An efficient FE-implementation of implicit gradient-enhanced damage models to simulate ductile failure

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We present a strategy which allows to implement a fully coupled, gradient-enhanced damage law into commercial FEM-codes with little effort. This enables a robust simulation of practical engineering problems avoiding spurious mesh dependency due to damage influence. The method is applied to a model for shear dominated, ductile damage of metals, which is used by engineers and often available in its local formulation within FEM-programs; e.g., ABAQUS. The model consists of a damage initiation criterion, followed by a damage evolution law which is coupled to the elastic-plastic constitutive equations. Convergence studies show the applicability of the implementation for 2D and 3D boundary value problems. Crack growth simulations of a benchmark problem show reasonable results compared to similar approaches from literature.

Keywords: gradient-enhanced damage; finite element implementation; ductile damage

1. Introduction

Nowadays, the principles of Continuum Damage Mechanics (CDM) are widely used to predict crack initiation in structures subjected to various loading conditions; e.g., [1, 2, 3]. However, the major problem of the local approach to fracture is the spurious mesh dependency, which is well known.

Early studies have shown, that a non-local averaging of variables related to strain softening leads to mesh independent results [4]. Such integral-type, non-local damage models are frequently investigated and improved [5]. As a drawback, the integral-type approach is difficult to handle within the Finite-Element-Metho d (FEM) [6]. Therefore, the implicit gradient approach has been derived by Peerlings et al. [6], which has been termed as gradient-enhanced non-local approach later on. As deduced by Forest [7], the gradient-enrichment is also related to the micromorphic approach. The initial proposal of gradient-enhancement has successfully been applied to various damage models in the FEM-framework (Gurson-type model [8], Rousselier-type model [9] and others [10, 11, 12]).

For engineering purposes, non-local damage models are still difficult to tackle. The considerable effort for implementing such models in FE-programs hinders its application to practical problems. The development of user-defined finite element formulations and advanced material routines are necessary; see e.g., [9, 13, 8]. Towards this issue, Mediavilla et al. [14] have proposed a method to implement a gradient-enhanced damage model into the commercial FEM-code MSC.MARC using an incrementally staggered operator-split approach.

The aim of this work is to explore a simple and comfortable method to realize a fully coupled gradient-enhanced implementation using commercial FE-codes. The idea is based on the observation that the additional governing equation of the gradient-enhanced approach and the well known heat equation
exhibit a useful similarity. This similarity is outlined in detail in the second section of the paper. We discuss a possibility to use this feature in conjunction with built-in solution methods of the commercial FEM-code ABAQUS. Similar implementation attempts have recently been applied for simulations of phase transitions within the phase-field theory [15].

In the third section of the paper, the gradient-enhanced framework and the solution method are applied to a prototype model for ductile damage of metallic materials, see [16]. The considered model contains a description of the elastic-plastic deformation behavior, a damage initiation criterion and a damage evolution law depending only on plastic deformation, which leads to material degradation; i.e., strain softening. Related local models are already successfully applied to engineering materials (see [17, 18]), which qualifies them to be non-locally enhanced. As it is well known, damage initiation and final fracture are dependent on the stress-state [19]. Therefore, a simple stress-triaxiality dependent damage initiation criterion together with the strain-driven damage evolution is tested. The advantage of the suggested modeling approach is manifested in its efficiency: No user-defined finite element or complete material routine is necessary. A convergence study is performed to show the reliability of the method.

The last part of the paper is dedicated to crack growth simulation. The problem of crack formation in a double-notched tensile test is considered, which has also been discussed by Mediavilla et al. [16].

2. Gradient-enhanced framework

Peerlings et al. [6] have derived an implicit-gradient formulation starting from an integral-type averaging approach. This leads to a field equation of Helmholtz-type:

\[ \varepsilon_d - L^2 \nabla^2 \varepsilon_d = \varepsilon_d \quad \text{in } \Omega. \quad (1) \]

Therein, \( \varepsilon_d \) denotes a scalar local variable, \( \bar{\varepsilon}_d \) is the non-local counterpart and \( \Omega \) is the currently occupied domain of the material body, respectively. The internal length \( L \) is introduced as additional material parameter. The spatial Laplacian is denoted as \( \nabla^2 \).

The natural boundary condition

\[ \nabla \cdot \bar{\varepsilon}_d \cdot \hat{n} = 0 \quad \text{on } \partial \Omega, \quad (2) \]

is utilized at all boundaries \( \partial \Omega \), as proposed by Peerlings et al. [6]. The normal vector to the boundary and the spatial Nabla-operator are denoted by \( \hat{n} \) and \( \nabla \), respectively. Nabla-operator and Laplacian are defined with respect to the current configuration. Therewith, the overall mean values of the local and non-local variables are equal:

\[ \int_{\Omega} \varepsilon_d d\Omega = \int_{\Omega} \varepsilon_d d\Omega. \quad (3) \]

This can be shown by applying the divergence theorem to Eq. (2) and using Eq. (1).

As usual in solid mechanics, the main equation to solve for is the balance of linear momentum (static case, without body forces)

\[ \nabla \cdot \sigma = 0 \quad \text{in } \Omega, \quad (4) \]

with appropriate boundary conditions. The Cauchy-stress tensor is denoted as \( \sigma \).

A user-defined finite element formulation (e.g. UEL-subroutine in ABAQUS) becomes necessary, because the FEM-form of the additional field equation Eq. (1) is not available in commercial FEM-programs by default. However, fully-coupled thermomechanical simulations are standard, for example
in ABAQUS, see \cite{20}. This leads to the following approach: We consider the special case of stationary heat conduction. Fourier’s law is chosen to define the heat flux $\vec{q}$:

$$\vec{q} = -\xi \nabla T.$$ \hfill (5)

The heat conduction parameter is denoted as $\xi$, with $\xi = \text{const.} \neq 0$. Thus, the field equation for the temperature $T$ reads

$$\xi \nabla^2 T + r = 0 \quad \text{in } \Omega.$$ \hfill (6)

A volumetric heat source $r$ is assumed. Homogeneous Neumann-boundary conditions for the heat flux $\vec{q}$ are prescribed on all boundaries $\partial \Omega_o$:

$$\vec{q} \cdot \vec{n} = 0 \quad \text{on } \partial \Omega_o.$$ \hfill (7)

The last two equations yield a striking analogy with respect to Eqn. (1) and (2) of the gradient-enhanced framework. The following renaming of variables is introduced:

$$T = \varepsilon_d,$$ \hfill (8)

$$r = -\varepsilon_d + \varepsilon_d.$$ \hfill (9)

The heat conduction parameter $\xi$ is related to the internal length $L$:

$$\xi = L^2.$$ \hfill (10)

Therewith, the stationary heat conduction problem defined by Eqn. (6) and (7) is transformed into the Helmholtz-equation (1) with the boundary condition (2).

With this knowledge at hand, fully coupled thermomechanical analysis of commercial FEM-programs can be used to perform simulations incorporating gradient-enhanced damage models. The modifications of the original stationary heat equation (see Eqn. (8) - (10)) are comfortably incorporated into the FEM-program ABAQUS with help of user-defined routines (UMAT, UHARD and HETVAL) as discussed within the subsequent sections. Compared to the coding via user-defined elements (UEL), the implementation of gradient-enhanced damage models via built-in thermomechanical elements has the advantage that the shape functions, the integration of stiffness matrices and the right-hand-side contributions are already implemented. Moreover, the tools for post-processing of the commercial software can be used directly.

To the author’s knowledge, the similarities between the presented field equations of gradient-enhanced damage and stationary heat conduction have not been utilized by other authors for implementation purposes before. Furthermore, the method will probably work for special cases of other advanced gradient-enhanced approaches (e.g. \cite{21}) and phase-field models for fracture (e.g. \cite{22, 23}). The technique fails if the gradient of the non-local variable directly occurs e.g. in criterion functions of plastic yielding or damage. A dependency of the internal variable $L$ on the non-local value $\varepsilon_d$ is possible.

The detailed implementation of the original field equations (1) and (4) within the FEM-framework can be found in [12, 16, 8]. For coupled temperature-displacement problems the same steps are performed. We mention the main ingredients briefly: Firstly, the strong forms of the governing equations (1) and (4) are rewritten in their weak forms. Secondly, the discretization is done by introducing interpolation functions for the degrees of freedom ($\vec{u}, \varepsilon_d$). The isoparametric ansatz is often applied. We follow the standard procedure of ABAQUS for large deformation analysis, where a so-called updated Lagrangian formulation is used, see \cite{24}. Finally, a consistent linearization leads to the system of algebraic equations to be solved in every incremental step.
3. Damage model

In the following, the gradient-enhanced framework is applied to a typical model for isotropic ductile damage. The local formulation is provided in similar forms by FEM-programs for engineering purposes (see "ductile damage" option in Abaqus [20]). Starting point is the model of Mediavilla et al. [12]. They have derived an elastic-plastic constitutive law coupled to damage based on the effective stress concept as well as the principle of equivalent strain, see [2]. In its original format, both the elastic properties and the plastic yielding are affected by damage evolution. A comparison with a simplified model, where just the strain hardening is decreased, yielded no significant differences for monotonic loading conditions under prescribed stress states, see [12]. This remains true for reasonable material parameters keeping the elastic strains small. These findings are incorporated in what follows.

Elasto-plasticity at finite deformations is handled via a hypo-elastic framework. As a constitutive assumption, the rate of deformation tensor $D$ is additively split into an elastic and a plastic part, $D_{el}$ and $D_{pl}$, respectively:

$$D = D_{el} + D_{pl}. \quad (11)$$

The hypo-elastic stress-strain relation

$$(\sigma)^{\circ} = C : D_{el} \quad (12)$$

is utilized in this study, neglecting damage influence on elastic properties. The Jaumann-rate $\dot{(\cdot)}^{\circ}$ is used as objective time derivative of the Cauchy-stress tensor $\sigma$:

$$\dot{(\sigma)^{\circ}} = \dot{\sigma} + \sigma \cdot W - W \cdot \sigma. \quad (13)$$

The fourth-order tensor of isotropic elastic stiffness is denoted by $C$. The definitions of the rate of deformation tensor $D$ and the spin tensor $W$ are given in A.

Rate-independent plastic behavior is assumed employing the yield function

$$f = \sigma_{eq} - (R(\varepsilon_{eq}) + \sigma_0)(1 - D) \leq 0, \quad (14)$$

where $\sigma_{eq}$ denotes the von Mises equivalent stress. The definition of $\sigma_{eq}$ is given in A, Eq. (43). The current yield stress, consisting of the initial yield stress $\sigma_0$ as well as the strain hardening $R(\varepsilon_{eq})$, is degraded by the damage state $D$, $0 \leq D \leq D_c$. A linear, isotropic hardening rule is adopted (single parameter $H$):

$$R(\varepsilon_{eq}) = H \varepsilon_{eq}. \quad (15)$$

Evolution laws for the internal variables have to be formulated. Here, the plastic rate of deformation $D_{pl}$ as well as the rate of the equivalent plastic strain $\dot{\varepsilon}_{eq}$ are defined in A.

In general, ductile damage is known as mechanism driven by plastic deformation. We follow Mediavilla et al. [16]: Therefore, the equivalent plastic strain $\varepsilon_{eq}$ is chosen as variable $\varepsilon_d$ for the gradient-enhancement. Other choices are possible: Linse et al. [8] introduce $\varepsilon_d$ as volumetric plastic strain in their non-local Gurson-model. Furthermore, $\varepsilon_d$ can be defined as the local damage variable itself, see [9, 13]. However, not all possibilities lead to satisfying results, as stressed by the assessments of Jirásek and Rolshoven [25] and Andrade et al. [5]. For example locking phenomena may occur, i. e., no complete material failure is reached, which do not arise if the non-local counterpart $\bar{\varepsilon}_d$ of $\varepsilon_d = \varepsilon_{eq}$ is considered as damage driving variable, see [25]. The following modified definition of $\varepsilon_d$ is formulated:

$$\dot{\varepsilon}_d = \begin{cases} 0, & \varepsilon_{eq} < \varepsilon_1(\sigma) \\ \dot{\varepsilon}_{eq}, & \text{once } \varepsilon_{eq} \geq \varepsilon_1(\sigma) \end{cases} \quad \text{during loading history.} \quad (16)$$
Therewith, damage initiation remains a local event controlled by $\varepsilon_{eq}$. The initiation strain $\varepsilon_i(\sigma)$ is not merely a fixed value in general, but rather a function of the stress state, which allows the designation "damage initiation locus", see [17, 18].

During loading history, healing effects have to be excluded; i.e., $\dot{D} \geq 0$. Therefore, an additional history variable $\kappa$ is defined via the Kuhn-Tucker-conditions

$$\dot{\kappa} \geq 0, \quad \kappa (\dot{\varepsilon}_d - \kappa) = 0, \quad \dot{\varepsilon}_d - \kappa \leq 0. \quad (17)$$

Hence, $\kappa$ is related to the non-local variable $\dot{\varepsilon}_d$ with restrictions. Damage evolves as function of the additional variable $\kappa$:

$$\dot{D} = h_D(D) \dot{\kappa}. \quad (18)$$

Therewith, the conditions in Eq. (17) ensure that $\kappa$ and $D$ cannot decrease, even when $\dot{\varepsilon}_d < 0$. This becomes possible if volume vanishes during numerical simulation using element deletion to handle crack growth. The reader is referred to the discussion in Section 6.

The shape of the damage law is dictated by $h_D(D)$, which is chosen as in Geers et al. [26] and Mediavilla et al. [16]:

$$h_D(D) = D_c \frac{3}{\tanh(3)} \frac{1}{\varepsilon_c} \left(1 - \tanh^2(3)(2D-1)^2\right). \quad (19)$$

The integrated form of Eq. (18) using Eq. (19) yields

$$D = D_c \left(1 + \frac{1}{\tanh(3)} \tanh \left(\frac{6 \kappa}{\varepsilon_c} - 3\right)\right), \quad (20)$$

see [26]. This particular damage law gives a slow growth of damage at the initiation of softening and near material failure $D_c$, respectively, see [26]. The material is undamaged as long as $\kappa = 0$ and completely failed at $\kappa = \varepsilon_c$. Complete material failure is therefore reached at a discrete value and not just asymptotically.

The complete material failure is defined by $D = D_c = 1$, see [27]. However, $D_c = 0.99$ is chosen in this study for numerical reasons. The first occurrence of $D = D_c$ in a considered material body marks the formation of an incipient crack located at the critical material point.

4. Numerical implementation of the damage model in ABAQUS

As discussed in the previous sections, the features of ABAQUS (version 6.14-2 and higher) are used to set up a framework for non-local damage modeling. Although the user-definition of a finite element is prevented, the implementation of the aforementioned material model is necessary. Also the source-like term $r$ (Eq. (9)) needs to be defined. We present two implementation strategies, depending on the complexity of the model:

1. Implementation of a user-defined material and a heat source (complete material routine, UMAT & HETVAL)
2. Implementation of a user-defined hardening and a heat source (minimal model, UHARD & HETVAL)

4.1. Complete material routine (UMAT)

The proposed damage model needs the definition of a material routine returning the current stress $\sigma$ and the definition of the current source term $r$. 

5
The hypo-elastic relation Eq. (12) is solved by applying an objective algorithm based on the notion of a rotated configuration. The underlying theory is extensively presented in the textbook of Simo and Hughes [28], section 8.3. The reader is referred to B for a short summary, Eqn. (46)-(56).

For implementation purposes, we change our notation to a vector-matrix-format, see B. As input in the incremental step $n \rightarrow n + 1$, ABAQUS provides the new strain increment $\Delta E$. Furthermore, the old rotated stresses $\sigma^\text{rot}$, the old non-local variable $\varepsilon_d^n$ and its increment $\Delta \varepsilon_d$ as well as the saved internal variables are transferred; e.g., $\varepsilon_{eq}^n$. The definitions of $\sigma^\text{rot}$ and $\Delta E$ are summarized in B, Eqn. (53) and (55).

The indices for the current values $n + 1$ are neglected in what follows. The stress $\sigma$ and the source term $r$ (defined by Eqn. (9) and (16)) are calculated for the fully elastic-plastic-damage response as

\[
\sigma = \sigma^w - C \cdot \Delta \sigma_{\text{pl}}
\]

\[
r = \mathbf{I} \cdot \left( - (\varepsilon_d^n + \Delta \varepsilon_d) \right) - (\varepsilon_{eq}^n - \varepsilon_{\text{fix}} + \Delta \varepsilon_{eq}) \quad , \quad \varepsilon_{eq} < \varepsilon_{\text{i}}(\sigma) \quad \text{once} \quad \varepsilon_{eq} \geq \varepsilon_{\text{i}}(\sigma).
\]

The trial-stress $\sigma^w$ is calculated as

\[
\sigma^w = \sigma^\text{rot} + C \cdot \Delta E.
\]

Further usage of superscript "tr" indicates values which are calculated from the trial-stress. If damage is initiated once, then the auxiliary-variable $\varepsilon_{\text{fix}}$ is fixed to the value of $\varepsilon_{\text{i}}(\sigma)$ at initiation. Only then, the local contribution to the damage driving variable starts. At the end of each increment, damage initiation is tested; i.e., $\varepsilon_{eq} \geq \varepsilon_{\text{i}}(\sigma)$.

The non-linear equations at the global FE-level are usually treated by the Newton-Raphson-method. Therefore, different entries of the so-called consistent material tangent have to be calculated in addition to the stress and source term update:

\[
K = \frac{d \sigma}{d \Delta E} + \mathbf{J} \cdot \frac{d \sigma}{d \Delta \varepsilon_d} \cdot \frac{d \sigma}{d \Delta \varepsilon_d} \cdot \frac{d \sigma}{d \Delta \varepsilon_d}.
\]

The stress tangent $K$ takes an unusual form, which is necessary in ABAQUS for hypo-elastic material laws (see [20] and B regarding the terms $J$ and $d \sigma / d \Delta E$). This results in a non-symmetric matrix $K$. The determinant of the deformation gradient is denoted by $J$, which is associated with change of volume.

Actually, the UMAT-interface provides a possibility to define the source term $r$. However, simulations are not possible with these source terms, that strongly depend on the temperature degree of freedom (non-local variable $\varepsilon_d$ in our case), for unknown technical reasons. Problems occur if the material tangent entry $d r / d \varepsilon_d$ is non-zero. Fortunately, ABAQUS enables to define a user-prescribed source term via subroutine HETVAL. All user-defined variables can be transferred from UMAT to HETVAL. The solution strategy turns out as follows: All updates and material tangent entries are calculated in UMAT. The source term $r$ is split:

\[
r = r_1 + r_2, \quad r_1 = - \varepsilon_d, \quad r_2 = \varepsilon_d.
\]

The part $r_1$ and the derivative $d r / d \varepsilon_d$ are transferred to HETVAL; $d r / d \Delta \varepsilon_d$ is set to zero in the UMAT data return. Especially the derivative $d r / d \Delta E$ is still returned by UMAT to keep a full coupling. The interaction of the utilized subroutines with the main program of ABAQUS is illustrated in Fig. 1 for the fully coupled modeling approach. For the current non-local model, the new damage state $D$ is evaluated at first and in every case using Eqn. (20) and (17).

As usual for rate-independent plasticity, the material’s behavior can be divided into a purely elastic and an elastic-plastic response, see the Kuhn-Tucker-conditions in Eq. (45). An operator-split is applied. Therefore, the yield function is tested with the trial stress and new damage state:

\[
f^w = \sigma_{eq}^w - (R(\sigma_{eq}^n) + \sigma_0)(1 - D).
\]
4.1.1. Elastic response

Purely elastic behavior is valid for \( f^{tr} < 0 \). The variable \( \kappa \) and the damage \( D \) have to be updated, because they are driven by the non-local variable \( \varepsilon_d \). All other output values read:

\[
\sigma = \sigma^{tr}, \quad r = \begin{cases} 
- (\varepsilon_0^d + \Delta \varepsilon_d) & , \varepsilon_{eq} < \varepsilon_i (\sigma) \\
- (\varepsilon_0^d + \Delta \varepsilon_d) + (\varepsilon_{eq}^{\text{fix}} - \varepsilon_i^{\text{fix}}) & , \text{once } \varepsilon_{eq} \geq \varepsilon_i (\sigma).
\end{cases}\]

The material tangent entries are

\[
\mathcal{K} = \mathcal{C} + \frac{1}{J} \sigma \cdot \frac{d J}{d \Delta E}, \quad \frac{d \sigma}{d \Delta \varepsilon_d} = 0, \quad \frac{d r}{d \Delta \varepsilon_d} = -1. \tag{29}
\]

4.1.2. Elastic-plastic response

Elastic-plastic behavior has to be considered for \( f^{tr} \geq 0 \). The solution of the elastic-plastic response as previously introduced is a standard procedure, called radial-return-method. Therefore, we refer to textbooks; e.g., [28]. A brief summary is given: The evolution Eqn. (41) and (44) are discretized in time via the Euler-backward method. Subsequently, the problem is condensed to one unknown value, here the increment of the Lagrange-multiplier \( \Delta \Lambda \). For the general case of non-linear hardening \( R (\varepsilon_{eq}) \), the only non-linear equation to be solved is the yield condition \( f (\Delta \Lambda) = 0 \). Again, the Newton-Raphson-method is employed at the material point level. The residual equation reads

\[
f = \sigma_{eq}^{tr} - 3 \mu \Delta \Lambda - \left( R (\varepsilon_{eq}^{tr} + \Delta \Lambda) + \sigma_0 \right) (1 - D). \tag{30}\]

The shear modulus is denoted by \( \mu \). The numerical solution is standard and therefore given in B. Therein, the material tangent entries for the elastic-plastic response are deduced:

\[
\mathcal{K} = \left( \mathcal{I} - \mathcal{C} \cdot N^{tr} \cdot \Delta \varepsilon - \Delta \Lambda \mathcal{C} \cdot \Phi \right) \cdot \mathcal{C} + \frac{1}{J} \sigma \cdot \frac{d J}{d \Delta E}, \tag{31}\]
\[ \frac{d \sigma}{d \Delta \varepsilon} = -\Lambda \bar{\varepsilon} \cdot \Delta \bar{\varepsilon}, \quad (32) \]

\[ \frac{d r}{d \Delta \varepsilon} = \begin{cases} 0^T, & \varepsilon_{\text{eq}} < \varepsilon_i (\sigma) \\ \frac{A_T}{C}, & \text{once } \varepsilon_{\text{eq}} \geq \varepsilon_i (\sigma), \end{cases} \quad (33) \]

\[ \frac{d r}{d \Delta \varepsilon} = \begin{cases} -1, & \varepsilon_{\text{eq}} < \varepsilon_i (\sigma) \\ \frac{\Lambda}{\varepsilon_i - 1} (\Lambda - 1), & \text{once } \varepsilon_{\text{eq}} \geq \varepsilon_i (\sigma). \end{cases} \quad (34) \]

### 4.2. Minimal model (UHARD)

Considering the special case, that the damage initiation should not depend on the stress state, a simpler implementation strategy of the damage model becomes feasible. The numerical framework of ABAQUS for elastic-plastic materials can be used (elastic-plastic behavior following von Mises with isotropic hardening, see ABAQUS-manual). The strain hardening \( \sigma_{\text{yield}} \) has to be defined in the user subroutine UHARD, including damage influence:

\[ \sigma_{\text{yield}} = (R (\varepsilon_{\text{eq}}) + \sigma_0) (1 - D (\bar{\varepsilon})). \quad (35) \]

Likewise, the damage evolution Eq. (20) can be updated, because \( \varepsilon_{\text{eq}} \) and \( \bar{\varepsilon} \) (prior the temperature degree of freedom) and their increments are available. The conditions in Eq. (17) have to be checked.

All ingredients for the source term \( r \) and its derivatives can be transferred to the user-subroutine HETVAL. The interaction of the subroutines is illustrated in Fig. 1. Only the contribution to the material tangent \( d r / d \varepsilon_{\text{eq}} \) corresponding to the term \( d r / d \Delta E \) of the UMAT-approach is not available. But no obstructive convergence problems were detected for all simulations up to crack initiation presented in this study. Problems regarding crack growth are discussed within the next section. As a remark: the source code of this minimal, non-local damage model contains of just a few lines. On the other hand, if additional coupling of the elastic properties to damage should be considered, the minimal model is not feasible anymore.

Whenever the default plasticity model of ABAQUS is used, Kirchhoff-stresses \( \tau = J \sigma \) are internally computed, which coincide with Cauchy-stresses \( \sigma \) only for incompressible material behavior. Therefore, the model equations given above and the minimal model are not identical. Nonetheless, for the considered damage law the volume is nearly preserved, because of using incompressible von Mises-plasticity and negligible elastic volume changes.

### 5. Benchmark test simulations until formation of an incipient crack

Both model implementations, via UMAT and the minimal version (UHARD), are tested by several examples. As stated by Mediavilla et al. [16], the considered type of damage model driven by equivalent plastic strain does especially apply to shear dominated loading situations; e. g., blanking. Therefore, a specimen leading to a pronounced shear band formation proposed by Samal et al. [9] is considered. Nonetheless, a smooth, cylindrical tensile test applied by Geers et al. [26] and a 3D plate-with-hole example investigated by Kiefer et al. [21] are additionally discussed to reveal some special properties of the non-local damage model, see geometric setup in Fig. 2. Slightly modified dimensions of the original specimens are used without influencing the conclusions. The material parameters as summarized in Tab. 2 are utilized within this section.

#### 5.1. Preliminaries

In all cases, quadratic shape functions for approximating the displacements and linear shape functions for the non-local variable are used within the finite element formulation. A reduced integration scheme
Figure 2: Benchmark specimen geometries and boundary conditions. Dimension are given in mm. Displacement controlled loading ($\bar{u}$) applied: (a) Shear band specimen with geometrical imperfection, plane strain state (2D), thickness $t = 1$ mm, finite element type CPE8RT, see [9]. (b) 3D plate-with-hole test, symmetries utilized, half thickness $t = 0.5$ mm, finite element type C3D20RT, see [21]. (c) Cylindrical tensile test, rotational symmetry utilized (2D), finite element type CAX8RT, see [26].
Table 1: Parameters of the damage initiation criterion (Eq. (39)) and non-local strain at crack formation \( \varepsilon_c \) for the stress-independent (S-1) and stress-dependent case (S-2).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Case S-1</th>
<th>Case S-2</th>
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<tr>
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<td>( \varepsilon_c )</td>
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Table 2: Material parameters.

<table>
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<th>Description</th>
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<td>( \nu )</td>
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<tr>
<td>( H )</td>
<td>hardening modulus</td>
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<tr>
<td>( L )</td>
<td>internal length</td>
<td>[mm]</td>
<td>0.5</td>
</tr>
<tr>
<td>( D_c )</td>
<td>damage at crack formation</td>
<td>[-]</td>
<td>0.99</td>
</tr>
</tbody>
</table>

is chosen; the ABAQUS internal notations of the element types are mentioned in Fig. 2. Stationary coupled temperature-displacement simulations are conducted.

Convergence studies concerning the spatial discretization are performed for all examples. For a gradient-enhanced Gurson-model, Linse et al. [8] have proposed to use a maximum element size (edge-length \( b_e \) of 2D square-shaped element) of \( b_e \leq L/4 \) to achieve converged results. Therefore, we choose the discretization variants (2D-square elements: \( b_e \times b_e \), 3D-cubic elements: \( b_e \times b_e \times b_e \)) in the vicinity of damage zones as

\[
\frac{b_e}{L} = \left\{ 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16} \right\}.
\]

The simulations are interrupted when damage reaches the final value \( D_c \) (corresponding to total material failure) the first time at the most critical integration point. This is interpreted as formation of an incipient crack.

5.2. Results of the benchmark tests

5.2.1. Shear band specimen (plane strain state, 2D)

The boundary value problem with underlying geometry of Fig. 2 a) is considered. For this example, a localized shear band is expected in the vicinity of damage, as shown by Samal et al. [9]. Simulations are conducted for the parameter set S-1; i.e., the stress-state independent damage initiation criterion (see Tab. 1). Damage starts right from the beginning of plastic deformation, because \( \varepsilon_i = 0 \). A local version of the damage model, the non-local complete material model (UMAT) and the non-local minimal model (UHARD) are compared in the following.

The convergence behavior of the non-local damage model in terms of its global response is illustrated with help of the force vs. displacement curves in Fig. 3. Refining the discretization for the non-local model leads to coincident curves, see Fig. 3. Nearly a complete unloading of the specimen is achieved, although no crack growth is present. Acceptable results can already be produced with \( \frac{b_e}{L} \leq 1/4 \), as proposed by Linse et al. [8]. The curves of the full implementation (UMAT) and the minimal model (UHARD) give the same results, as revealed in Fig. 3 for \( \frac{b_e}{L} = 1/8 \).

Contrary, the force drop becomes steeper while decreasing the ratio \( \frac{b_e}{L} \) for the local version of the damage model. Especially the force state, when the first material point is fully degraded (\( D = 1 \), seems
Figure 3: Normalized force ($F$) vs. displacement ($\bar{u}$) curves of the shear band specimen up to formation of an incipient crack ($D = D_c$ firstly met at an integration point). (see Fig. 2 a), $A_0 = 5 \times 1 \, \text{mm}^2$, $l_0 = 15 \, \text{mm}$). Different ratios of characteristic element dimension $b_c$ to internal length $L$ are considered. Curves are shown for the local and non-local damage model as well as for the minimal model (UHARD).

Figure 4: Non-local vs. local version of the damage model: Damage distribution at the formation of an incipient crack ($D = D_c$ firstly met at an integration point) for different discretization levels $b_c/L$. Stress-state independent damage initiation criterion (parameter set S-1).
Table 3: Global convergence behavior using the minimal model (UHARD) and complete model (UMAT).
Necessary steps (top values in the cells), increment cutbacks (mid values) and average iteration steps (bottom values) depending on the global tolerance refinements are compared. Premature termination is marked by ×. Omitted cases are denoted by –.

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not to converge to a certain value for the considered discretization. Further decrease of the element size will lead to the situation, that no difference between the force level at the localization of damage and the first occurrence of complete material failure can be detected. The necessary energy for the transition from the beginning of damage localization up to the formation of an incipient crack becomes infinitesimally small.

Additionally, the non-local character of the proposed damage model can impressively be illustrated by the damage distribution in the developed shear band, see Fig. 4. A finite width of the damage zone evolves for the non-local case despite of decreasing $b_\varepsilon/L$, whereas damage narrows down into a band with a thickness of one finite element for the local version of the model.

5.2.2. Convergence behavior during global iterations of the Newton-Raphson scheme

A convergence study is conducted in order to test the reliability of the implementation variants (UHARD, UMAT) within the framework of a monolithic Newton-Raphson-scheme, which is used to solve the coupled field problem. Especially the role of the missing material tangent entry using the UHARD-implementation should be clarified.

A simulation of the shear band specimen (see Fig. 2 a)) is considered in order to analyze the convergence properties of the implementations. The element size is chosen as $b_\varepsilon = L/4 \approx 4800$ elements, $\approx 35000$ degrees of freedom. The time stepping is prescribed in order to allow a maximum displacement
increment $\Delta \bar{u} = 0.01 \bar{l}_0$, where $\bar{l}_0$ denotes the height of the specimen. The final displacement considered in the step is $\bar{u} = 0.1 \bar{l}_0$. Cutbacks of the increment size due to convergence problems and increase of the step size in case of fast convergence are allowed. The initial increment is equal to the maximum increment $\Delta \bar{u} = 0.1 \bar{l}_0$.

The residual force vector and the residual flux vector shall be denoted as $R_u$ and $R_\varepsilon$, respectively. In each loading increment, iterations are performed until the residuals fall below a bound

$$\max(R_u) < \epsilon_u = \alpha_u \bar{F}, \quad \max(R_\varepsilon) < \epsilon_\varepsilon = 3 \cdot 10^{-6} \alpha_\varepsilon \bar{L}^2. \quad (37)$$

In the present convergence study, $\bar{F}$ is fixed to a value which has been determined from a purely elastic-plastic calculation of the considered example ($\bar{F} = 8$ N). The parameters $\alpha_u$ and $\alpha_\varepsilon$ are pre-factors which are determined in what follows. ABAQUS prescribes a default value $\alpha_u = 5 \cdot 10^{-3}$. Following Hütter et al. [29], the bound $\epsilon_\varepsilon$ is chosen proportional to the internal length $\bar{L}$ in the present convergence study, see Eq. (37).

The required load increments, the iterations per increment and possible cutbacks are investigated for different termination criteria in order to assess the convergence behavior. As reference, the suggestions of Hütter [30] are considered: $\alpha_u = 2 \cdot 10^{-3}$, $\alpha_\varepsilon = 1.0$. Additionally, smaller tolerances are applied. The cases are summarized as:

$$\alpha_u = 2 \cdot 10^{-3}; 2 \cdot 10^{-4}; 2 \cdot 10^{-5} \quad \alpha_\varepsilon = 1.0; 1 \cdot 10^{-1}; 1 \cdot 10^{-2}. \quad (38)$$

Simulations are conducted with the UHARD and UMAT-based models considering damage (parameter set S-1 from Tab. 1), whereby the tolerances are systematically varied as illustrated in Tab. 3. Along the rows of the table, the tolerance for the force residual $\epsilon_u$ is decreased at constant $\epsilon_\varepsilon$. Following the columns, the tolerance $\epsilon_\varepsilon$ is decreased at constant $\epsilon_u$. The case of decreasing both tolerances can be found along the major diagonal.

The following conclusions can be drawn from Tab. 3: The UMAT-approach shows a comparable behavior for all considered cases. Simulation up to formation of an incipient crack is consistently possible. Eight cutbacks of the increment size are necessary. In Fig. 5, the number of iterations are plotted against the loading history for the most restrictive case. Some cutbacks are visible as points of many iterations. It is possible to identify the occurrence of cutbacks and the necessity of many

Figure 5: Global convergence behavior of the complete model (UMAT) over normalized loading for the most restrictive tolerance (bottom-right-case in Tab. 3).
Table 4: Comparison of the global convergence behavior of the two implementation variants for pure elastic-plastic behavior. Necessary steps (top values in the cells), increment cutbacks (mid values) and average iteration steps (bottom values) depending on the global tolerance refinements are compared. Premature termination is marked by ×.

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iterations (Fig. 5) with critical points in the load-displacement-curves (Fig. 3): Cutbacks occur clearly near the transition from linear force-displacement response to non-linear (elastic-plastic) behavior and at the beginning of the load drop. The low number of necessary iterations ($\approx 5$) to fulfill also the most restrictive termination criterion may be seen as an indicator for a reasonable convergence. The average size of the displacement increment has been determined as $\approx 0.06 l_0$, which is near to the (target) maximum displacement increment $\Delta u = 0.01 l_0$. A higher maximum increment has been tried, but more cutbacks occurred and the number of overall increments didn’t decrease significantly.

Concerning the UHARD-approach, decreasing the tolerance $\bar{\epsilon}_u$ and keeping $\epsilon_u$ at the reference value enables the simulation until formation of an incipient crack. But especially for the tightest tolerance, a remarkable degradation of the performance indicators is visible. This can be attributed to the missing tangent entry. Reducing the force residual tolerance or both tolerances simultaneously leads to premature termination of the simulations, i.e., the UHARD-approach fails.

The ABAQUS-internal formulation of elastic-plastic material behavior seems to have problems with tight tolerances of the force residual. Therefore, purely elastic-plastic simulations without damage have been conducted, see Tab. 4. Interestingly, the UMAT-implementation manages all refinements, whereas the UHARD aborts again. Also the ABAQUS-intrinsic possibility of prescribing the (linear!) hardening law in a tabular manner, instead of using the user-defined hardening routine, yields no satisfying result.

For all upcoming simulations, the bounds proposed by Hütter et al. [29] are applied. The average force $\bar{F}$ is taken as provided by ABAQUS.

5.2.3. Plate-with-hole test (3D)

To take a stress dependency of the damage initiation into account, the Johnson-Cook’s model of fracture as used by Bai and Wierzbicki [19] is considered:

$$
\varepsilon_1 (h) = C_1 + C_2 \exp \left( -C_3 h \right). 
$$

Therewith, damage initiation is a function of the stress triaxiality $h$ (see Eq. (43)) in an exponential manner. The parameters of the stress-state dependent case S-2 are chosen to yield $\varepsilon_1 (h = 1/3) = 0.4$ and $\varepsilon_1 (h = 1) = 0.1$, see Tab. 1. The geometry and boundary conditions of the considered plate-with-hole example are given in Fig. 2 b).

The global responses of the local and non-local model are shown in Fig. 6 as force vs. displacement curves. The simulations are stopped when a crack is formed, similar to the shear band simulations.

A pronounced force drop is visible for the non-local model. Refining the discretization leads again to coincident curves with same level of force and displacement at formation of an incipient crack. In case of the local model, nearly no load drop due to damage exists up to crack formation. The contour plot in Fig. 7 shows, that damage strongly evolves in a couple of finite elements for the local model. Contrary, the simulations using the gradient-enhanced model exhibit a finite size of the damage zone.
Figure 6: Normalized force ($F$) vs. displacement ($\bar{u}$) curves of plate-with-hole specimen up to formation of an incipient crack ($D = D_c$ firstly met at an integration point). (see Fig. 2 b), $A_0 = 10 \times 0.5$ mm$^2$, $b_0 = 10$ mm). Different ratios of characteristic element dimension $b_e$ to internal length $L$ are considered. Curves are shown for the local and non-local damage model.

during mesh refinement. As for the 2D-case, a mesh size $b_e/L = 1/4$ seems to be a good choice to get converged results.

5.2.4. Smooth tensile test (axi-symmetric, 2D)

The smooth tensile test example is considered next (see Fig. 2 c)). The gradient-enhanced implementation with stress-triaxiality dependent damage initiation is applied, as for the 3D-example (S-2, see Tab. 1).

As shown by the contour plot in Fig. 8, damage develops in the center of the tensile specimen, where the incipient crack is finally created. The damage zone is spread over several layers of finite elements due to the non-local character of the underlying model. Also necking occurs prior to crack formation.

A questionable property of the damage model is revealed by the results summarized in the diagram of Fig. 8: Only the strain hardening is reduced by damage, which directly dictates the permissible equivalent stress $\sigma_{eq}$ via the yield condition Eq. (14). Consequently, the deviatoric stresses vanish. On the other hand, hydrostatic stresses are not directly restricted, which leads to the "residual" stress $\sigma_{zz}$ at the specimen’s center, see the curves of $\sigma_{xx}$ and $\sigma_y$ in Fig. 8. An additional coupling of the elastic properties to damage may also have a similar effect, because high volumetric stresses can occur in the undamaged (effective) configuration, which still produce considerable stresses in the damaged configuration although $D$ approaches a high value ($D \approx 0.99$). To overcome this issue, a damage-coupled dependency of the yield condition on hydrostatic stress with associated volumetric plastic strain can be taken into account, which additionally restricts the permissible stress state. This would lead to a Gurson-type model, where $\sigma_{eq} = \sigma_y = 0$ at the fully damaged state.

6. Crack growth modeling by element deletion

For crack growth simulations, a transition from continuous damage to a discontinuous material separation is necessary. During crack growth, new surfaces are generated which have to be handled with appropriate techniques, see [26, 11, 29, 14, 16]. Keeping actually damaged regions active during crack
growth analysis raises some disadvantageous effects: highly distorted elements, unrealistic high damage growth in the crack surroundings leading to increasing crack width, see [31].

One crude possibility to model crack growth is the element deletion technique. This method is often used in the context of local damage models applied within explicit FEM-codes, see [17, 18]. Also in the non-local framework element deletion has been considered, see [31]. In ABAQUS, element deletion is also available during a quasi-static, implicit analysis. Therefore, its applicability towards crack growth simulation in combination with the non-local damage model should be studied.

On the one hand, deleting a fully damaged element automatically yields the trivial natural boundary conditions for the non-local field equation (see Eq. (2)), which has been suggested by Peerlings et al. [27] for evolving crack contours. On the other hand, no sharp crack can be introduced by deleting an element of finite size. Imposing the trivial natural boundary condition may generate a jump-like contribution due to the instantaneous change of the flux leading to numerical problems as stated by Hütter et al. [29]. Subsequently, a redistribution of the non-local variable occurs due to the vanishing volume during element deletion, due to the diffusional character of the field equation and due to the new natural boundary condition, which could induce questionable effects, see [29]. As a further consequence, mass is lost which may not influence quasi-static simulations, but plays a role in dynamic simulations. Furthermore, a fully damaged state of all integration points within a single element is a necessary condition for deletion in ABAQUS. Until complete failure of an element, a high contribution to the non-local strain can occur leading to an overestimation of damage growth. Peerlings [31] has shown,
that a crack may not form completely due to crack-bridging elements. A small element size in crack growth regions has to be ensured to counterbalance the method’s drawbacks.

Besides the general issues concerning the non-local variable during element deletion, the specific problem of non-zero stresses at actually fully damaged states for the considered damage model may also lead to numerical problems as discussed in the previous section for the smooth tensile test: Deleting the fully damaged element during simulation causes an artificial force jump. This issue may not severally occur for cracks growing from free surfaces or for shear dominated problems, see [16]. As a pragmatic method, numerical damping is used to overcome critical force jumps in the present study.

6.1. Numerical example

A double-notched tensile specimen is considered as proposed by Brokken [32] and Mediavilla et al. [16]. Geometry and boundary conditions are depicted in Fig. 9. The plane strain state is assumed.

Different mesh-refinements $h_0/L$ are tested. In order to have a considerable crack growth instead of softening due to necking and damage, a smaller internal length ($L = 0.25$ mm) and a higher strain hardening ($H = 600$ MPa) are chosen compared to the previous simulations. The set of damage parameters S-1 is used, see Tab. 1. The full-model version (UMAT) is utilized. Numerical damping by adding viscous forces is applied as described in ABAQUS [20] (option "stabilize"). The damping forces are automatically computed with the assumption of a unity density, the velocity at the FE-nodes (global prescribed velocity $\dot{u} = 1$ mm/s) and a constant damping factor $c$, $c = 0.0002$. With these damping parameters, no differences between the undamped and damped case were recognized up to the initiation of an incipient crack. Crack growth simulations with the minimal model (UHARD) gave no satisfying results, because convergence problems regarding the force equilibrium occurred after some crack advance. In order to keep the simulations running, a very small size of the load increment becomes necessary. The issues can be attributed to the questionable convergence properties of the default elastic-plastic modeling in ABAQUS, see Section 5.2.2.
Figure 9: Double-notched tensile test (see [32, 16]). Displacement controlled loading $\bar{u}$. Dimensions in mm. Plane strain state (2D) with thickness $t=1$ mm. Finite element type CPE8R T.

6.2. Results

Force vs. displacement curves for three mesh resolutions are plotted in Fig. 10. A gradual force drop is already induced by damage until formation of an incipient crack (highlighted by a circle). Afterwards, stable crack growth takes place. A smooth curve is obtained during element deletion. Just small force jumps occur, which become visible only at high magnification of the curves. At $\bar{u}/L_0 \approx 0.049$ a sudden decrease of the force appears, which may mark the unstable crack extension and failure of the specimen. Nonetheless, a reasonable result of the global response is already available with a coarse mesh of $b_0/L = 1/2$, although the crack contour is crude, see Fig. 11.

The crack contour prior to unstable crack growth ($\bar{u}/L_0 \approx 0.049$) is illustrated for all meshes in Fig. 11. For the coarse mesh, element erosion in some distance to the current crack tip occurs and crack bridging elements are visible. Since the employed finite element formulation contains several integration points per element the crack can be bridged at single nodes as long as one active integration point exists. Crack extension and growth direction coincide for all meshes. For all simulations of this shear dominated problem the crack width is partly formed by deleting some layers of elements. However, no severe blunting of the cracks occurs (see Fig. 11 and Fig. 12).

The crack propagation is illustrated in Fig. 12 for the mesh $b_0/L = 1/4$. At first, a shear band with high damage is formed. The crack initiates at the upper right notch followed by a second crack at the bottom notch. The second crack seems to grow faster and both cracks unify near the center of the specimen.

6.3. Discussion

Similar results of the double-notched tensile test problem have been obtained by Mediavilla et al. [16] (remeshing technique to simulate crack growth) as well as Ambati et al. [23] (phase-field approach to ductile fracture, small deformation theory). In our study, extremely distorted elements are avoided by choosing suitable values of the damage law ($\varepsilon_c, L$). Mediavilla et al. [16] have investigated cases, where very large local deformations occur until material failure is reached. Then, the remeshing approach seems to be a better choice.

The presented example aims at shear dominated failure (here crack Mode I). Similar local formulations of the damage model are also used for crack growth configurations of Mode I in ductile materials.
Figure 10: Normalized force ($F$) vs. displacement ($\bar{u}$) curves of the double-notched specimen up to final structural failure. $A_0 = 10 \times 1$ mm$^2$, $l_0 = 10$ mm. Different ratios of characteristic element dimension $b_e$ to internal length $L$ are considered. The circle $\circ$ labels the crack initiation.

Figure 11: Crack contour for different mesh refinements $b_e/L$ prior to the sudden force drop at $\bar{u}/l_0 \approx 0.049$. $l_0 = 10$ mm.
Figure 12: Crack growth and damage distribution ($D$) for different loading stages $\bar{u}/l_0$ of the double-notched tensile test for $b_0/L = 1/4$. $l_0 = 10$ mm.
see [18]. The applicability of the discussed gradient-enhanced model to Mode I dominated problems needs to be evaluated. Typically, a damage mechanism dominated by void growth is expected, which is strongly influenced by stress triaxiality and not only by equivalent plastic strain. For the Mode I configuration under plane strain conditions, the plastic zone develops perpendicular to the crack growth direction; see textbooks [33]. Therefore, some unrealistic blunting effects may arise if damage and finally element deletion are only driven by equivalent plastic strain. Drawbacks of the model concerning damage evolution have already been revealed by the simulation of a simple tensile test, see previous section. Some extensions are necessary, especially concerning the influence of hydrostatic stress on yielding and plastic flow as well as the damage evolution as function of the stress state. Some improvements have been suggested by Mediavilla et al. [12] towards damage evolution, but further steps are highly recommended.

Finally a remark on the computational costs: To obtain the results of crack growth using element deletion, small loading increments are necessary when deletion starts during implicit, quasi-static analysis. These rather simple crack growth simulations need therefore a considerable high amount of computational power and time. For the example shown in Fig. 12, a few thousand load increments were needed.

7. Conclusions

The framework of implicit gradient-enhancement of Peerlings et al. [6] in combination with the damage model of Mediavilla et al. [16] is utilized as example to demonstrate the implementation method. The following key-ideas and findings should be emphasized:

- Due to the gradient-enhanced framework, an additional partial differential equation has to be solved, which describes the evolution of a scalar non-local variable. Fortunately, similarities between the additional field equation and the stationary heat equation can be successfully used for implementation purposes. The standard framework of implicit, fully-coupled temperature-displacement simulations provided by commercial FE-codes can be applied to solve boundary value problems incorporating the gradient-enhancement of damage. The necessary modifications of the heat equation can be realized if a general volumetric heat source can be defined as function of temperature and strain in the available commercial FE-code as a subroutine. The subsequent key-idea is a simple renaming of degrees of freedom: The non-local variable substitutes the temperature. The method circumvents the coding of a user-defined element, which usually requires a high programming effort and exhibits post-processing drawbacks.

- The implementation of the specific gradient-enhanced damage model of Mediavilla et al. [16] into the commercial FE-program ABAQUS is demonstrated. In its simplest form, the gradient-enhanced prototype model can be implemented as a user-defined strain-hardening routine UHARD in ABAQUS (a few lines of source code). This turns out to be sufficient for simulations up to formation of an incipient crack. A more general implementation, which is appropriate for crack growth simulations, is accessible via the user-defined material interface UMAT. This still needs less effort than a complete user-defined element coding.

- A stress-state dependent damage initiation criterion, as proposed by Lian et al. [18], is tested within the gradient-enhanced damage framework. The simulation results of different 2D and 3D examples exhibit the desired mesh-independent properties of the approach.

- Crack growth simulations using the element deletion technique can be conducted in ABAQUS. The use of (small) numerical damping enables to model a large amount of crack propagation. As numerical example, crack growth in a double-notched tensile test is considered. The results are in qualitative agreement with similar simulations from literature.
In future studies, the implementation method allows a relatively fast testing and comparison of different gradient-enhanced damage models to evaluate their advantages and drawbacks. The developed subroutines are provided by the authors as supplementary material [34].

Acknowledgments

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References


The rate of deformation tensor \( D \) and the spin tensor \( W \), as symmetric and skew-symmetric parts of the velocity gradient \( L \), are defined as:

\[
L = \dot{F} \cdot F^{-1}, \quad D = \frac{1}{2} \left( L + L^T \right), \quad W = \frac{1}{2} \left( L - L^T \right).
\] (40)

The deformation gradient is denoted as \( F \).

An associated flow rule is assumed, i. e.,

\[
D_{pl} = \dot{\Lambda} \frac{\partial f}{\partial \sigma} = \dot{\Lambda}N
\] (41)

with the yield normal

\[
N = \frac{3}{2\sigma_{eq}}S.
\] (42)

We define some typical quantities related to the stress tensor \( \sigma \):

\[
\sigma_h = \frac{\text{tr} (\sigma)}{3}, \quad S = \sigma - \sigma_h \delta, \quad \sigma_{eq} = \sqrt{\frac{3}{2} S : S}, \quad h = \frac{\sigma_h}{\sigma_{eq}}.
\] (43)

These are the hydrostatic stress \( \sigma_h \), the stress deviator \( S \), the von Mises equivalent stress \( \sigma_{eq} \) and the stress triaxiality \( h \). The second-order unity tensor is denoted as \( \delta \).

The rate of equivalent plastic strain is calculated as usual

\[
\dot{\varepsilon}_{eq} = \sqrt{\frac{2}{3} D_{pl} : D_{pl}} = \dot{\Lambda},
\] (44)
which coincides with the Lagrange-multiplier $\dot{\Lambda}$. The evolution of the hardening variable is assumed to be equal to the equivalent plastic strain $\dot{\varepsilon}_{eq}$.

The elastic-plastic model is completed by the Kuhn-Tucker-conditions

$$\dot{\Lambda} \geq 0, \quad \dot{A} f = 0, \quad f \leq 0.$$  \hspace{1cm} (45)

**B.**

The integration of the hypo-elastic relation (12) is conducted in a rotated configuration, where only the material time derivative has to be performed. The stress and the elastic part of the rate of deformation tensor in the rotated configuration are denoted as

$$\dot{\tilde{\sigma}} = Q^T \cdot \sigma \cdot Q, \quad \dot{\tilde{D}}_{el} = Q^T \cdot D_{el} \cdot Q.$$ \hspace{1cm} (46)

The orthogonal tensor $Q$ is given by the evolution equation

$$\dot{Q} = \Omega \cdot Q, \quad Q(t = 0) = \delta.$$ \hspace{1cm} (47)

The skew-symmetric tensor $\Omega$ is chosen as $\Omega = W$. The numerical integration of Eqs. (47) and (48) to obtain $Q^{n+1}$ is performed by the algorithm proposed by Hughes and Winget [35].

The hypo-elastic relation can be rewritten in the rotated configuration as

$$\dot{\tilde{\sigma}} = C : \tilde{D}_{el}.$$ \hspace{1cm} (49)

The time derivative of the rotated stress Eq. (46) yields after some manipulations

$$\dot{\tilde{\sigma}} = Q^T \cdot (\sigma)\circ \cdot Q.$$ \hspace{1cm} (50)

Therewith, one recognizes that rotation of the hypo-elastic relation (12) using $Q$ leads to the setting (49).

The needed kinematic quantities are approximated starting from the deformation gradient as known quantity: The velocity gradient is approximated at $n + \alpha$ ($0 \leq \alpha \leq 1$) as

$$L^{n+\alpha} = \frac{(F^{n+1} - F^n)}{\Delta t} \cdot \left((1 - \alpha) \left(F^n\right)^{-1} + \alpha \left(F^{n+1}\right)^{-1}\right).$$ \hspace{1cm} (51)

The approximation of the rate of deformation tensor $D$ and the spin tensor $W$ follow as

$$D^{n+\alpha} = \frac{1}{2} \left(L^{n+\alpha} + (L^{n+\alpha})^T\right), \quad W^{n+\alpha} = \frac{1}{2} \left(L^{n+\alpha} - (L^{n+\alpha})^T\right).$$ \hspace{1cm} (52)

The stress-strain relation in the rotated configuration given by Eq. (49) can be numerically integrated (here Euler-backward method). After some manipulations the stress in the spatial configuration can be found:

$$\sigma^{n+1} = \Delta Q \cdot \sigma^n \cdot \Delta Q^T \cdot \sigma^{n+1} + C : (\Delta E - \Delta E_{pl})$$ \hspace{1cm} (53)

The old stress $\sigma^n$ is incrementally rotated by $\Delta Q$, which is defined as

$$\Delta Q = Q^{n+1} \cdot (Q^n)^T.$$ \hspace{1cm} (54)
In Eq. (53), the incremental strain tensor $\Delta E$ and the incremental plastic strain $\Delta E_{pl}$ are defined as

$$\Delta E = D^{n+\alpha} \Delta t, \quad \alpha = \frac{1}{2}$$

$$\Delta E_{pl} = D_{pl} \Delta t,$$

following the conventions of ABAQUS with $\Delta t$ as time increment.

Vector-matrix notation is used for the numerical solution. Symmetric second-order tensors $A$ are represented by appropriate column vectors $\mathbf{A}$; fourth-order tensors with certain symmetry properties $A$ are represented by square-matrices $A$; e.g., elastic stiffness tensor. All operations on tensors are rewritten as matrix multiplication designated by a center-dot ($\cdot$). The identity matrix is denoted by $\mathbf{I}$; the second-order unity tensor $\mathbf{\delta}$ is cast into a column vector; e.g., for the 3D-case as

$$\mathbf{\delta} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}^T.$$  

(57)

The transpose of a matrix is highlighted by the superscript "T".

The equivalent stress $\sigma_{eq}^{tr}$ is given by

$$\sigma_{eq}^{tr} = \sqrt{\frac{3}{2}} (S^{tr})^T \cdot \mathbf{P} \cdot S^{tr}$$

with the deviator of the trial-stress

$$S^{tr} = \left( \mathbf{I} - \mathbf{\delta} \cdot \frac{1}{3} \mathbf{\delta}^T \right) \cdot \sigma^{tr}.$$  

(59)

An appropriate diagonal scaling matrix $\mathbf{P}$ is inserted in Eq. (58) to reproduce the tensor operation introduced in Eq. (43). The scaling matrix $\mathbf{P}$ yields in the 3D-case

$$\mathbf{P} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}.$$  

(60)

The non-linear equation $f(\Delta \Lambda) = 0$ is solved as follows: The residual Eq. (30) can be approximated by a Taylor-expansion:

$$f(\Delta \Lambda + \Delta \Lambda) \approx f(\Delta \Lambda) + \frac{\partial f}{\partial \Delta \Lambda} \Delta \Lambda.$$  

(61)

The total differential of $f$ with respect to $\Delta \Lambda$ provides

$$df = \frac{\partial f}{\partial \Delta \Lambda} d \Delta \Lambda = \left( -3\mu - (1 - D) \frac{\partial R}{\partial \Delta \Lambda} \right) d \Delta \Lambda.$$  

(62)

According to the Newton-Raphson-algorithm, the Taylor-expansion of $f$ is used to find a root $f = 0$ iteratively. In every iteration $k \rightarrow k + 1$ the update algorithm

$$\Delta \Delta \Lambda = - \frac{f^k}{\frac{\partial f}{\partial \Delta \Lambda}|_k},$$

$$\Delta \Lambda^{k+1} = \Delta \Lambda^k + \Delta \Delta \Lambda$$

(63)

(64)
runs until convergence (\(|f| < \epsilon \) and \(|\Delta \Delta \Lambda| < \epsilon\), where \(\epsilon \ll 1\)). The iterative update of \(\Delta \Lambda\) is denoted as \(\Delta \Delta \Lambda\).

After a solution has successfully been found, the stress and the source term are updated:

\[
\sigma = \sigma^{tr} - \frac{C}{\lambda} \Delta \Lambda N^{tr},
\]
\[
r = \begin{cases} 
-(\varepsilon_{d}^{\alpha} + \Delta \varepsilon_{d}), & \varepsilon_{eq} < \varepsilon_{i}(\sigma) \\
-(\varepsilon_{d}^{\alpha} + \Delta \varepsilon_{d}) + \left(\varepsilon_{eq}^{\alpha} + \Delta \Lambda - \varepsilon_{x}^{\alpha}\right), & \text{once } \varepsilon_{eq} \geq \varepsilon_{i}(\sigma).
\end{cases}
\]

The material tangent entries are deduced as follows: Firstly, the total differentials of Eqn. (65) and (66) are computed. The independent variables are now \(\sigma^{tr}, \Delta \varepsilon_{d}\) and \(\Delta \Lambda\):

\[
d\sigma = d\sigma^{tr} - \frac{C}{\lambda} \left(d\Delta \Lambda N^{tr} + \Delta \Lambda d N^{tr}\right),
\]
\[
dr = \begin{cases} 
-d\Delta \varepsilon_{d}, & \varepsilon_{eq} < \varepsilon_{i}(h) \\
-d\Delta \varepsilon_{d} + d \Delta \Lambda, & \text{once } \varepsilon_{eq} \geq \varepsilon_{i}(h).
\end{cases}
\]

The expression for \(d \Delta \Lambda\) can readily be found from the total differential of Eq. (30), \(d f = 0\). The result reads

\[
d \Delta \Lambda = \frac{\partial^{\alpha} \varepsilon_{d}^{\alpha} \Delta \Lambda}{3\mu + \frac{\partial R}{\partial \Delta \Lambda}(1 - D)} d \sigma^{tr} + \frac{\partial R}{\partial \Delta \Lambda}(1 - D) d \varepsilon_{x}.,
\]

The derivative of \(N^{tr}\) with respect to \(\sigma^{tr}\) yields:

\[
d N^{tr} = \Phi \cdot d \sigma^{tr}
\]

with

\[
\Phi = \frac{3}{2\sigma_{eq}^{\alpha}} \left(I - \frac{1}{3} \delta \cdot \delta^{T} - \frac{3}{2 (\sigma_{eq}^{\alpha})^{2}} S^{tr} \cdot (S^{tr})^{T} \cdot P\right).
\]

Finally, \(d \sigma^{tr}\) is needed, which is straightforward:

\[
d \sigma^{tr} = \frac{C}{\lambda} d \Delta \varepsilon_{x}.
\]

Within the material tangent entries Eq. (31), the proper definition of the determinant of the deformation gradient \(J = \det(F)\) is needed. Its rate formulation is known from basic continuum mechanics as \(J = J^{tr}(D)\). A numerical integration can be performed as

\[
J^{n+1} = J^{n} \exp\left(\text{tr} \left(\Delta t \mathcal{D}^{n+\alpha}\right)\right) = J^{n} \exp\left(\text{tr} \left(\Delta E\right)\right).
\]

Thereafter, a direct relation of \(J\) and \(\Delta E\) is established. The matrix-vector-notations of \(J^{n+1}\) and \(d J/\Delta E\) follow as \((n + 1)\) dropped

\[
J = J^{n} \exp\left(\Delta E^{T} \cdot \delta^{T}\right),
\]
\[
\frac{d J}{\Delta E} = J \delta^{T}.
\]

Combining Eqn. (67) – (74) and reordering enables to write down the desired material tangent entries for the elastic-plastic case, see Eqn. (31) – (34), as well as the stress tangent of the elastic case, see Eq. (29).