon_p \frac{1}{1 + \Delta \varepsilon_p}. \tag{47}
$$

For an equivalent plastic strain in the matrix material, we can write

$$
\Delta \varepsilon^{pl}_m = \frac{-\Delta \varepsilon_p p^\alpha + \Delta \varepsilon_q q^\alpha}{(1 - f) \sigma_y(\varepsilon^{pl}_m)}, \tag{48}
$$

$$
\sigma_y = (1 + 3\mu \varepsilon^{pl}_m) N + \alpha \tanh(\Delta \varepsilon^{pl}_m \tau_1 / \Delta t), \tag{49}
$$

where $\varepsilon^{pl}_m = (\varepsilon^{pl}_m)_t + \Delta \varepsilon^{pl}_m$.

Equations (48) and (49) are solved with given values of $\Delta \varepsilon_p$ and $\Delta \varepsilon_q$.

The problem of integrating the elastoviscoplastic equations reduces to the solution of the set of equations: (18), (44), (46) – (49). These equations are solved using Newton’s method.

Projecting equation (19) onto $n$ and taking into account that $n$ is collinear with $s^r/q^r$ and $\dot{e}^{pl} = \dot{\varepsilon}_q n$, we find

$$
q^r + \frac{2\mu_2}{\tau_2} Q \left(q^r - q_f^r\right) = 3\alpha \varepsilon_q. \tag{50}
$$

We use the backward Euler scheme to integrate this equation. Taking into account that $Q$ is supposed to be a linear function of its argument, we can write

$$
\Delta q^r + \frac{2\mu_2}{\tau_2} \frac{\Delta t}{\tau_2} \left(q^r - q_f^r\right) = 3\alpha \Delta \varepsilon_q, \tag{51}
$$

where we suppose that $2\mu_2 = G$. Solving this equation, we find

$$
q^r = q_f^r + \left(q_0^r - q_f^r\right) \left(1 + y\right), \tag{52}
$$

where $q_0^r = q_f^r + 3\alpha \Delta \varepsilon_q = G \Delta t / \tau_2$.

Residual stress tensor is written in the form

$$
s^r = \frac{2}{3} q^r n. \tag{53}
$$

Finally, the solution of the problem is determined by equations (14), (45) and (48).
6. Numerical example
The results of the finite element analysis of a micromechanical model are represented in Figure 1. The elastic-plastic properties of the matrix material common for all calculations are specified by \( A = 500, \nu = 0.3, \sigma_{y0} = 1, \mu_1 = 5, N = 0.4, a = 1, q_1 = 1.5, q_2 = 0.2, q_3 = 2.25, q_f = 0.01 \); for \( a, b \) and \( c \): \( a = 1, q_c = 0.05 \); for \( a \) and \( b \): \( r_2 = 30 \); for \( c \): \( n = 5 \); for \( d \): \( a = 5, q_c = 0.3, \tau_1 = 1, \tau_2 = 10 \).

Figure 1.

Figure 1a shows that smaller stain rate leads to larger voids growth, i.e. material damage occurs sooner in smaller strain rates. Figure 1b illustrates a correlation between the active and full equivalent stress. The micromechanical model describes a large variety of material properties.

7. Conclusions
Application of the splitting method to the Gurson’s and Kukudzhanov’s models has been demonstrated in this paper. It was shown that the computational advantages of splitting method (as compared with standard methods) are achieved due to at the correction step, some equations can be integrated analytically. Constitutive relations of the micromechanical model, based on the phenomenological theory of dislocations, were integrated using splitting and backward Euler methods. It was shown that this model describes a large variety of materials as it involves kinematic hardening with residual stress relaxation after voids nucleation and viscosity.

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