ZESZYTY NAUKOWE POLITECHNIKI ŚLĄSKIEJ 2004
Seria: BUDOWNICTWO z. 102 Nr kol. 1644

Tomasz ŻEBRO*
Politechnika Krakowska

A COMPARISON OF TWO GRADIENT PLASTICITY FORMULATIONS AND ALGORITHMS FOR LOCALIZATION SIMULATIONS

Summary. The paper compares two formulations of the plastic flow theory regularized by the presence of higher-order gradients of an internal variable in the yield function. The computation is limited to small strains. The physical and theoretical background of the localization phenomena is briefly presented. The boundary value problem of gradient dependent plasticity is described. Two different solution algorithms are compared.

PORÓWNANIE DWÓCH SFORMUŁOWAŃ I ALGORYTMÓW GRADIENTOWEJ PLASTYCZNOŚCI DLA ANALIZY LOKALIZACJI

Streszczenie. W artykule porównano dwa sformułowania teorii plastyczności zregularyzowanej przez gradient wyższego rzędu wewnętrznego parametru $\underline{\kappa}$ w funkcji plastyczności. Rozważania prowadzone są przy założeniu małych odkształceń. W pracy krótko przedstawiono fizyczne i teoretyczne aspekty zjawiska lokalizacji. Oba sformułowania opisane są za pomocą problemu sprzężonego, w którym dyskretyzowane są dwie niezależne zmienne: przemieszczenie $\underline{u}$ i κ. W podejściu de Borsta i Mühlhausa [1] w funkcji plastyczności występuje laplasjan zmiennej κ. Jego obecność wymaga przy dyskretyzacji użycia funkcji o klasie ciągłości C^1. Poszukiwanie obszaru plastycznego odbywa się przez lokalne sprawdzenie warunku plastyczności w każdym punkcie numerycznego całkowania. W drugim z prezentowanych podejść, zaproponowanym przez Liebe i Steinmanna [3], dla określenia obszaru plastycznego sprawdzane są warunki obciążenia/odciążenia w formie słabej na poziomie węzłów. Dzięki temu do dyskretyzacji zmiennej κ wykorzystywane są funkcje o ciągłości C^0.

1. Motivation of gradient plasticity theory

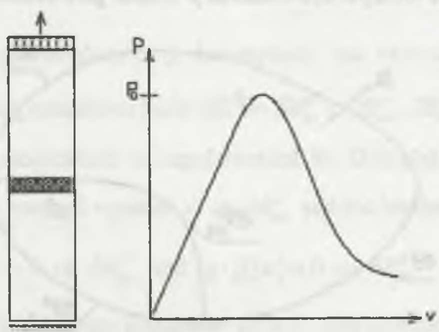

Fig. 1. Tensile bar, load versus displacement diagram for a softening material
Rys. 1. Pręt rozciągany, wykres obciążenie-przemieszczenie dla materiału z osłabieniem

* Opiekun naukowy: Dr inż. Jerzy Pamin

Localization phenomena are often noticed in the mechanical behavior of materials. The localization is a specific type of deformation in which, starting from a certain moment in the loading history, the whole deformation is concentrated in one or more narrow bands. The place and direction in which these bands develop depend on the shape of the body, loading and boundary conditions, but the phenomenon itself is a result of the material properties. The localization phenomena can have different character depending on the examined material: in ductile and frictional materials (steel, polymers, soil) we observe necking, shear bands or slip planes, in brittle materials (concrete, ceramics) we observe fracture bands and discrete cracks.

The strain localization is a physical result of the heterogeneity (microstructure) of real materials and is triggered at a place where the material is weaker or damaged. In macroscopic modeling such behavior is induced by unstable (softening) constitutive relation, see Figure 1. The classical models which express a hardening relation between average stresses and strains lead to smooth deformation and exclude strain localization.

The paper deals with the theoretical and algorithmic formulation of gradient plasticity. The aim is a reliable numerical simulation of localized plastic deformation. The gradient plasticity theory according to [3] is presented, and compared with the theory derived in [1]. Linear kinematic relations are assumed.

The gradient plasticity formulation can be derived from the free Helmholtz energy incorporating the gradient of an internal history variable [3]. Since the model is based on the postulate of maximum plastic dissipation, the associated flow rule is implied. In contrast to the algorithm derived in [1, 2], the algorithm proposed in [3] is based on a weak satisfaction of the loading-unloading conditions (at the nodal point level).

2. Strong form of the coupled boundary value problem

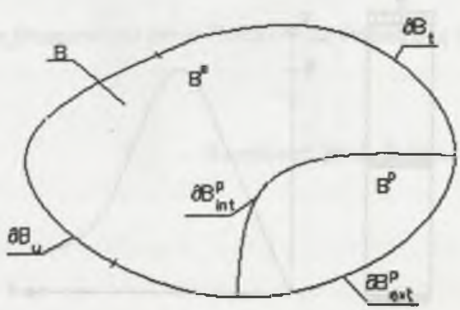

Fig. 2. Elastic-plastic body
Rys. 2. Ciało sprężysto - plastyczne

We assume that a body B is divided into elastic and plastic parts, see Figure 2. A displacement field $\underline{u}(x)$ and a history variable $\kappa(x)$ (which is in the considered case proportional to plastic multiplier λ) are parameterized in terms of placement $x \in B$. These two primary variables are governed by partial differential equations and a set of Kuhn-Tucker complementarity conditions.

Firstly, the equilibrium subproblem is written as:

$$\mathrm{div}\underline{\sigma}(\underline{u},\kappa)+\underline{b}=\underline{0} \text{ in } B, \tag{1}$$

where $\underline{\sigma}$ is the stress tensor and $\underline{b}$ is the body force per unit volume in B. The total boundary ∂B of domain B is decomposed as follows: $\partial B = \partial B_u \cup \partial B_t, \partial B_u \cap \partial B_t = \varnothing$. Dirichlet and Neumann boundary conditions are prescribed ($\underline{n}$ is an outer normal vector) on the boundary parts:

$$\underline{u}=\underline{u}_p \text{ on } \partial B_u \text{ and } \underline{n}\cdot\underline{\sigma}=\underline{t}_p \text{ on } \partial B_t \tag{2}$$

When a part of the body in the loading process yields, the standard elastic-plastic constitutive equation relates the stress and strains rates. The constitutive subproblem is governed by the gradient-dependent yield condition:

$$F=\varphi(\underline{u},\kappa)-\overline{Y}(\kappa,\nabla\kappa)=0 \text{ in } B, \tag{3}$$

where $\varphi(\underline{u},\kappa)$ is an equivalent stress measure, the gradient enhanced yield strength $\overline{Y}(\kappa,\nabla\kappa)=Y(\kappa)-\mathrm{div}\underline{H}(\kappa)$, and $\underline{H}$ is the hardening flux. In the special case when $\underline{H}=c\nabla\kappa$ with a constant coefficient c, we obtain $\overline{Y}(\kappa,\nabla\kappa)=Y(\kappa)-c\nabla^2\kappa$.

Moreover, the corresponding Kuhn-Tucker complementarity conditions hold:

$$F\le 0,\ \dot{\kappa}\ge 0,\ \dot{\kappa}F=0, \tag{4}$$

The boundary of the plastic subdomain is decomposed into external part ∂B^p_{ext} and internal one ∂B^p_{int} and the following conditions hold: $\partial B^p = \partial B^p_{int} \cup \partial B^p_{ext}, \partial B^p_{int} \cap \partial B^p_{ext} = \varnothing$.

The constitutive subproblem is supplemented by Dirichlet and Neumann boundary conditions in terms of the internal variable $\dot{\kappa}$ on ∂B^p_{int} and the hardening flux $\underline{H}$ on ∂B^p_{ext}:

$$\dot{\kappa}=0 \text{ on } \partial B^p_{int} \text{ and } \underline{n}\cdot\underline{H}(\kappa)=0 \text{ on } \partial B^p_{ext}. \tag{5}$$

The Kuhn-Tucker complementarity condition $\dot{\kappa}F=0$ can alternatively be postulated by a decomposition of the total domain into a subdomain of elastic or inactive states and a subdomain of plastic (active) states, respectively:

$$B^e = \{x \in B : F \leq 0, \dot{\kappa} = 0\} \text{ and } B^p = \{x \in B : F = 0, \dot{\kappa} > 0\}, \tag{6}$$

with additional requirements: $B = B^e \cup \partial B^p$, $B^e \cap B^p = \varnothing$.

3. Weak form of the coupled boundary value problem

In order to solve the coupled boundary value problem using a finite element discretization, the above equations are reformulated into a weak form.

In a first step, which is standard and common for both approaches, the equilibrium equation (1) and corresponding Neumann boundary condition $\underline{n} \cdot \underline{\sigma} = \underline{t}_p$ are tested by a virtual displacement $\delta \underline{u}$. As a result, the virtual work expression can be written as:

$$G^u = \int_{\partial B^t} \delta \underline{u} \cdot \underline{t}^p \mathrm{d}A + \int_B [\delta \underline{u} \cdot \underline{b} - \nabla \delta \underline{u} : \underline{\sigma}] \mathrm{d}V = 0 \tag{7}$$

where A and V denote the surface and volume of body B, respectively.

3.1. Approach of de Borst and Mühlhaus

Secondly, the yield condition is tested by $\delta\kappa$ and an integral over the plastic part of the solution domain gives the following equation [1, 2]:

$$G^F = \int_{B^p} \delta\kappa F(\underline{\sigma}, \kappa, \nabla^2 \kappa) \mathrm{d}V = \int_{B^p} \delta\kappa [\varphi(\underline{u}, \kappa) - Y(\kappa) + c\nabla^2 \kappa] \mathrm{d}V = 0. \tag{8}$$

The decomposition of the solution domain into elastic and plastic subdomains is as specified in eq. (6). The yield condition (3) is invoked locally to decide whether a point is in an elastic or plastic state.

3.2. Approach of Liebe and Steinmann

In the second approach the Kuhn-Tucker condition $F \leq 0$ and Neumann boundary condition $\underline{n} \cdot \underline{H} = 0$ are tested by $\delta\kappa(\delta\kappa > 0)$ and additionally the condition $\dot{\kappa} \geq 0$ is tested by δF. Finally, we obtain their weak forms:

$$G^F = \int_B \{\delta\kappa [\varphi(\underline{u}, \kappa) - Y(\kappa)] - \nabla \delta\kappa \cdot \underline{H}(\kappa)\} \mathrm{d}V \leq 0, \tag{9}$$

$$\dot{G}^\kappa = \int_B \delta F \dot{\kappa} \mathrm{d}V \geq 0. \tag{10}$$

Equation (9) can be interpreted as a weak form of the yield condition and eq. (10) assures positive increments of internal variable κ.

The global definitions of inactive and active subdomains are written as:

$$B^e = \{x \in B : G^F \leq 0, \dot{G}^\kappa = 0 \ \forall \delta\kappa, \delta F > 0\}, \tag{11}$$

$$B^p = \{x \in B : G^F = 0, \dot{G}^\kappa > 0 \ \forall \delta\kappa, \delta F > 0\}. \tag{12}$$

4. Time and space discretization of the problem

The above sets of governing equations (7), (8) or (7), (9), (10) have to be discretized in time and space. In order to compute $\underline{u}_{n+1}$ and κ_{n+1} at the end of time step $(n+1)$ the discrete equilibrium equation is written as:

$$G^u_{n+1} = \int_{\partial B^t} \delta\underline{u} \cdot \underline{t}^p_{n+1} \mathrm{d}A + \int_B [\delta\underline{u} \cdot \underline{b}_{n+1} - \nabla\delta\underline{u} : \underline{\sigma}_{n+1}] \mathrm{d}V = 0. \tag{13}$$

Next, the equation is discretized in space. The standard Bubnov-Galerkin finite element method is applied and domain B is decomposed into finite elements B_e. Using shape functions N^k_u for nodes k in an element we write:

$$\underline{u}^h = N^k_u \underline{u}_k \in H^1(B), \tag{14}$$

where summation over k is performed and H^l denotes the Sobolev function space. The discrete representation of strains $\underline{\varepsilon}^h = \nabla_s \underline{u}^h$, where ∇_s is a suitable linear differential operator, can be written as:

$$\underline{\varepsilon}^h = \nabla_s N^k_u \underline{u}_k . \tag{15}$$

We define the set of all nodes in the discretized domain as $\hat{B} = \{K : K = 1, n_{np}\}$, where n_{np} is the total number of nodal points. The discrete equilibrium equation written for each node K is:

$$\underline{R}^u_K = \mathop{A}_e \int_{\partial B_e} N^k_u \underline{t}^p_{n+1} \mathrm{d}A + \int_{B_e} [N^k_u \underline{b}_{n+1} - \nabla N^k_u \cdot \underline{\sigma}_{n+1}] \mathrm{d}V = 0, \tag{16}$$

where $\mathop{A}_e$ denotes the assembly operator adding contributions of all finite elements, i.e. eq. (16) represents the assembly of respective element residuals $\underline{R}^u_K = \mathop{A}_e \underline{R}^u_k$.

4.1. Approach of de Borst and Mühlhaus

The time discretization of the weak form of the yield condition in eq. (8) gives:

$$G^F_{n+1} = \int_{B^p} \delta\kappa F_{n+1}(\underline{\sigma}_{n+1}, \kappa_{n+1}, \nabla^2\kappa_{n+1}) \mathrm{d}V = 0. \tag{17}$$

The decomposition of the solution domain into elastic and plastic parts is obtained by writing eqs (6) for time step $(n+1)$.

Next, eq. (17) is discretized in space. Due to the presence of the second order gradient of the internal variable we have to introduce C^1-continuous shape functions N_κ^k for this field:

$$\kappa^h = N_\kappa^k \kappa_k \in H^2(B), \tag{18}$$

where H^2 denotes the relevant Sobolev space. The discrete representation of the Laplacian of internal variable κ can be written as:

$$\nabla^2 \kappa = \nabla^2 N_\kappa^k \kappa_k . \tag{19}$$

The discretized yield condition (17) is:

$$R_K^F = \underset{e}{A} \int_{B_e^p} F\left(\underline{u}_{n+1}, \kappa_{n+1}, \nabla^2 \kappa_{n+1}\right) N_\kappa^k \mathrm{d}V = 0, \tag{20}$$

where K is the number of a node in the subset of $\hat{B}$ which contains only the points in plastic state.

4.2. Approach of Liebe and Steinmann

The time discretization is performed in a similar way as in the previous subsection. The algorithmic Kuhn-Tucker complementarity conditions are:

$$G_{n+1}^F = \int_B \left\{ \delta\kappa \left[\varphi\left(\underline{u}_{n+1}, \kappa_{n+1}\right) - Y\left(\kappa_{n+1}\right) \right] - \nabla\delta\kappa \cdot \underline{H}\left(\kappa_{n+1}\right) \right\} \mathrm{d}V \le 0, \tag{21}$$

$$\Delta G_{n+1}^\kappa = \int_B \delta F\left(\kappa_{n+1} - \kappa_n\right) \mathrm{d}V \ge 0. \tag{22}$$

The algorithmic form of elastic-inactive and active subdomains is obtained by writing eqs (11) and (12) for time step (n+1).

The set of equations is now discretized in space. The displacement field $\underline{u}$ and the internal variable κ are now interpolated using similar shape functions N_u^k according to eq. (14), and N_κ^k as follows:

$$\kappa^h = N_\kappa^k \kappa_k \in H^1(B), \tag{23}$$

The discrete representation of plastic strain gradient $\underline{\kappa}^h = \nabla\kappa^k$ can be written as:

$$\underline{\kappa}^h = \nabla N_\kappa^k \kappa_k . \tag{24}$$

Finally, the discretized set of integral equations is composed of eq. (16) and the following two:

$$R_K^F = \underset{e}{A} \int_{B_e^p} \left\{ N_\kappa^k \left[\varphi\left(\underline{u}_{n+1}^h, \kappa_{n+1}^h\right) - Y\left(\kappa_{n+1}\right) \right] - \nabla N_\kappa^k \cdot \underline{H}\left(\kappa_{n+1}^h\right) \right\} \mathrm{d}V \leq 0, \tag{25}$$

$$\Delta R_K^\kappa = \underset{e}{A} \int_{B_e^p} N_\kappa^k \left(\kappa_{n+1}^h - \kappa_n^h\right) \mathrm{d}V \geq 0, \tag{26}$$

where K is a node number in the subset of $\hat{B}$ which contains only the points which exhibit plasticity.

5. Comparison of solution algorithms

In the incremental-iterative solution algorithm the task is as follows: given $\underline{u}_K^{(0)}, \kappa_K^{(0)}$ at all nodes and $\underline{\sigma}^{(0)}$ in all elements at the end of previous time step (n), compute the updated values $\underline{u}_K, \kappa_K, \underline{\sigma}$ at time ($n+1$). The comparison of the algorithms for the two discussed versions of the gradient plasticity theory is given in Figure 3.

The Newton algorithm is employed, which requires consistent linearization and computation of the tangent operator $\underline{K}$. In Figure 3 the symbol 'Δ' denotes the total increment of a quantity within an incremental step of external load $\Delta \underline{F}_{ext}$, and '$d$' denotes an iterative correction of a quantity. The elastic stiffness tensor is denoted by $\underline{D}$. Moreover, $\underline{K}_{kl}$ denotes the block of the element tangent matrix related to nodes k and l, while $\underline{K}_{KL}$ denotes the block of the global tangent matrix related to nodes K and L.

<table>
<tr>
<td>
The algorithm for the gradient plasticity formulation of de Borst and Mühlhaus [1, 2]:
Structural level (for each node):
1. Compute $\underline{R}_K^u = \Delta \underline{F}_{ext}$,
2. Solve for $d\underline{u}_K, d\kappa_K$ update $\Delta \underline{u}_K, \Delta \kappa_K$

Element level (for each integration point):
3. Constitutive update
$\Delta \underline{\varepsilon} = \nabla_s N_u^k \Delta \underline{u}_k$,
$\Delta \kappa = N_\kappa^k \Delta \kappa_k$,
$\kappa = \kappa_0 + \Delta \kappa$,
$\nabla^2 \kappa = \nabla^2 N_\kappa^k \Delta \kappa_k$,
$\underline{\sigma}_t = \underline{\sigma}_0 + \underline{D} \cdot \Delta \underline{\varepsilon}$,
</td>
<td>
The algorithm for the gradient plasticity formulation of Liebe and Steinmann [3]:
Structural level (for each node):
1. Compute $\underline{R}_K^u = \Delta \underline{F}_{ext}$,
2. Solve for $d\underline{u}_K, d\kappa_K$ update $\Delta \underline{u}_K, \Delta \kappa_K$
If $\Delta \kappa_K < 0$ then $\Delta \kappa_K = 0$
Element level (for each integration point):
3. Constitutive update
$\Delta \underline{\varepsilon} = \nabla_s N_u^k \Delta \underline{u}_k$,
$\Delta \kappa = N_\kappa^k \Delta \kappa_k$,
$\kappa = \kappa_0 + \Delta \kappa$,
</td>
</tr>
</table>

If $F(\underline{\sigma}_t, \kappa, \nabla^2\kappa) > 0$, then plastic state $\underline{\sigma} = \underline{\sigma}_t - \Delta\kappa \underline{D} : \left.\frac{\partial F}{\partial \underline{\sigma}}\right\|_{\underline{\sigma}_t}$, else elastic state, $\underline{\sigma} = \underline{\sigma}_t$. 4. Compute $\underline{R}^u_k, R^F_k, \underline{K}_{kl}$ **Structural level** (for each node) 5. Assemble $\underline{R}^u_K, R^F_K, \underline{K}_{KL}$ 6. Check global convergence criteria, if not satisfied go back to 2.	$\underline{\sigma}_t = \underline{\sigma}_0 + \underline{D} \cdot \Delta\underline{\varepsilon}$, $\underline{\sigma} = \underline{\sigma}_t - \Delta\kappa \underline{D} : \left.\frac{\partial F}{\partial \underline{\sigma}}\right\|_{\underline{\sigma}_t}$ 4. Compute $\underline{R}^u_k, R^F_k, \underline{K}_{kl}$ **Structural level** (for each node) 5. Assemble $\underline{R}^u_K, R^F_K, \underline{K}_{KL}$ If node K is elastic and $R^F_K > 0$ then mark K as plastic If node K is plastic, $R^F_K < 0$ and $\Delta\kappa_K = 0$ then mark K as unloading 6. Check global convergence criteria, if not satisfied go back to 2.

Fig. 3. Comparison of solution algorithms
Rys. 3. Porównanie dwóch algorytmów

6. Conclusions

In the paper two theoretical and algorithmic formulations of gradient plasticity, designed for the simulations of localized deformations, have been compared. In both the considered approaches the coupled boundary value problem is discretized using two independent primary variables $\underline{u}$ and κ. In the approach of de Borst and Mühlhaus [1,2] the yield condition is invoked locally, i.e. at each integration point the verification is performed whether the constitutive equations of elasticity of plasticity are satisfied. The presence of the Laplacian of internal variable κ in the yield condition sets the requirement of C^1-continuity of the shape functions for κ. This means that only a limited set of finite elements can be applied in one- and two-dimensional problems, and three-dimensional ones are practically intractable. In the concept of Liebe and Steinmann [3] the algorithm involves a weak satisfaction of the loading-unloading condition (at the nodal point level). As a result, C^0-continuous shape functions are sufficient for the discretization of internal variable κ. Standard Lagrange interpolation (e.g. quadratic) can be used for both $\underline{u}$ and κ, and three-dimensional problems can be solved.

REFERENCES

1. Borst R. de, Mühlhaus H.-B.: Gradient-dependent plasticity: Formulations and algorithmic aspects. Int. J. Numer. Meth. Engng 1992;35:521-539.
2. Borst R. de, Pamin J.: Some novel developments in finite element procedures for gradient-dependent plasticity. Int. J. Numer. Meth. Engng 1996;39:2477-2505.
3. Liebe T., Steinmann P.: Theory and numerics of a thermodynamically consistent framework for geometrically linear gradient plasticity. Int. J. Numer. Meth. Engng 2001;51:1437-1467.

Recenzent: Dr hab. Zbigniew Sikora, prof. Pol. Gdańskiej