

Theory and numerics of gradient-extended damage coupled with plasticity

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Für meine Familie

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Summary

Numerical simulations for predicting damage and failure of materials and structures are of fundamental importance in many engineering disciplines, since they usually reduce the number of costly and time-consuming practical experiments and allow for deeper insights into processes that would otherwise not or only hardly be possible. The significance of such simulations depends to a large extent on the quality of the applied material models which are themselves constantly being further developed to take more and more phenomena and effects into account that occur in real materials. In this context, the coupled modeling of the complex material phenomena ‘damage’ and ‘plasticity’ can be mentioned as a challenging and practically relevant subject the scientific literature has been dealing with for quite some time already. There is still a pressing need for further research in this scientific field.

The present cumulative dissertation aims at making a valuable contribution in this regard. It essentially represents a compilation of several published works of the author (and his coauthors) related to the topic. The overall goal is the development and investigation of novel gradient-extended damage-plasticity material models, both for the geometrically linear and nonlinear regime, which are based on a so-called ‘two-surface’ approach. The latter means that damage and plasticity are modeled as truly distinct (but coupled) dissipative mechanisms by taking separate damage loading and plastic yield criteria as well as loading / unloading conditions into consideration, respectively. Nonlinear Armstrong-Frederick kinematic hardening, nonlinear Voce isotropic hardening and nonlinear damage hardening are also accounted for by the models that can quite flexibly be adapted to various situations in which the considered real material shows either a (quasi-)brittle-type, ductile-type or possibly a mixed-type damaging behavior. The gradient-extension of damage (based on a micromorphic approach) is used to avoid pathological mesh sensitivity issues in finite element simulations that otherwise typically occur when using conventional models involving material softening behavior.

After an introductory part with a literature overview and a more detailed clarification of the research-relevant questions, the thesis begins with two works that are concerned with a numerical comparison of two different and competing kind of formulations for large deformation plasticity: hypo- and hyperelastic-based plasticity formulations that rely upon an additive decomposition of the rate of deformation tensor or a multiplicative split of the deformation gradient. At this point, no damage is being considered, yet. The main purpose for the thesis is to clarify whether one of the two formulations should generally be preferred when it later comes to an extension of the geometrically linear gradient-enhanced damage-plasticity model to large deformations. Various simulations with single finite elements finally reveal

that the results, which are obtained using the respective modeling approaches, can indeed significantly differ from each other under extreme conditions and that an incautious use of hypoelastic-based plasticity formulations can even lead to physically implausible model behavior. However, in more application-oriented structural simulations these problems are nearly insignificant and the results show a good agreement which suggests that, in principal, both formulations are well-suited for the development of new material models involving large plastic deformations.

Afterwards, two works are presented that deal with the theory and numerics of two slightly different two-surface gradient-extended damage-plasticity models for the geometrically linear regime. Among other things, the following topics are discussed: the application of the micro-morphic approach to achieve the gradient-extension of the models, the derivation of the strong and weak form of the underlying boundary value problem, the thermodynamically consistent derivation of the evolution equations, the models' implementation into finite element codes, the algorithmic handling of the discretized equations at the integration point level and the computation of the consistent tangent operators which are necessary to retain a quadratic rate of convergence of the Newton scheme at the global finite element level. The results of numerous structural simulations demonstrate the good practical performance and mesh regularizing properties of the models in finite element simulations involving material softening.

In the last part of the thesis, the model formulation is extended for its application to geometrically nonlinear problems. For this, a hyperelastic-based plasticity framework is used which relies upon an additional multiplicative split of the plastic part of the deformation gradient in order to allow for the modeling of nonlinear Armstrong-Frederick kinematic hardening at large deformations and which utilizes exclusively symmetric internal variables. Besides the theory, also many numerically relevant topics are discussed, such as a suitable time integration scheme for the evolution equations that preserves both the plastic incompressibility and symmetry of the tensorial internal variables, or the implementation of the model formulation into finite element codes. Finally, the functionality of the geometrically nonlinear model is exemplified by a structural finite element simulation.

Zusammenfassung

Numerische Simulationen zur Vorhersage der Schädigung und des Versagens von Werkstoffen und Strukturen sind in vielen Ingenieurdisziplinen von grundlegender Bedeutung, da sie oftmals die Zahl kosten- und zeitintensiver Experimente reduzieren können und tiefgehendere Einblicke in Prozesse erlauben, die ansonsten nicht oder nur schwer möglich wären. Die Aussagekraft solcher Simulationen hängt dabei wesentlich von der Güte der verwendeten Materialmodelle ab, die selbst ständig weiterentwickelt werden, um immer mehr Phänomenen und Effekten, die in realen Werkstoffen auftreten, Rechnung zu tragen. In diesem Zusammenhang sei beispielsweise die gekoppelte Modellierung der komplexen Materialphänomene „Schädigung“ und „Plastizität“ als ein anspruchsvolles und praxisrelevantes Thema genannt, mit dem sich die wissenschaftliche Literatur seit geraumer Zeit beschäftigt. Hier besteht auch weiterhin dringender Forschungsbedarf.

Die vorliegende kumulative Dissertation möchte dazu einen wertvollen Beitrag leisten. Sie repräsentiert im Wesentlichen eine Zusammenstellung mehrerer bereits veröffentlichter Arbeiten des Autors (und seiner Koautoren) zum Themengebiet. Das übergeordnete Ziel ist die Entwicklung und Untersuchung neuartiger gradientenerweiterter Schädigungs-Plastizitätsmodelle, sowohl im Rahmen einer geometrisch linearen als auch nichtlinearen Theorie, die auf einem sogenannten „Zwei-Flächen“-Ansatz basieren. Hierbei werden Schädigung und Plastizität jeweils als eigenständige (aber gekoppelte) dissipative Mechanismen aufgefasst und mittels separater Schädigungs- und Fließflächen sowie Be- und Entlastungsbedingungen modelliert. Zudem werden nichtlineare kinematische Armstrong-Frederick Verfestigung, nichtlineare isotrope Voce Verfestigung und nichtlineare Schädigungsverfestigung durch die Modelle berücksichtigt, die sehr flexibel an verschiedene Gegebenheiten angepasst werden können, in denen der betrachtete reale Werkstoff entweder ein (quasi-)sprödes, duktiler oder möglicherweise gemischtes Schädigungsverhalten aufweist. Die Gradientenerweiterung der Schädigung (basierend auf einem mikromorphen Ansatz) wird dazu genutzt, pathologische Netzabhängigkeitsprobleme in Finite-Elemente-Simulationen zu vermeiden, die sonst üblicherweise beim Einsatz von konventionellen Modellen mit Materialerweichungsverhalten auftreten.

Nach einem Einleitungsteil mit einem Literaturüberblick und einer detaillierteren Klärung der forschungsrelevanten Fragen, beginnt die Dissertation mit zwei Arbeiten, die sich beide mit einem numerischen Vergleich zweier unterschiedlicher, konkurrierender Formulierungen für Plastizität bei großen Verformungen befassen: hypo- und hyperelastische Plastizitätsformulierungen, die auf einer additiven Zerlegung des Deformationsgeschwindigkeitstensors bzw. einer multiplikativen Zerlegung des Deformationsgradienten basieren. Hierbei wird zu-

nächst noch keine Schädigung betrachtet. Der Hauptzweck für die Dissertation besteht darin, zu klären, ob eine der beiden Formulierungen grundsätzlich bevorzugt werden sollte, wenn das geometrisch lineare gradientenerweiterte Schädigungs-Plastizitätsmodell zu einem späteren Zeitpunkt auf große Deformationen erweitert wird. Verschiedene Simulationen mit einzelnen finiten Elementen zeigen schließlich, dass sich die Ergebnisse, die mit beiden Modellierungsansätzen erzielt werden, im Extremfall deutlich voneinander unterscheiden können und dass ein unsachgemäßer Einsatz hypoelastischer Plastizitätsformulierungen sogar nicht-physikalisches Modellverhalten hervorrufen kann. In anwendungsorientierteren Strukturrechnungen sind diese Probleme jedoch nahezu unbedeutend und die Ergebnisse zeigen eine gute Übereinstimmung, was darauf hindeutet, dass prinzipiell beide Formulierungen für die Entwicklung neuer Materialmodelle zur Beschreibung großer plastischer Verformungen geeignet sind.

Anschließend werden zwei Arbeiten präsentiert, die sich mit der Theorie und Numerik zweier leicht unterschiedlicher gradientenerweiterter Schädigungs-Plastizitätsmodelle für den geometrisch linearen Fall befassen und welche beide auf dem oben genannten Zwei-Flächen-Ansatz basieren. Unter anderem werden folgende Themen besprochen: die Anwendung des mikromorphen Ansatzes zur Realisierung der Gradientenerweiterung der Modelle, die Ableitung der starken und schwachen Form des zugrundeliegenden Randwertproblems, die thermodynamisch konsistente Herleitung der Evolutionsgleichungen, die Implementierung der Modelle in Finite-Elemente-Codes, die algorithmische Behandlung der diskretisierten Gleichungen auf Integrationspunktebene sowie die Berechnung der konsistenten Tangentenoperatoren zur Gewährleistung der quadratischen Konvergenz des Newton-Verfahrens auf globaler Finite-Elemente-Ebene. Die Ergebnisse zahlreicher Strukturrechnungen belegen schließlich die gute Praxistauglichkeit und netzregularisierenden Eigenschaften der Modelle in Finite-Elemente-Simulationen, in denen Materialerweichungsverhalten auftritt.

Im letzten Teil der Dissertation wird die Modellformulierung erweitert, um sie auf geometrisch nichtlineare Problemstellungen anwendbar zu machen. Hierzu wird ein hyperelastisches Plastizitätsmodell als „Gerüst“ verwendet, das eine zusätzliche multiplikative Zerlegung des plastischen Anteils des Deformationsgradienten zur Abbildung nichtlinearer kinematischer Armstrong-Frederick Verfestigung bei großen Verformungen nutzt und das von ausschließlich symmetrischen inneren Variablen Gebrauch macht. Neben der Theorie werden auch viele numerisch relevante Themen besprochen, wie z. B. ein geeignetes Zeitintegrationsschema für die Evolutionsgleichungen, das sowohl die plastische Inkompressibilität als auch die Symmetrie der tensoriellen inneren Variablen bewahrt, oder auch die Implementierung der Modellformulierung in Finite-Elemente-Codes. Schließlich wird die Funktionalität des geometrisch nichtlinearen Modells anhand einer Finite-Elemente-Strukturrechnung beispielhaft illustriert.

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1 | Introduction

1.1 Motivation and research-relevant questions

Nowadays, simulation tools based on the finite element method play an essential role during the planning, implementation and execution phases of many industrial processes. This is particularly true for those areas of application in which the creation of prototypes and conduction of numerous experiments are considered either too costly or time-consuming. With today's computing power at hand, large-scale simulations under ever-more realistic conditions can be carried out such that the number of experiments can be reduced to a necessary minimum. As one example of an industrial sector to which all of the above mentioned statements apply, forming technology can be mentioned.

From a material modeling point of view, forming is especially interesting since the employed workpieces, for instance sheet metals, usually undergo large strains and rotations during the processing and care needs to be taken in order to prevent damaging of the desired end-product. The latter fact emphasizes a true need for advanced material models in the simulations which are able to properly capture complex inelastic phenomena, as, e. g., (possibly coupled) plasticity and damage in a geometrically nonlinear framework, a topic which is far from being trivial even for the geometrically linear case and subject to intensive research in both the academic and industrial community.

Concerning plasticity, several formulations for the geometrically nonlinear case are known in the literature, none of which is universally recognized as the 'best' by all parts of the mechanics community alike. The two most popular types in this field are probably hypoelastic- and hyperelastic-based plasticity formulations which both inherently differ in the description of plastic flow, the definition of the elastic properties as well as the utilized stress and strain measures, respectively. The former type can be considered a natural extension of the classical infinitesimal formulation and is characterized by the fundamental kinematic hypothesis that the symmetric part of the velocity gradient, also referred to as the 'rate of deformation' tensor, can be additively split into purely elastic and plastic parts as well as by the assumption of a hypoelastic constitutive equation for an (in principle arbitrary) objective stress rate.

On the contrary, the latter type assumes a multiplicative split of the deformation gradient into elastic and plastic parts as well as a hyperelastic constitutive equation for the stress itself (as opposed to its rate). Historically, hypoelastic-based plasticity models are older than their hyperelastic-based counterparts and are rejected by some of today's experts within the mechanics community, due to several problems that were encountered in the past. However, on the one hand, new developments in more recent years considerably improved the situation and, on the other hand, hypoelastic-based plasticity models are still widely used in commercial finite element programs nowadays, sometimes they even constitute the exclusive option for the end-user. Thus, before the one or the other modeling approach is chosen for the development of a new elastoplastic material model, it seems worthwhile to study and directly compare their respective performances in application-oriented structural examples with each other.

Concerning damage, it can be stated that, due to the variety of physical mechanisms causing damage in real materials and due to the differing views on to which detail damaging effects need to be captured by a particular material model, a vast amount of damage formulations was developed in the literature. Approaches based on the concept of continuum damage mechanics, for instance, make use of (possibly multiple) scalar- or tensor-valued internal variables and corresponding phenomenological evolution equations that account for the effects of damage in an averaged sense only. These variables usually degrade the stiffness, strength and / or other properties of the material such that 'softening' behavior occurs, meaning that the material response is weakened. In the idealized case in which the defects in the material are assumed to occur in a purely isotropic manner during the deformation, a single scalar variable is usually sufficient for the modeling. However, the particular way how the influence of this variable is finally incorporated into the constitutive formulation still strongly depends on the context and the damage behavior of the considered material, whether it is, e. g., brittle-like or ductile-like. It would be desirable to have a damage formulation at hand which can flexibly be adapted to different modeling conditions by adjusting the material parameters accordingly.

A general problem of conventional 'local' material models showing softening behavior is the fact that their application in finite element simulations can lead to highly mesh-dependent results, both with respect to the used element sizes and element types but also with respect to the 'structure' of the mesh, i. e., the particular shape and orientation of individual elements. Unexpected artifacts can be the consequence in damage simulations, such as a physically implausible shrinking of the damage process zone accompanied by an ever-decreasing energy dissipation, or a change in the propagation direction of damage, merely upon mesh refinement. It seems clear that such issues can easily render finite element results useless for subsequent meaningful analyses. Even worse, these problems cannot be simply cured by using a different

numerical method since their origin lies inherently in the material formulation itself which is in some sense too simplistic.

Different solution strategies were proposed in the past in order to overcome the above mentioned shortcomings of the classical ‘local’ damage formulations. From a conceptual point of view, one of the most promising approaches is to rely on ‘nonlocal’ integral-type or gradient-extended damage material models which implicitly introduce internal material length scales into the formulation that act as ‘localization limiters’, essentially preventing damage process zones from shrinking below a tolerable lower bound and curing the spurious mesh orientation issue. Especially gradient-extended models are popular since they are comparatively easy to implement into existing ‘standard’ finite element codes. Many of these models assume the existence of an additional partial differential equation, next to the classical balance of linear momentum, which needs to be solved for a newly introduced ‘nonlocal’ global variable that is treated analogously to the displacements. Through the differential equation and constitutive interdependencies within the model, a complex interplay between this variable and the evolution of damage at ‘local’ material points is introduced into the formulation, leading to a ‘nonlocal’ character of damage which is the key for curing the problem. Nevertheless, at least two open questions remain at this point: how to properly choose the particular partial differential equation and how to exactly incorporate the influence of the ‘nonlocal’ variable into the constitutive formulation? In the past, modeling decisions in this regard were often made on a ‘trial-and-error’ basis. It seems advantageous to tackle the problem more systematically by using a procedure which answers the mentioned questions in some way ‘automatically’.

The goal of this dissertation is the development and implementation of novel thermodynamically consistent gradient-extended damage-plasticity models with combined nonlinear kinematic and isotropic hardening. First of all, two geometrically linear models are established, one of which is later extended to the geometrically nonlinear regime on the basis of a specific hyperelastic-based plasticity formulation that was developed earlier by other members of the author’s workgroup. The models’ underlying formulation is based on a ‘two-surface’ approach in which damage and plasticity are treated as distinct (but coupled) dissipative mechanisms by using independent damage and plastic yield criteria as well as corresponding sets of loading / unloading conditions, respectively. The latter fact makes the models especially flexible in the sense that both plasticity and damage can be switched off, if desired, by choosing the material parameters accordingly. In this way, various situations can be accounted for in which the considered material’s behavior is either (quasi-)brittle-like, ductile-like or possibly anything in between. The models’ gradient-extension is derived on the basis of the micromorphic theory according to Forest [2009, 2016] which can, very practically speaking,

be considered a systematic and convenient approach for converting existing ‘local’ material models to corresponding ‘nonlocal’ variants. Only few basic assumptions are necessary, after which the influence of the gradient-extension on the constitutive equations becomes in each case self-explanatory and apparent. A main objective of the dissertation is also the practical confirmation of the models’ mesh regularizing properties in several finite element test simulations. For this, the models are firstly implemented as new user elements into the academic finite element program FEAP. Many important algorithmic aspects are discussed, as, for instance, the steps necessary to retain a quadratic rate of convergence in a Newton iteration at the global finite element level or the time discretization of the models’ evolution equations and other related topics, respectively.

1.2 State-of-the-art in the continuum mechanical modeling of combined damage and plasticity

Continuum mechanical models for the description of combined damage (or failure) and plasticity in materials can roughly be classified into ‘uncoupled’ and ‘coupled’ formulations. Uncoupled formulations make use of phenomenological / empirical failure criteria or damage variables which measure the degree of deterioration at a material point in a certain sense (e. g., by means of ‘strain-to-failure’ curves that depend on the stress state, strain rate, temperature and / or other quantities). If such a failure criterion is met or damage reaches a certain pre-defined limit during the computation, the material element is considered to fail which usually means that the corresponding finite element is eliminated from the mesh or the equivalent stress is set to zero at the integration point. The actual reason for the terminology ‘uncoupled’ stems from the fact that damage has no effect whatsoever on the constitutive response of the model. As such, uncoupled models are also not subject to the same mesh objectivity issues which are present for conventional ‘local’ damage models showing softening behavior.

One of the oldest criteria in this field is the one by Coulomb [1776] and Tresca [1864] which is still widely used in many civil engineering applications nowadays. It assumes that fracture occurs at a material point whenever the maximum shear stress reaches or exceeds a predefined value. In contrast to that, the classical Mohr-Coulomb criterion (see Mohr [1914] and the aforementioned reference) states that material fails due to a critical combination of both shear and normal stresses and not due to a maximum of one of the two alone. It was mainly utilized in the past in order to describe the failure behavior of brittle geomaterials since it accounts for the dependence of fracture on hydrostatic pressure and the Lode angle parameter which

is in turn related to the third deviatoric stress invariant (Lode [1925]). Bai and Wierzbicki [2010] extended the scope of application of the Mohr-Coulomb criterion later also to the failure behavior of ductile materials. Recently, presuming the condition of plane stress, Jia and Bai [2016] developed an ‘all-strain based’ variant that can predict the fracture strain in dependence of the strain ratio and strain state angle only, both of which can be measured directly via digital image correlation such that additional finite element based studies can be avoided. Another popular fracture model, originally developed for bulk forming operations by Cockcroft and Latham [1968] and later further modified by Oh et al. [1979], postulates that failure happens when a critical amount of plastic work has been done by the (normalized) maximum principal tensile stress along the path of the equivalent plastic strain. It is frequently available as built-in model in many of today’s commercial finite element codes and successfully used, e. g., for the simulation of the perforation of metal plates, of warm / hot cross-wedge rolling and sheet metal forming processes (see Børvik et al. [2009], Huang et al. [2017], Tarigopula et al. [2008], respectively). The same holds true for the famous fracture model by Johnson and Cook [1985] which considers a dependence of failure on the stress triaxiality (defined as the ratio between the mean stress and the von Mises equivalent stress), strain rate and temperature and which is used, for instance, in simulations of machining metal matrix composites (Ghandehariun et al. [2016]). Wilkins et al. [1980] suggested a ductile failure criterion which takes into account the influences of hydrostatic tension, of the maximum ratio between deviatoric principal stresses and of a characteristic length of the microstructure of the material. Later, this criterion was further enhanced and implemented into the commercial finite element code PAM-CRASH by Kamoulakos et al. [2003]. An exemplary area of application is the prediction of different failure modes in spotwelded metals (Nguyen et al. [2012]). Based on experimental and numerical insights, Bao and Wierzbicki [2004] concluded that the fracture strain should not be considered a monotonic but a piecewise function of the stress triaxiality and proposed a criterion with three distinct ‘branches’ and possible slope discontinuities in the respective transition regimes. Bai and Wierzbicki [2008], Wierzbicki and Xue [2005], Xue [2007] incorporated also the important effect of the Lode angle parameter into the expression. Recently, Buchkremer et al. [2016] proposed a further extension of the model and a novel non-iterative procedure for its calibration which were successfully applied in the 3D finite element simulation of chip breakage in metal cutting. Another failure model which is often used, e. g., in automotive industry is CrachFEM (Hooputra et al. [2003, 2004]). It is mainly employed to describe the fracture behavior of thin sheets and distinguishes between three different failure mechanisms: ductile normal fracture, ductile shear fracture and tensile instability. Above all, the prediction of sheet instabilities can be considered the special feature of the model. Since

CrachFEM is a commercial software distributed by the company MATFEM in Munich, Germany, its exact mode of operation remains to some extent unclear. It is, however, known that it can be understood as a further development of the well-known model by Marciniak and Kuczyński [1967] which is used for the calculation of the forming limits of sheet metals due to localized necking under proportional loadings. CrachFEM is said to be able to predict the forming limit curve also for non-proportional loading paths (see, e. g., Dell et al. [2001, 2007], Heath et al. [2013]).

In general, the predictive capabilities of uncoupled models are considered limited, especially in cases in which pronounced fractured or damaged zones occur in the material, such that the influence of damage on the material behavior itself should not be neglected anymore. For this reason, coupled formulations were developed. The latter are often further categorized into two main groups which will be described in what follows.

Models belonging to the first group are micromechanically motivated and make use of (one or maybe more) internal variables that represent the volume fraction of voids within the material. These variables and corresponding evolution equations account for the main microscopic mechanisms responsible for ductile damage which are the nucleation, growth and coalescence of microvoids during plastic deformation. Usually, these variables are incorporated into the yield function(s) of the formulation and a stress decrease is induced whenever the volume fraction of voids increases in the material. For brevity, the related literature review here solely concentrates on the class of Gurson-type plasticity models for porous materials (for a more comprehensive treatment, see, e. g., Besson [2010]).

McClintock [1968] and Rice and Tracey [1969] studied and modeled the evolution of microvoids within in an elastoplastic matrix and observed that the void growth is mainly governed by the stress triaxiality. Inspired by these observations, Gurson [1977] carried out approximate limit analyses of a single cylindrical and spherical pore embedded in a perfectly plastic von Mises cylinder and sphere, respectively, and developed a constitutive model for ductile porous materials in which the void volume fraction is used as an internal damage variable that affects the yield function and leads to material softening. Tvergaard [1981, 1982*b*] introduced adjustable parameters into Gurson's original yield function in order to improve the model's flexibility and accuracy. Tvergaard [1982*a*] proposed to include an additional term in the evolution law of the damage variable which describes the average macroscopic effect of final material failure by void coalescence and which becomes only active when a critical value of the void volume fraction is exceeded. The particular choice for this term suggested by Tvergaard and Needleman [1984] is probably the most popular one and the corresponding model is commonly referred to as the Gurson–Tvergaard–Needleman (GTN) model in the literature.

Since then, the model was continuously developed further in many respects. For instance, void shape effects were accounted for in the model by Gologanu et al. [1993, 1994, 1997], Madou and Leblond [2012*a,b*], void size effects by Wen et al. [2005] and void shear effects by Xue [2008], among others. Kinematic hardening was incorporated and studied by, e. g., Arndt et al. [1997], Besson and Guillemer-Neel [2003], Klingbeil et al. [2016], Leblond et al. [1995], Mear and Hutchinson [1985], Mühlich and Brocks [2003] and Ristinmaa [1997]. Other interesting aspects which were implemented and investigated are plastic anisotropy (Benzerga and Besson [2001], Keralavarma and Benzerga [2008, 2010], Monchiet et al. [2006, 2008], Morin et al. [2015]), strain rate sensitivity (Needleman and Tvergaard [1984], Pan et al. [1983]) and the effects of inclusions upon void growth (Siruguet and Leblond [2004]). Nonlocal integral-type extensions of the GTN model were proposed by Leblond et al. [1994] who studied bifurcation phenomena in porous ductile materials and by Sun and Hönl [1994] who simulated damage development in shear bands, necking regions and at crack tips. Later, Enakoutsa et al. [2007] focused on the numerical implementation of the former model and compared the results with experiments. Tvergaard and Needleman [1995] developed a rate-dependent nonlocal integral-type variant of the GTN model and investigated the influence of the material length scale in the computations. A purely mechanically motivated nonlocal gradient-type extension of the GTN model was proposed by Ramaswamy and Aravas [1998] who incorporated a spatial gradient of porosity into the formulation which resulted in a new diffusion-like evolution equation of the void volume fraction. In contrast to that, Reusch et al. [2003*a,b*] followed a thermodynamic approach suggested by Svendsen [1999] in which a new field quantity (and its gradient) was introduced into the formulation that can be considered a continuum microstructural field or generalized phase field. The conceptual benefit of this approach is that the evolution of the void volume fraction, and therefore also its physical interpretation, remain unchanged compared to the original GTN model. Later, Reusch et al. [2008] used this model to simulate ductile crack initiation and propagation in metal matrix composites. Nonlocal gradient-extended GTN models based on the implicit gradient approach according to Peerlings et al. [1996] were developed and utilized by, e. g., Linse et al. [2012] and Hütter et al. [2013, 2014]. Recently, Aldakheel et al. [2017] and Miehe, Kienle, Aldakheel and Teichtmeister [2016] coupled a modified Gurson-type plasticity model with the phase field approach of fracture in a geometrically nonlinear framework.

The second group of models is based on the continuum damage mechanics (CDM) concept. Here, scalar- or tensor-valued internal variables are introduced into a standard continuum mechanics framework that account for the complex dissipative effects of damage in an averaged sense only by causing material softening in a certain way. In contrast to the micromechani-

cally motivated models described in the above, damage and its evolution are usually described in a purely phenomenological manner. The constitutive equations of the model are then derived on the basis of rigorous thermodynamic considerations, the concept of ‘effective stress’ and / or other ‘effective variables’ as well as a hypothesis of equivalence between the damaged and a fictitious undamaged state of the material. The specific physical meaning of the damage variable(s) clearly depends on the particular context.

The origin of CDM is usually attributed to Kachanov [1958] who utilized a scalar internal variable to characterize the gradual deterioration of metals in the case of creep and who introduced already the notion of ‘effective stress’ (in this context as the ratio between the maximum tensile stress at a considered material point and a scalar function measuring the degree of damage). Later, Rabotnov [1963, 1969] had the idea to identify the reduction of the cross section area due to microcracking in the material with an increase of the internal damage variable, thus equipping the latter with a clearer physical interpretation. The ideas laid down by the latter authors were then the starting point for intensive developments in the scientific field of CDM and various problems were investigated. For instance, Lemaitre [1971] dealt with low cycle fatigue damage in metals, Leckie and Hayhurst [1974] and Hult [1974] were concerned with the coupling between damage and (cyclic) creep, respectively, Chaboche [1974] worked on high cycle fatigue damage, whereas Lemaitre and Chaboche [1975] created a model for creep-fatigue damage interaction, to name only a few related publications during this time. In the following years, more and more effort was spent to embed CDM consistently in the general framework of thermodynamics of irreversible processes and to establish it as a sound and general theory on its own (for a pioneering reference in this context, see, e. g., Chaboche [1978]). Among other things, this enabled also the development of a large number of different models to describe anisotropic damage. For instance, Chaboche [1981, 1984] developed a model for creep damage in which the damage variable is assumed to be an unsymmetric fourth-order tensor in the most general anisotropic case. In contrast to that, Betten [1986], Chow and Lu [1989*b,a*], Cordebois and Sidoroff [1982], Murakami [1988] and Murakami and Ohno [1981], among others, proposed formulations for anisotropic damage based on a symmetric second-order damage tensor. Even formulations with first- and eighth-order damage tensors were developed (see, e. g., Krajcinovic and Fonseka [1981] and Chaboche [1978, 1982], respectively). A model for the prediction of isotropic ductile damage in metals which gained widespread popularity in the CDM community is the one proposed by Lemaitre [1984, 1985*a,b*]. As a consequence of the effective stress concept and the hypothesis of strain equivalence, damage is defined as a reduction of the elastic stiffness properties which can generally more easily be measured in experiments than the reduction of load-carrying area due to mi-

crocracking. The evolution equation of damage is derived from a dissipation potential and is strongly influenced by the stress triaxiality ratio. The model is based on a ‘single-surface’ formulation in which damage is not truly regarded as an own ‘mechanism’ but can only develop further if plasticity evolves as well (i. e., formally, a yield criterion and loading / unloading conditions for plasticity are present in the model but no corresponding counterparts for damage). Later, the original Lemaitre model was modified and extended to account for, e. g., ageing effects (Marquis and Lemaitre [1988]), damage anisotropy (Lemaitre et al. [2000]), crack closure effects (Andrade Pires et al. [2003], Bouchard et al. [2011], Desmorat and Cantournet [2008]) and large deformations (de Souza Neto et al. [1998]). More recently, also the Lode angle effect was incorporated into the formulation (Lian et al. [2014]). Other coupled elastoplastic damage models based on a ‘two-surface’ approach with separate yield and damage criteria as well as loading / unloading conditions, respectively, were developed by Hansen and Schreyer [1994], Ju [1989], Simo and Ju [1987] for a geometrically linear setting and by Voyiadjis and Kattan [1992], Zhu and Cescotto [1995] for a geometrically nonlinear setting. Menzel et al. [2005] developed a large deformation anisotropic continuum damage model coupled to elastoplasticity with kinematic hardening which is based on a single-surface formulation. Nonlocal integral-type formulations of a simplified Lemaitre-type damage model (neglecting kinematic hardening) were presented by Andrade et al. [2009] for the geometrically linear case and by Andrade et al. [2011] for the geometrically nonlinear case (based on a multiplicative split of the deformation gradient). In contrast to that, Brepols et al. [2015b,a] suggested a nonlocal implicit-gradient Lemaitre-type damage model with nonlinear kinematic hardening and César de Sá et al. [2006] an implicit-gradient variant of the Lemaitre model which accounts also for crack closure effects. Other gradient-enhanced CDM models coupled with elastoplasticity were presented by, e. g., de Borst et al. [1999] and Nedjar [2001]. Saanouni and Hamed [2013] proposed a gradient-enhanced damage-plasticity model for large deformations and investigated its practical behavior in several 2D finite element simulations. In their single-surface formulation, damage is modeled by means of a Lemaitre-type ansatz and the gradient-extension is derived on the basis of the micromorphic approach according to Forest [2009, 2016]. Brepols et al. [2017, 2018] developed two slightly different regularized micromorphic damage-plasticity models which are based on a two-surface approach and which allow for both nonlinear plastic and damage hardening, respectively. In their papers, the latter authors discussed several related theoretical and numerical aspects, as, for instance, a significant simplification of the otherwise non-trivial algorithmic treatment of the model at the integration point level based on the Fischer-Burmeister complementarity function (for more details, see Chaps. 4 and 5 in the present thesis). A conceptually quite similar model

and approach were utilized by Kiefer et al. [2018]. Micromorphic gradient-extended damage models coupled to crystal plasticity for small and large deformations were suggested and investigated by Aslan, Cordero, Gaubert and Forest [2011], Aslan and Forest [2009] and Aslan, Quilici and Forest [2011]. Other nonlocal implicit-gradient CDM models which are coupled to elastoplasticity and in which damage reduces the yield stress (as opposed to the elastic stiffness properties in the Lemaitre model, for example) were proposed by Engelen et al. [2002] for the geometrically linear case and by Geers [2004], Geers et al. [2001, 2003] for the geometrically nonlinear case, respectively. Recently, formulations were developed which couple gradient damage with gradient plasticity (see, e. g., Dimitrijevic and Hackl [2011] and the works by Miehe, Aldakheel and Raina [2016], Miehe, Teichtmeister and Aldakheel [2016] who utilized the phase field approach).

1.3 Outline of the dissertation

The present cumulative dissertation is organized as follows. Chapters 2 and 3 represent two of the author's (and his coauthors') published works which are concerned with a numerical comparison of hypoelastic- and hyperelastic-based approaches for large deformation elastoplasticity with combined nonlinear kinematic and isotropic hardening. Goal of the studies is to provide new insights into whether one of the two approaches should generally be preferred to the other in numerical simulations or not (this question is relevant for the extension of the gradient-enhanced damage-plasticity formulation developed in Chaps. 4 and 5 to the geometrically nonlinear regime which will be discussed in Chap. 6). The hypoelastic-based framework considered in Chaps. 2 and 3 is the same. An equal objective rate for the stress and the back stress tensor is assumed in the corresponding constitutive equations (either the Jaumann, Green-Naghdi or logarithmic rate, respectively). In contrast to that, the hyperelastic-based models in the two chapters differ from each other. While the one in Chap. 2 makes use of a Hencky-type elastic energy in terms of a logarithmic elastic strain measure and an objective rate equation for the back stress (in order to model nonlinear Armstrong-Frederick kinematic hardening), the model in Chap. 3 is based on a Neo-Hookean elastic energy and a more sophisticated approach for nonlinear kinematic hardening in which an additional multiplicative split of the plastic part of the deformation gradient is assumed. The hypoelastic- and hyperelastic-based models are directly compared to each other in several one element tests but also in quite complex finite element simulations of industrially-relevant forming processes. It is shown that, although pronounced differences appear in the individual one element tests, the particular modeling approach for large deformation elastoplasticity plays, in more application-

oriented examples at the structural level, a less significant role than originally expected.

Chapters 4 and 5 represent two other of the author's (and his coauthors') published works which are concerned with the theoretical development and numerical implementation of two gradient-extended damage-plasticity material models in a CDM framework. The focus lies in both cases on a 'two-surface' approach in which damage and plasticity are modeled as, in principle, independent dissipative mechanisms and the micromorphic theory is used to derive the gradient-extension of the model. At this point, a geometrically linear theory is assumed to study the models' behavior in the simplest context possible. The particular models discussed in the two chapters are conceptually very similar to each other but differ in some details. More precisely, in Chap. 4, the underlying damage formalism is based on the hypothesis of total energy equivalence and two dissipation potentials for damage and plasticity are introduced from which thermodynamically consistent evolution equations of the strain-like internal variables are derived, respectively. On the contrary, the model discussed in Chap. 5 is formally based on the hypothesis of strain equivalence and no additional dissipation potentials are introduced which leads to different constitutive equations than in the other case. Especially in Chap. 4, many algorithmic and numerical aspects are highlighted, as, e. g., the implementation of the gradient-extended damage-plasticity model into finite element codes, the algorithmic treatment of the discretized equations at the integration point level (which requires special considerations due to the presence of two independent sets of loading / unloading conditions), and the derivation of the consistent tangent operators that are necessary to retain a quadratic rate of convergence in a Newton scheme at the global finite element level. Furthermore, in Chap. 5, a general procedure is presented to enforce stress constraints for (general) 3D gradient-extended material models at the integration point level. The latter makes it possible, for instance, to integrate such models consistently into beam or shell elements or to carry out 2D plane stress computations. Both chapters conclude with a detailed discussion of several numerical examples which are used to illustrate the influence of the damage material parameters in the formulation and to practically prove the models' mesh regularizing properties in finite element simulations.

Finally, Chap. 6 deals with the extension of the gradient-enhanced damage-plasticity model presented in Chap. 5 to the large deformation regime. The basis for that is a well-established and thermodynamically motivated hyperelastic-based plasticity formulation which was developed earlier by other members of the author's workgroup. It makes use of an additional physically motivated multiplicative decomposition of the plastic part of the deformation gradient in order to model nonlinear Armstrong-Frederick kinematic hardening. The model's derivation is presented in great detail. For instance, it is shown how the two-surface strategy for

damage-plasticity and the micromorphic approach for the model's gradient-extension can be adopted also in a geometrically nonlinear framework. Furthermore, many numerical aspects are discussed, as, e. g., the time integration of the evolution equations by means of an exponential map algorithm that preserves both the plastic incompressibility and the symmetry of the tensorial internal variables, as well as the model's implementation into finite element codes. At the end, the functionality of the model is illustrated in a numerical benchmark example in which large plastic deformations and damage play a significant role.

2 | **Article 1:**

Comparison of hyper- and hypoelastic-based formulations of elastoplasticity with applications to metal forming

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Disclosure of the individual authors’ contributions to the article:

T. Brepols reviewed the relevant existing literature, implemented all material models considered in this study into ABAQUS / Standard (via the UMAT interface), performed all simulations, interpreted the results and wrote the article. I. N. Vladimirov provided an ABAQUS input file for the cylindrical cup drawing simulation of Sect. 2.5.2. Furthermore, he and S. Reese gave conceptual advice, contributed to the discussion of the results, read the article and gave valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

2.1 Abstract

The aim of this work is to examine two specific finite strain elastoplasticity models in terms of their applicability in metal forming processes, namely a hyperelastic-based model which relies upon a multiplicative decomposition of the deformation gradient into elastic and plastic parts and a hypoelastic-based model which makes use of an additive elastic-plastic split of the rate of deformation tensor. Both models allow for nonlinear isotropic and kinematic hardening and were implemented as user material subroutines (UMAT) into ABAQUS / Standard. Various sample calculations were performed to assess the respective properties and capabilities of the models. The FE simulation of a deep drawing process produced nearly congruent results for both models which suggests that they are equally well-suited for modeling metallic materials in metal forming processes.

2.2 Introduction

A number of alternative formulations exist for the extension of the infinitesimal elastoplasticity theory to the finite strain regime, all of which are identical in the ‘small strain limit’ but which differ substantially in the kinematic description of plastic flow, the description of the elastic behavior as well as the choice of the stress and strain measures. In the past, there have been intensive debates in the scientific community as to whether there is a specific formulation which should be preferred over the others to model elastoplastic materials or not (see, e. g., Casey and Naghdi [1981]). Although each formulation has its own advantages and disadvantages, the hyperelastic-based approach relying upon a multiplicative decomposition of the deformation gradient into elastic and plastic parts has gained widespread acceptance over the last two decades and can be considered as ‘state-of-the-art’ (de Souza Neto et al. [2008]). However, even nowadays many commercial finite element codes exploit a hypoelastic-based approach which relies upon an additive elastic-plastic split of the rate of deformation tensor when it comes to the modeling of finite strain elastoplasticity, especially if small elastic strains are assumed (see, e. g., N. N. [2010]). Available literature seems to be mainly concerned with the theoretical aspects and differences of both approaches (Xiao et al. [2006]), thus it is still worthwhile and interesting to examine their respective practical capabilities in more application-oriented examples. For that reason, the present work discusses and compares two specific hyper- and hypoelastic-based plasticity models with nonlinear isotropic and kinematic hardening which are comparatively easy to implement. Both models are implemented as user material subroutines (UMAT) into ABAQUS / Standard and are first tested on the Gauss-point

level to investigate their general behavior and basic properties. Afterwards, the models are also deployed in a structural deep drawing simulation to estimate their suitability in the case of metal forming processes.

2.3 Hypoelastic-based constitutive model

2.3.1 Objective stress rates

Constitutive laws should be formulated in accordance with the principle of material frame-indifference. Therefore, Eulerian rate type hypoelastic-plastic laws are formulated in terms of objective rates of Eulerian stress measures, as, e. g., of the Kirchhoff stress $\boldsymbol{\tau}$. More generally, for an arbitrary Eulerian second-order tensor $\mathbf{t}$, the special class of co-rotational rates can be defined by

$$\overset{\circ}{\mathbf{t}}^* := \dot{\mathbf{t}} - \boldsymbol{\Omega}^* \mathbf{t} + \mathbf{t} \boldsymbol{\Omega}^*. \quad (2.1)$$

In the latter definition, $\dot{\mathbf{t}}$ denotes the material time derivative of $\mathbf{t}$ and $\boldsymbol{\Omega}^*$ is some second-order skew-symmetric (spin) tensor which characterizes the specific kind of objective rate. Two classical examples of co-rotational rates are the well-known Jaumann (J) and Green-Naghdi (GN) rates which are defined, respectively, by the spin tensors

$$\boldsymbol{\Omega}^J = \mathbf{w} \quad (2.2)$$

$$\boldsymbol{\Omega}^{\text{GN}} = \dot{\mathbf{R}} \mathbf{R}, \quad (2.3)$$

where $\mathbf{w} = \frac{1}{2} (\mathbf{I} - \mathbf{I}^T)$ is the skew-symmetric part of the spatial velocity gradient $\mathbf{I} = \nabla_x \mathbf{v}$ and $\mathbf{R}$ is the rotation tensor in the polar decomposition of the deformation gradient $\mathbf{F} = \mathbf{v} \mathbf{R} = \mathbf{R} \mathbf{U}$. More recently, in the context of the self-consistent Eulerian theory developed mainly by the workgroup of Bruhns, Xiao and Meyers (see, e. g., Bruhns et al. [1999]), specific attention has been paid also to the co-rotational logarithmic (LOG) rate defined by

$$\boldsymbol{\Omega}^{\text{LOG}} = \mathbf{w} + \sum_{i \neq k}^m \left(\frac{1 + (b_i/b_k)}{1 - (b_i/b_k)} + \frac{2}{\ln(b_i/b_k)} \right) \mathbf{b}_i \mathbf{d} \mathbf{b}_k, \quad (2.4)$$

where b_i denotes the i th eigenvalue of $\mathbf{b} = \mathbf{F} \mathbf{F}^T$, $\mathbf{b}_i$ the i th eigenprojection of $\mathbf{b}$, m the number of distinct eigenvalues of $\mathbf{b}$ and $\mathbf{d} = \frac{1}{2} (\mathbf{I} + \mathbf{I}^T)$ is the symmetric part of the spatial velocity gradient, also termed rate of deformation tensor. A co-rotational rate $\overset{\circ}{\mathbf{t}}^*$ can be interpreted as the conventional material time derivative of the quantity $\mathbf{t}$ observed in an associated $\boldsymbol{\Omega}^*$ -

spinning frame (Bruhns [2009]).

2.3.2 Additive split of the rate of deformation tensor and stress-strain relationship

Hypoelastic-based formulations assume that the rate of deformation tensor $\mathbf{d}$ can additively be decomposed into elastic and plastic parts according to

$$\mathbf{d} = \mathbf{d}_e + \mathbf{d}_p, \quad (2.5)$$

where $\mathbf{d}_e$ and $\mathbf{d}_p$ are called the elastic and plastic rate of deformation tensor, respectively. It should be noted that these quantities are objective Eulerian tensors which may be used in formulating constitutive relationships (Simo and Hughes [1998]). Based on this, hypoelastic-plastic material models are typically defined by

$$\overset{\circ}{\boldsymbol{\tau}}^* = \mathcal{C}[\mathbf{d}_e] = \mathcal{C}[(\mathbf{d} - \mathbf{d}_p)], \quad (2.6)$$

in which $\overset{\circ}{\boldsymbol{\tau}}^*$ is some co-rotational rate of the Kirchhoff stress according to definition (2.1) and $\mathcal{C}$ denotes the standard constant fourth-order elasticity tensor of the infinitesimal theory

$$\mathcal{C} = \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \mathcal{I}. \quad (2.7)$$

In the latter relation, λ and μ denote the first Lamé parameter and the shear modulus, respectively, $\mathbf{I}$ is the second-order identity tensor and $\mathcal{I}$ is the fourth order symmetric identity tensor. The constitutive relationship (2.6) is reasonable for metal-like materials in which the elastic strains are orders of magnitudes smaller than their plastic counterparts.

2.3.3 Yield criterion, flow rule and hardening laws

A yield function Φ is introduced which defines the set of all admissible states

$$\bar{\mathbb{E}} := \{(\boldsymbol{\tau}, \boldsymbol{\chi}, \kappa) \mid \Phi(\boldsymbol{\tau}, \boldsymbol{\chi}, \kappa) \leq 0\}, \quad (2.8)$$

where the deviatoric second-order back stress tensor $\boldsymbol{\chi}$ and the scalar accumulated plastic strain κ are connected to kinematic and isotropic hardening of the material, respectively. The principle of frame indifference demands the yield function Φ to be an isotropic function of the stress (Simo and Hughes [1998]). Without loss of generality, it can be taken as the standard

von Mises yield criterion

$$\Phi = \|\boldsymbol{\tau}^D - \boldsymbol{\chi}\| - \sqrt{\frac{2}{3}} (\sigma_{y0} + R), \quad (2.9)$$

where $\boldsymbol{\tau}^D$ is the deviatoric part of the Kirchhoff stress, σ_{y0} is the initial yield stress and

$$R = Q(1 - e^{-\beta\kappa}) \quad (2.10)$$

accounts for nonlinear isotropic hardening of Voce type (Voce [1955]) (Q and β are material parameters). An associative flow rule is defined by

$$\mathbf{d}_p = \dot{\gamma} \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \quad (2.11)$$

where $\dot{\gamma}$ is the usual plastic multiplier. Furthermore, (objective) evolution equations for $\boldsymbol{\chi}$ and κ are defined by

$$\overset{\circ}{\boldsymbol{\chi}}^* = \dot{\gamma} c \frac{\partial \Phi}{\partial \boldsymbol{\tau}} - \dot{\gamma} b \boldsymbol{\chi} \quad (2.12)$$

$$\dot{\kappa} = \dot{\gamma} \sqrt{\frac{2}{3}}, \quad (2.13)$$

in which c and b are material parameters and (2.12) accounts for nonlinear kinematic hardening of Armstrong-Frederick type (Armstrong and Frederick [1966]). As was pointed out by Bruhns [2009], Prager's yielding stationarity criterion implies that the objective rates $\overset{\circ}{\boldsymbol{\tau}}^*$ and $\overset{\circ}{\boldsymbol{\chi}}^*$ must be co-rotational rates of the same kind, i. e., their defining spin tensors according to expression (2.1) should be chosen equally. Finally, the hypoelastic-based plasticity model is supplemented by the usual Kuhn-Tucker conditions

$$\Phi \leq 0, \quad \dot{\gamma} \geq 0, \quad \Phi \dot{\gamma} = 0. \quad (2.14)$$

2.3.4 Self-consistent Eulerian model

Classical hypoelastic-plastic material models do not assume the existence of an underlying free-energy potential. As a consequence, dissipation of energy may be predicted by the model even in the absence of plastic flow which is clearly an undesirable feature. In the past, the discoveries of spurious shear oscillations that can arise in cases of large simple shear deformations raised questions on the physical soundness and general applicability of the hypoelastic-based material model (Nagtegaal and De Jong [1981]). These doubts were reinforced by Simo

and Pister [1984] who demonstrated that, for any of the then-known objective rates (including the Jaumann and Green-Naghdi rates but not the logarithmic rate), the widely used hypoelastic relation (2.6) is not exactly integrable, except for some particular instances of the elastic constants.

To address these issues, the workgroup by Bruhns, Xiao and Meyers developed in a number of publications (see, e. g., Bruhns et al. [1999]) the self-consistent Eulerian model of finite elastoplasticity which is based upon a newly developed ‘elastic integrability criterion’ which demands that, for every process of elastic deformations with $\mathbf{d}_e = \mathbf{d}$, the rate equation (2.6) must be exactly integrable to deliver a dissipationless elastic relation that really characterizes recoverable elastic material behavior. One of the most important results in the foregoing references was the demonstration that there is one and only one choice for the objective stress rate in (2.6) which renders the elastic integrability criterion satisfied, namely the co-rotational logarithmic rate which is defined by the logarithmic spin tensor (2.4). With this, the issues of elastic dissipation and non-uniqueness of the theory with respect to the choice of the objective rate could be removed.

2.4 Hyperelastic-based constitutive model

2.4.1 Multiplicative split of the deformation gradient

The finite strain hyperelastic-based plasticity model is based on the fundamental hypothesis that the total deformation gradient $\mathbf{F}$ can multiplicatively be decomposed into elastic and plastic parts according to

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p, \quad (2.15)$$

where $\mathbf{F}_e$ and $\mathbf{F}_p$ are called the elastic and plastic deformation gradients, respectively. The decomposition implicitly assumes the existence of a (local) unstressed intermediate configuration which is defined by the plastic deformation gradient $\mathbf{F}_p$ (Simo and Hughes [1998]).

2.4.2 Constitutive relationships

Based on the principle of material objectivity, the Helmholtz free energy per unit volume is given in the form

$$\Psi = \Psi_e(\tilde{\boldsymbol{\varepsilon}}_e) + \Psi_{\text{kin}}(\boldsymbol{\xi}) + \Psi_{\text{iso}}(\kappa), \quad (2.16)$$

where $\Psi_e = \frac{1}{2} \tilde{\boldsymbol{\varepsilon}}_e \cdot \mathcal{C}[\tilde{\boldsymbol{\varepsilon}}_e]$ represents the elastic energy stored in the material which is assumed to be a quadratic function of the logarithmic elastic strain $\tilde{\boldsymbol{\varepsilon}}_e = \frac{1}{2} \ln(\mathbf{F}_e \mathbf{F}_e^T)$. Moreover,

$\Psi_{\text{kin}} = \frac{1}{2} c \boldsymbol{\xi} \cdot \boldsymbol{\xi}$ and $\Psi_{\text{iso}} = Q(\kappa + \frac{e^{-\beta\kappa}}{\beta})$ are stored energies related to nonlinear kinematic hardening of Armstrong-Frederick type and nonlinear isotropic hardening of Voce type. The latter are functions of the inner variables $\boldsymbol{\xi}$ and κ , respectively.

Using the Clausius-Duhem form of the second law of thermodynamics $-\dot{\Psi}(\tilde{\boldsymbol{\varepsilon}}_e, \boldsymbol{\xi}, \kappa) + \boldsymbol{\tau} \cdot \mathbf{d} \geq 0$ and assuming that the Helmholtz free energy is an isotropic function of its arguments, the following constitutive relationships for the stress $\boldsymbol{\tau}$ and the thermodynamic conjugate forces $\boldsymbol{\chi}$ and R can be derived, namely

$$\boldsymbol{\tau} = \frac{\partial \Psi_e}{\partial \tilde{\boldsymbol{\varepsilon}}_e} = \mathbf{C}[\tilde{\boldsymbol{\varepsilon}}_e] \quad (2.17)$$

$$\boldsymbol{\chi} = \frac{\partial \Psi_{\text{kin}}}{\partial \boldsymbol{\xi}} = c \boldsymbol{\xi} \quad (2.18)$$

$$R = \frac{\partial \Psi_{\text{iso}}}{\partial \kappa} = Q(1 - e^{-\beta\kappa}). \quad (2.19)$$

2.4.3 Yield criterion, flow rule and hardening laws

An isotropic yield function Φ is introduced which defines the set of all admissible states as in (2.8) and again the Von Mises yield criterion (2.9) is used. Furthermore, by assuming that the skew-symmetric part of the plastic velocity gradient $\mathbf{l}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}$ vanishes, i. e., $\mathbf{w}_p = \frac{1}{2}(\mathbf{l}_p - \mathbf{l}_p^T) = \mathbf{0}$, and that a dissipation potential $\Xi = \Phi + \frac{1}{2} \frac{b}{c} \boldsymbol{\chi} \cdot \boldsymbol{\chi}$ exists, the following flow rule and evolution equations for the inner variables can be derived (see de Souza Neto et al. [2008]), viz.,

$$\mathbf{d}_p = \dot{\gamma} \mathbf{R}_e^T \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \mathbf{R}_e \quad (2.20)$$

$$\overset{\circ}{\boldsymbol{\xi}}^* = -\dot{\gamma} \frac{\partial \Xi}{\partial \boldsymbol{\chi}} = \dot{\gamma} \frac{\partial \Phi}{\partial \boldsymbol{\tau}} - \dot{\gamma} \frac{b}{c} \boldsymbol{\chi} \quad (2.21)$$

$$\dot{\kappa} = -\dot{\gamma} \frac{\partial \Xi}{\partial \kappa} = \dot{\gamma} \sqrt{\frac{2}{3}}. \quad (2.22)$$

The evolution equation for the second-order tensor variable $\boldsymbol{\xi}$ is formulated in terms of an (arbitrary) co-rotational rate to maintain objectivity of the formulation. Finally, the hyperelastic-based plasticity model is supplemented by the usual Kuhn-Tucker conditions (2.14).

2.5 Results and discussion

2.5.1 Elliptical closed path deformation of a single element

A cubic C3D8R finite element in ABAQUS was subjected to a repeated elliptical closed path deformation in which the displacements of the nodes were prescribed according to Fig. 2.1.

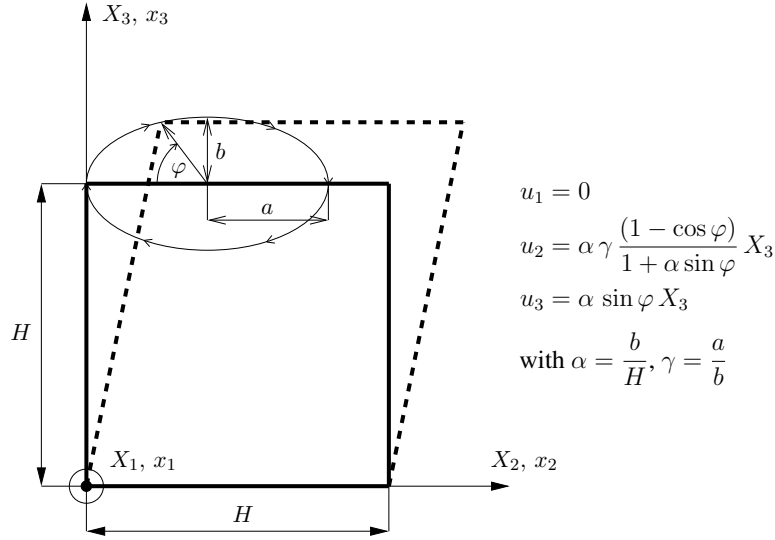
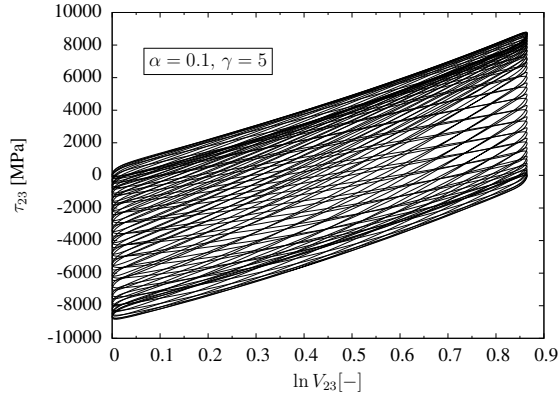


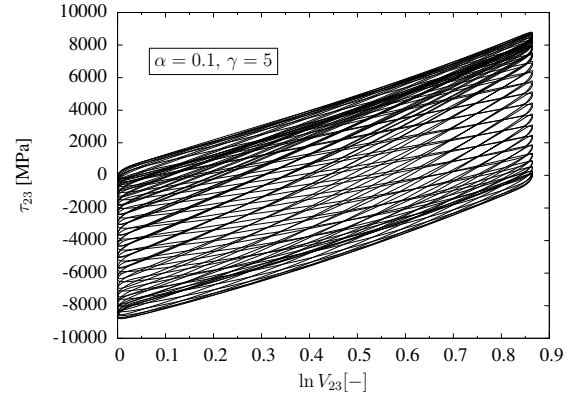
Figure 2.1: Elliptical closed path deformation

The material response was assumed to be hypoelastic-plastic or hyperelastic-plastic with either the Jaumann, Green-Naghdi or the logarithmic rate and the material parameters were specified as $\mu = 80000$ [MPa], $\lambda = 119999.67$ [MPa], $\sigma_{y0} = 800$ [MPa], $Q = 0$ [MPa], $\beta = 0$ [-], $c = 20000$ [MPa] and $b = 0$ [-]. The parameters Q , β and b were set to zero such that an elastoplastic material with linear kinematic hardening was assumed. The idea for this example was given by Eshraghi [2009].

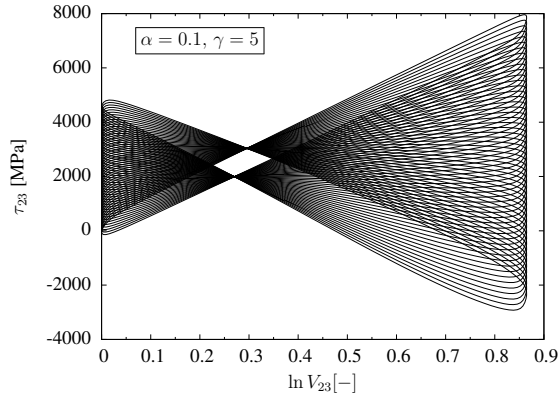
Figure 2.2 shows the shear stress-strain responses of the element at the integration point for 50 subsequent elliptical cycles by using either the hypoelastic- or hyperelastic-based model. In these plots, a remarkable dependency of the results on the respective objective rates can be observed. Moreover, except for the case of the Jaumann rate, the hypoelastic- and hyperelastic-based model behave quite differently. Only in the case of the hypoelastic-based model with the logarithmic rate, a physically meaningful stabilized hysteresis loop can be observed which emphasizes the physical soundness of the self-consistent Eulerian model. It should be mentioned that the problems arise due to the extreme simple shear deformation in connection with the applied linear kinematic hardening model, an issue which was reported already earlier by Nagtegaal and De Jong [1981].



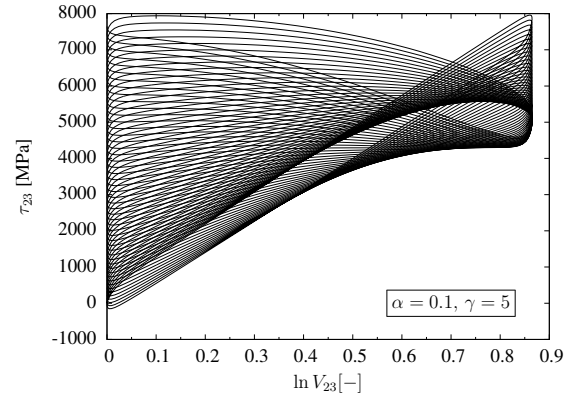
(a) Hypoelastic-based model: Jaumann rate



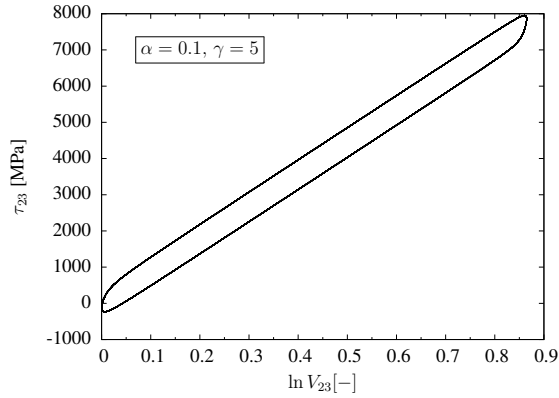
(b) Hyperelastic-based model: Jaumann rate



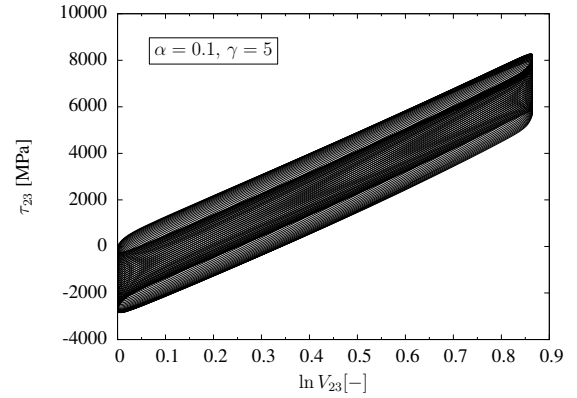
(c) Hypoelastic-based model: Green-Naghdi rate



(d) Hyperelastic-based model: Green-Naghdi rate



(e) Hypoelastic-based model: Logarithmic rate



(f) Hyperelastic-based model: Logarithmic rate

Figure 2.2: Stress-strain plots for 50 elliptical deformation cycles

2.5.2 Cylindrical cup drawing

A structural simulation of the cylindrical cup drawing process was performed in ABAQUS with both the hypoelastic- and hyperelastic-based plasticity models. It was the objective to determine whether there is really also a noticeable influence of the specific objective rate chosen in more realistic situations, e. g., in the case of a metal forming process or not. Deep drawing is an important process in the field of sheet metal forming. The basic tools for this process consist of a die, a blankholder and a punch which were modeled by rigid-body elements. In the process, the blank is mounted between the die and the blankholder and a downwards moving punch forms the blank into the die. A schematic view of the cylindrical cup drawing setup is given in Fig. 2.3.

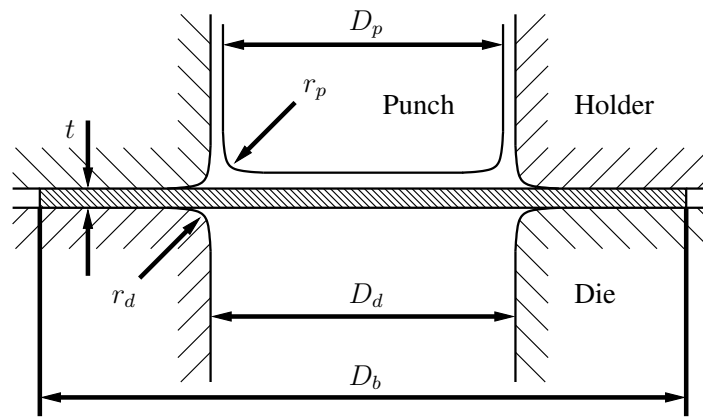


Figure 2.3: Schematic view of cylindrical cup drawing process

The process parameters and the dimensions of the tools were taken from Vladimirov et al. [2011] and are given in Table 2.1. The blank itself was discretized by 1274 C3D8I hexahe-

Parameter/Data	Value	Dimension
Punch diameter D_p	50	[mm]
Punch profile radius r_p	5	[mm]
Die opening diameter D_d	52.8	[mm]
Die profile radius r_d	5	[mm]
Blank diameter D_b	100	[mm]
Sheet thickness t	1	[mm]
Coloumb's coefficient of friction	0.02	[-]
Blankholder force	5	[kN]

Table 2.1: Process parameters and tool data

dral solid elements (2 elements were used in thickness direction). By exploiting symmetry

conditions, it was sufficient to model only a quarter of the blank. A combined nonlinear isotropic and kinematic hardening behavior was assumed, the material parameters were taken from Vladimirov et al. [2009] and specified as: $\mu = 72509.4$ [MPa], $\lambda = 140753.5$ [MPa], $\sigma_{y0} = 325$ [MPa], $c = 2600$ [MPa], $b = 12.5$ [-], $Q = 215$ [MPa] and $\beta = 8$ [-].

Figure 2.4 shows the calculated punch force plotted over the punch displacement for the hypoelastic- and hyperelastic-based plasticity model by using either the Jaumann, Green-Naghdi or logarithmic rate. The curves are almost indistinguishable from each other. Fig-

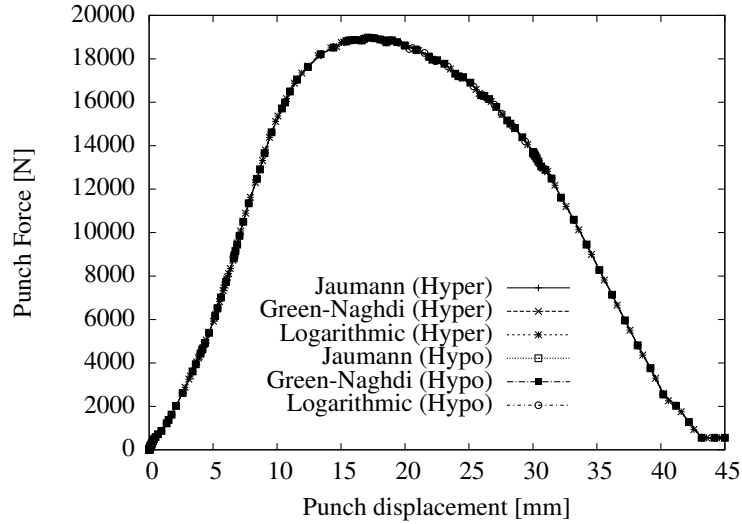


Figure 2.4: Punch force-punch displacement diagram

ure 2.5 shows a contour plot of the distribution of the accumulated plastic strain within the blank for different values of the punch displacement u . For brevity, these results are only plotted once since they are essentially the same for both models and all objective rates considered. The results create the impression that in the simulation of deep drawing processes the particular choice of objective rate used in the hypoelastic- or hyperelastic-based model is of minor importance. Moreover, from the viewpoint of accuracy it seems that neither of the two approaches is preferable over the other. This may be explained by the fact that simple shear deformations in the blank can be neglected and kinematic hardening does not play an important role since the loading is proportional. It should be mentioned that in real cup drawing experiments the formation of ‘cup-earrings’ can be observed, the reason for which lies in the anisotropy of the metal sheet that can not be considered by the discussed isotropic material models. This topic is out of the scope of this work and is treated elsewhere (see, e. g., Vladimirov et al. [2011]).

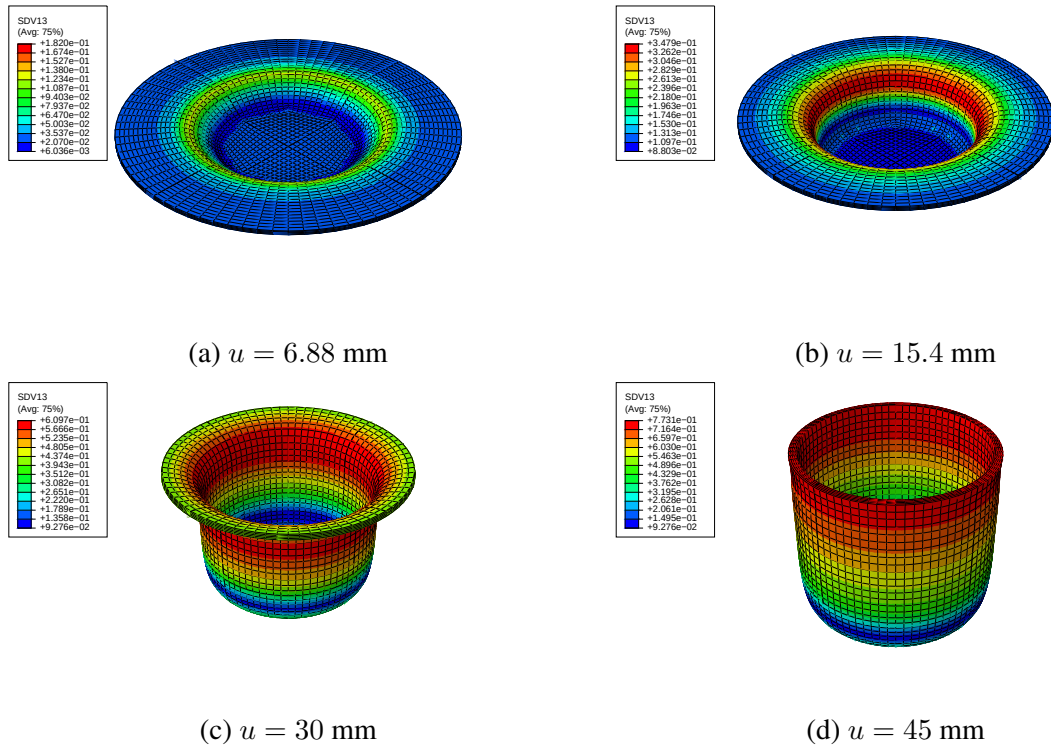


Figure 2.5: Accumulated plastic strain in blank at several punch displacements u

2.6 Conclusions

In this work, two specific hyperelastic- and hypoelastic-based models of finite strain elastoplasticity were examined in terms of their applicability in metal forming processes. Both models allow for nonlinear isotropic and kinematic hardening of Voce and Armstrong-Frederick type and were implemented as user material subroutines (UMAT) into ABAQUS / Standard. In agreement with the theory, simple shear dominated deformation tests on the Gauss-point level showed that the models can be remarkably influenced by the specific objective (back) stress rate chosen in the formulation if linear kinematic hardening is assumed. However, the FE simulation of a cylindrical cup drawing process with more realistic values for the material parameters delivered nearly congruent results for both models and all considered objective rates which suggests that the presented hyperelastic- as well as the hypoelastic-based plasticity model are well-suited for modeling metallic materials in metal forming processes.

3 | **Article 2:**

Numerical comparison of isotropic hypo- and hyperelastic-based plasticity models with application to industrial forming processes

This article was published as:

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Disclosure of the individual authors’ contributions to the article:

T. Brepols reviewed the relevant existing literature, implemented all hypoelastic-based material models and corresponding incrementally objective algorithms considered in this study into ABAQUS / Standard (via the UMAT interface), performed all simulations, interpreted the results and wrote the article. I. N. Vladimirov provided the user material subroutine of the hyperelastic-based plasticity model and ABAQUS input files for the forming simulations considered in Sects. 3.5.5.2 – 3.5.5.4. Furthermore, he and S. Reese gave conceptual advice, contributed to the discussion of the results, read the article and gave valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

3.1 Abstract

Industrial forming processes are usually characterized by large plastic strains and rotations of material elements. This emphasizes the importance of reliable finite strain elastoplasticity models in corresponding finite element simulations. The aim of this work is to review and numerically compare two inherently different types of formulations of finite strain elastoplasticity, namely hypoelastic- and hyperelastic-based plasticity models, with special reference to their applicability in forming processes. Both models allow for nonlinear isotropic and kinematic hardening of Voce and Armstrong-Frederick type and were implemented as user material subroutines (UMAT) into ABAQUS / Standard. Several numerical tests were conducted to assess their respective capabilities. Interestingly enough, although both models led to remarkably different results in shear-dominated single element deformation tests, the structural simulations of a deep drawing, draw bending and thermoforming process delivered nearly congruent results. This suggests that both models are well-suited for modeling elastoplastic materials in common industrial forming processes.

3.2 Introduction

The theoretical development of material models as well as their implementation into numerical methods, e. g., the finite element method, is a time-consuming and challenging task, especially in the context of a large deformation theory. Concerning elastoplastic material models, different strategies exist to extend the infinitesimal theory to the finite deformation range. Consequently, quite a high number of alternative formulations were proposed and discussed in the past (for an intensive yet interesting debate on that topic, see, e. g., Casey and Naghdi [1981]). All these formulations, though based on a completely different description of plastic flow, elastic properties as well as stress and strain measures, are identical in the ‘small strain limit’.

In the beginnings of the theory and application of large deformation elastoplasticity, models implemented into finite element codes relied exclusively on hypoelastic-based approaches which make use of an additive split of the rate of deformation tensor into elastic and plastic parts and a constitutive equation for objective stress rates. Pioneering papers in this field were published, e. g., by Argyris and Kleiber [1977], Argyris et al. [1978], Hibbitt et al. [1970], McMeeking and Rice [1975] and Nagtegaal and De Jong [1981], to name only a few. However, shortly afterwards several controversial issues appeared in this context, e. g., the non-uniqueness regarding the respective objective rate used in the formulation (Atluri [1984],

Nemat-Nasser [1982], Perić [1992]), the lack of objectivity of corresponding numerical integration schemes which led to the development of incrementally objective algorithms (Hughes [1984], Hughes and Winget [1980], Rubinstein and Atluri [1983]) and several artifacts, such as, e. g., the oscillatory shear stress response under monotonic shear loading (Dienes [1979], Lehmann [1972], Nagtegaal and De Jong [1982]) or artificial elastic dissipation (Kojić and Bathe [1987], Simo and Pister [1984]). The development of the so-called self-consistent Eulerian model (see, e. g., Bruhns et al. [1999], Xiao et al. [1997a, 2000]) based on the logarithmic stress rate shed new light on the topic since it does not suffer from the above mentioned problems. There is still active research in this area, see, e. g., Zhu et al. [2014] for the development of a logarithmic stress-based hypoelastic-plastic model relying upon a finite strain extension of the kinematic hardening rule by Abdel-Karim and Ohno [2000] for infinitesimal plasticity. Recently, the self-consistent Eulerian model has been used to describe the elastoviscoplastic damage behavior of mineral filled semi-crystalline polymers (Balieu et al. [2013]) or for modeling shape-memory alloys (see, e. g., Müller and Bruhns [2006], Teeriaho [2013], Xiao [2013]). Hypoelastic-based plasticity models taking into account elastic and/or plastic anisotropy in combination with nonlinear isotropic and kinematic hardening are also successfully employed in the metal forming community to simulate various industrial processes and predict phenomena such as springback (see, e. g., Firat et al. [2008], Haddag et al. [2007], Hama et al. [2008], Oliveira et al. [2007] and Yoshida and Uemori [2003], to name only a few). Even nowadays many in-built material models in commercial finite element codes exploit classical hypoelastic-based approaches to model finite strain elastoplasticity, especially if small elastic strains are assumed.

Owing to the problems described above, hyperelastic-based plasticity models emerged. They rely upon a multiplicative decomposition of the deformation gradient into elastic and plastic parts and a hyperelastic constitutive equation for the stress. Initial developments in this field were given by Simo [1985] and Simo and Ortiz [1985]. This type of models bypasses the aforementioned drawbacks observed in hypoelastic-based plasticity, as, e. g., elastic dissipation and incremental objectivity, since an underlying free energy potential is utilized and the principle of frame-indifference is satisfied in a trivial manner. Several models based on principal logarithmic strains were established which incorporate either isotropic or combined isotropic-kinematic hardening (see, e. g., Eterovic and Bathe [1990], Cuitiño and Ortiz [1992], Simo [1992], Weber and Anand [1990]). Due to an exponential map algorithm utilized to integrate the plastic flow rule, these models retain the simple small strain format return mapping of the infinitesimal theory. However, the mentioned concepts are mainly limited to isotropic elastoplasticity. Thermodynamically consistent formulations were presented which

are also amenable to elastic and/or plastic anisotropy of the material (among others, Chatti et al. [2001], Han et al. [2002, 2003], Sansour et al. [2006, 2008]) and/or kinematic hardening for arbitrary large deformations, see, e. g., Dogui and Sidoroff [1985], Haupt [1996], Lion [2000], Svendsen et al. [1998] and Tsakmakis [1996]. In this context, Arghavani et al. [2010, 2011], Dettmer and Reese [2004], Reese and Christ [2008] and Vladimirov et al. [2008, 2009] considered and discussed also several numerical examples on the structural level in detail. The hyperelastic-based approach to model finite elastoplasticity gained widespread acceptance over the last two decades and can nowadays be considered as ‘state-of-the-art’. As such, it is a matter of ongoing research in a variety of scientific areas, as, e. g., soil plasticity (see, e. g., Coombs et al. [2013]), damage mechanics (see, e. g., Ayoub et al. [2014], Badreddine et al. [2010], Vladimirov et al. [2014]) or crystal plasticity (see, e. g., Bargmann et al. [2011]). The application of anisotropic hyperelastic-based plasticity models in the simulation of structural metal forming processes which involve springback behavior of the material is nowadays likewise well-established (among others, see, e. g., Sansour et al. [2007] and Vladimirov et al. [2010, 2011]).

The available literature is mainly concerned with theoretical aspects of and differences between hypoelastic- and hyperelastic-based formulations (see, e. g., Xiao et al. [2006]). To the authors’ knowledge, the respective practical capabilities of both approaches have rarely been directly compared with each other in more application-oriented examples which seems however worthwhile and interesting (for one among the few counterexamples, see, e. g., Chatti [2010]). In this respect, the present work makes a contribution by discussing and comparing two specific hyper- and hypoelastic-based plasticity models with isotropic and kinematic hardening applied in the simulation of forming processes. The presented models are implemented as user material subroutines (UMAT) into the commercial finite element code ABAQUS / Standard. Various sample calculations, as, e. g., the simulation of a deep drawing, draw bending and thermoforming process, are performed to assess their respective capabilities.

The paper is structured as follows. Section 3.3 is concerned with the theory and algorithmic implementation of a general hypoelastic-based plasticity model with combined nonlinear isotropic and kinematic hardening. The main ingredients of the model are presented as the chosen objective stress rate, the split of the rate of deformation tensor into elastic and plastic parts, the yield function and further constitutive equations to close the model. Section 3.4 addresses a specific hyperelastic-based plasticity model with combined hardening. In addition to the multiplicative decomposition of the deformation gradient into elastic and plastic parts, this model is based on a further split of the plastic part in order to model nonlinear kinematic

hardening. The main issues such as kinematic assumptions, formulation of the Helmholtz free energy, thermodynamically-consistent derivation of the constitutive equations and the yield function are regarded. A numerical algorithm is discussed which preserves the plastic volume and the symmetry of the internal variables. Finally, numerical comparisons between the two models both on the Gauss point level and in various forming simulations are presented in Sect. 3.5.

3.3 Hypoelastic-based plasticity model

3.3.1 Objective corotational rates

In continuum mechanics, the constitutive equations are required to satisfy the principle of material frame-indifference (also called principle of material objectivity). According to this fundamental physical principle, material properties must be independent of the respective frame of reference or observer (see, e. g., Truesdell and Noll [1965]). In an Eulerian rate-type formulation of finite elastoplasticity, constitutive laws are therefore formulated in terms of objective rates of Eulerian stress measures, as, e. g., of the Kirchhoff stress tensor $\boldsymbol{\tau}$.

Generally speaking, objective rates may be classified into two different categories, namely corotational and non-corotational rates. Any corotational rate of a symmetric second-order Eulerian tensor $\mathbf{a}$ can be expressed as

$$\overset{\circ}{\mathbf{a}} \equiv \dot{\mathbf{a}} - \boldsymbol{\Omega} \mathbf{a} + \mathbf{a} \boldsymbol{\Omega} \quad (3.1)$$

where $\dot{\mathbf{a}}$ denotes the material time derivative of $\mathbf{a}$ and $\boldsymbol{\Omega}$ is a skew-symmetric second-order Eulerian quantity which is also called spin tensor. The particular form of $\boldsymbol{\Omega}$ characterizes the specific kind of corotational rate. Sufficient requirements for the spin to render $\overset{\circ}{\mathbf{a}}$ indeed an objective quantity for any time-differentiable $\mathbf{a}$ were given by Xiao et al. [1998].

Two classical examples of objective corotational rates are the well-known Jaumann and Green-Naghdi rates (see, e. g., Green and Naghdi [1965], Jaumann [1911] and Zaremba [1903]) which are defined, respectively, by the spin tensors

$$\boldsymbol{\Omega} = \mathbf{w} \quad (\text{Jaumann}) \quad (3.2)$$

$$\boldsymbol{\Omega} = \dot{\mathbf{R}} \mathbf{R}^T \quad (\text{Green-Naghdi}) \quad (3.3)$$

where $\mathbf{w} = \frac{1}{2} (\mathbf{l} - \mathbf{l}^T)$ is the skew-symmetric part of the spatial velocity gradient $\mathbf{l} = \dot{\mathbf{F}} \mathbf{F}^{-1}$

and $\mathbf{R}$ denotes the rotation tensor of the polar decomposition of the deformation gradient $\mathbf{F} = \mathbf{v} \mathbf{R} = \mathbf{R} \mathbf{U}$ ($\mathbf{v}$ and $\mathbf{U}$ are the left and right stretch tensor, respectively). More recently, in the context of the self-consistent Eulerian theory developed mainly by Bruhns, Xiao and Meyers (see, e. g., Bruhns et al. [1999]) specific attention has been paid to the corotational logarithmic rate defined by

$$\boldsymbol{\Omega} = \mathbf{w} + \sum_{i \neq k}^m \left(\frac{1 + (b_i/b_k)}{1 - (b_i/b_k)} + \frac{2}{\ln(b_i/b_k)} \right) \mathbf{b}_i \mathbf{d} \mathbf{b}_k \quad (\text{Logarithmic}) \quad (3.4)$$

where b_i denotes the i th eigenvalue of the left Cauchy-Green tensor $\mathbf{b} = \mathbf{F} \mathbf{F}^T$, $\mathbf{b}_i$ is the i th eigenprojection of $\mathbf{b}$ (see Appendix 3.7.1), m is the number of distinct eigenvalues of $\mathbf{b}$ and $\mathbf{d} = \frac{1}{2} (\mathbf{I} + \mathbf{I}^T)$ is the symmetric part of the spatial velocity gradient, also termed ‘rate of deformation tensor’.

3.3.2 Additive split of rate of deformation and hypoelastic constitutive law

In hypoelastic-based plasticity, the rate of deformation tensor $\mathbf{d}$ is assumed to be additively separable into elastic and plastic parts according to

$$\mathbf{d} = \mathbf{d}_e + \mathbf{d}_p \quad (3.5)$$

where $\mathbf{d}_e$ and $\mathbf{d}_p$ are objective Eulerian quantities which are labeled elastic and plastic rate of deformation tensor, respectively. Although sometimes considered to be an ‘ad hoc’ generalization of the additive decomposition of the strain tensor in the infinitesimal elastoplasticity theory, relation (3.5) can in fact be deduced from the hypothesis that the total stress work increment is composed of independent recoverable and irrecoverable parts during each process of elastoplastic deformation (for further details, see, e. g., Lehmann [1982, 1989] and Xiao et al. [2006]). Thus, the additive decomposition (3.5) is physically motivated.

Based on (3.5), the hypoelastic response of the material is expressed in terms of a linear relationship between an (arbitrary) objective rate of the Kirchhoff stress according to definition (3.1) and the elastic rate of deformation tensor, i. e.,

$$\overset{\circ}{\boldsymbol{\tau}} = \mathcal{H}(\boldsymbol{\tau}) [\mathbf{d}_e] = \mathcal{H}(\boldsymbol{\tau}) [\mathbf{d} - \mathbf{d}_p] \quad (3.6)$$

in which $\mathcal{H}$ is the fourth-order tensor of elastic moduli that may depend on the stress. The principle of frame-indifference demands $\mathcal{H}(\boldsymbol{\tau})$ to be an isotropic function of the Kirchhoff

stress tensor Truesdell and Noll [1965, p. 405]). One advantage of hypoelastic-based models is the ability to incorporate variable, state-dependent elastic moduli easily into the formulation. This feature is especially attractive for many geotechnical applications, see, e. g., Chen and Zhou [2013].

An important subclass of (3.6) constitute the so-called hypoelastic-based models of grade zero

$$\overset{\circ}{\boldsymbol{\tau}} = \mathcal{C} [\mathbf{d}_e] = \mathcal{C} [\mathbf{d} - \mathbf{d}_p] \quad (3.7)$$

where the elastic moduli tensor $\mathcal{C}$ is considered to be independent of the stress. A special choice for $\mathcal{C}$ suitable for modeling, e. g., metal elastoplasticity is given by the standard isotropic elasticity tensor of the infinitesimal theory

$$\mathcal{C} := \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \mathcal{I} \quad (3.8)$$

In the latter expression, λ and μ denote the Lamé parameters. The quantity $\mathbf{I}$ is the second-order identity tensor and $\mathcal{I}$ denotes the fourth order symmetric identity tensor.

3.3.3 Yield criterion, flow rule and hardening laws

A yield function Φ is assumed which defines the set of all admissible states

$$\bar{\mathbb{E}} := \{ (\boldsymbol{\tau}, \boldsymbol{\chi}, R) \mid \Phi(\boldsymbol{\tau}, \boldsymbol{\chi}, R) \leq 0 \} \quad (3.9)$$

where the deviatoric second-order back stress tensor $\boldsymbol{\chi}$ and the scalar stress-like quantity R are related to kinematic and isotropic hardening of the material, respectively. For the sake of a simple and meaningful comparison between the hypoelastic-based and the hyperelastic-based approaches, the von Mises yield criterion

$$\Phi = \sqrt{\frac{3}{2}} \|\boldsymbol{\tau}^D - \boldsymbol{\chi}\| - (\sigma_y + R) \quad (3.10)$$

will be considered in the following. The superscript D is used to denote the deviatoric part of a quantity, i. e., if $\mathbf{A}$ is a second-order tensor then the deviatoric part reads $\mathbf{A}^D := \mathbf{A} - \frac{1}{3} \text{tr}(\mathbf{A}) \mathbf{I}$. In expression (3.10), σ_y is the initial yield stress and

$$R = Q (1 - e^{-\beta \kappa}) \quad (3.11)$$

is related to nonlinear isotropic hardening behavior of Voce type where κ is the accumulated plastic strain and Q, β are material parameters (Voce [1955]). In the associative flow rule

$$\mathbf{d}_p = \dot{\gamma} \frac{\partial \Phi}{\partial \boldsymbol{\tau}} = \dot{\gamma} \sqrt{\frac{3}{2}} \frac{\boldsymbol{\tau}^D - \boldsymbol{\chi}}{\|\boldsymbol{\tau}^D - \boldsymbol{\chi}\|} \quad (3.12)$$

$\dot{\gamma}$ denotes the plastic multiplier and $\partial \Phi / \partial \boldsymbol{\tau}$ defines the ‘direction’ of plastic flow. Furthermore, (objective) evolution equations for $\boldsymbol{\chi}$ and κ are defined by

$$\dot{\boldsymbol{\chi}} = \dot{\gamma} \sqrt{\frac{3}{2}} \left(c \frac{\boldsymbol{\tau}^D - \boldsymbol{\chi}}{\|\boldsymbol{\tau}^D - \boldsymbol{\chi}\|} - b \boldsymbol{\chi} \right) \quad (3.13)$$

$$\dot{\kappa} = -\dot{\gamma} \frac{\partial \Phi}{\partial R} = \dot{\gamma} \quad (3.14)$$

in which c and b are material parameters and Eq. (3.13) represents nonlinear kinematic hardening of Armstrong-Frederick type (Armstrong and Frederick [1966]). Finally, as in the infinitesimal theory, the hypoelastic-based plasticity model is supplemented by the usual Kuhn-Tucker conditions

$$\Phi \leq 0, \quad \dot{\gamma} \geq 0, \quad \Phi \dot{\gamma} = 0 \quad (3.15)$$

More advanced or complex kinematic and isotropic hardening rules than (3.13) and (3.14) could be easily incorporated into the hypoelastic-based plasticity model described above. In particular, any evolution equation for the back stress tensor valid within the small strain theory can conveniently be extended to finite strains by replacing the relevant material time derivatives of the back stress by (in principle arbitrary) objective rates of the latter.

3.3.4 Elastic dissipation issue and self-consistent Eulerian model

It was noted by Prager [1961b] that relationship (3.6) is rate-independent as well as incrementally linear and reversible. Thus, small deformation increments about a finitely deformed state of the material cause stress and strain increments which are linearly related and reversible upon unloading. However, since hypoelastic-based models usually lack an underlying elastic potential, conservation of energy cannot be expected in general for large elastic deformations. For this reason, the work done in a closed deformation cycle is normally not zero. In other words, dissipation may be predicted even in the absence of plastic flow which is clearly physically implausible. Moreover, the discovery of spurious shear oscillations that may arise for large simple shear deformations (see, e. g., Dienes [1979], Lehmann [1972], Nagtegaal and De Jong [1982]) raised questions regarding the general applicability and physical soundness

of the hypoelastic-based material model. These doubts were reinforced by Simo and Pister [1984] who demonstrated that, for any of the then-known objective rates (including, e. g., the Jaumann and Green-Naghdi rates but not the logarithmic rate), the widely used hypoelastic relation (3.7) based on (3.8) is not exactly integrable, except for some particular instances of the elastic constants. Furthermore, no restriction is placed on the respective definition of $\overset{\circ}{\boldsymbol{\tau}}$ and $\overset{\circ}{\boldsymbol{\chi}}$, which means that in principle the objective rates can be chosen independently and differently from each other. These circumstances rendered the hypoelastic-based theory somewhat unsatisfactory in former times.

To overcome these issues, Bruhns and coauthors developed in a number of publications (see, e. g., Bruhns et al. [1999], Xiao et al. [1997*a,b*, 1999, 2000]) the self-consistent Eulerian model of finite elastoplasticity. They demonstrated that Prager's yielding stationarity criterion (Prager [1961*a*]) implies that $\overset{\circ}{\boldsymbol{\tau}}$ and $\overset{\circ}{\boldsymbol{\chi}}$ should be corotational rates of the same type, i. e., the respective spin tensors according to expression (3.1) should be chosen equally. Furthermore, they introduced the 'elastic integrability criterion' which demands that, for every process of purely elastic deformations with $\mathbf{d}_e = \mathbf{d}$, rate equation (3.6) must be exactly integrable to deliver a dissipationless elastic relation that really characterizes recoverable elastic material behavior.

One of the most important results in the foregoing references was the demonstration that there is one and only one choice for the objective stress rate in (3.7) which renders the elastic integrability criterion unconditionally satisfied, namely the corotational logarithmic rate which is defined by the logarithmic spin tensor (3.4). Moreover, it was shown that a hypoelastic model based on (3.8) and the logarithmic rate is in fact the equivalent rate form of the well-known isotropic hyperelastic model by Hencky (Hencky [1928, 1931, 1933]) and hence possesses an elastic potential. Concerning the more general hypoelastic relation (3.6), the complex integrability conditions originally developed by Bernstein [1960*a,b*] which are necessary for relating hypoelasticity to Cauchy-elasticity could substantially be simplified. With this, the issues of elastic dissipation and non-uniqueness of the theory with respect to the choice of the objective rate could be removed and the hypoelastic-based plasticity model could be equipped with a better physical soundness.

3.3.5 Algorithmic implementation

3.3.5.1 Main ideas

The algorithmic implementation of the hypoelastic-based plasticity model requires the usage of an incrementally objective integration algorithm (a term first introduced by Hughes and

Winget [1980]) to maintain the frame-indifference of the formulation also in the time-discrete range. The main idea is to map the constitutive equations, originally formulated in the current configuration, to a specific local configuration which is unaffected by any superposed spatial rigid body motion. Afterwards, a common time integration algorithm can be performed which leads to an algorithmic problem in this local configuration. Finally, the discrete equations are mapped back to the current configuration.

Basically, for the actual implementation two different types of methodologies are considered:

- On the one hand, the objective rate quantities in the spatial description can be transferred to a convective representation by appropriate tensorial transformations using the deformation gradient ('pull-back'). Here, the fact is exploited that objects in the convective representation remain unaltered under superposed spatial rigid body motions. From a mechanical point of view, this may be interpreted as going from the current to the reference configuration of the body. This approach will be used here to derive an objective algorithmic approximation for the rate of deformation tensor.
- On the other hand, the objective rate quantities in the spatial description can be transformed to a rotation-neutralized representation. This is achieved by transforming them to a locally rotating coordinate system which is constructed such that the rotated objects do not alter under superposed spatial rigid body motions. This approach is particularly suited for equations involving corotational objective rates.

In the following, a short summary of the numerical integration of the hypoelastic-based plasticity model described above will be given (for further details, refer, e. g., to Simo and Hughes [1998]).

3.3.5.2 Geometric setup

Let $\mathcal{B} \subset \mathbb{R}^3$ be the reference configuration of the continuum elastoplastic body under consideration and let any material point of the body be identified by its position vector $\mathbf{X} \in \mathcal{B}$. Furthermore, let $I = [t_0, t_{\text{end}}] \subset \mathbb{R}$ be the time interval of interest. The generally nonlinear mapping

$$\varphi : \begin{cases} \mathcal{B} \times I & \longrightarrow \mathbb{R}^3 \\ (\mathbf{X}, t) & \longmapsto \mathbf{x} = \varphi(\mathbf{X}, t) \end{cases} \quad (3.16)$$

is referred to as the motion. For any fixed time $t \in I$, the mapping $\varphi(\bullet, t) = \varphi_t : \mathcal{B} \longrightarrow \mathbb{R}^3$ is denoted as configuration. In the context considered here it is assumed that the configurations

at t_n and $t_{n+1} = t_n + \Delta t$, that is $\varphi_n : \mathcal{B} \rightarrow \mathbb{R}^3$ and $\varphi_{n+1} : \mathcal{B} \rightarrow \mathbb{R}^3$, are given. With these, a one-parameter family of configurations can be defined via

$$\varphi_{n+\alpha} = \alpha \varphi_n + (1 - \alpha) \varphi_{n+1}, \quad \alpha \in [0, 1] \quad (3.17)$$

The corresponding deformation gradient is given by the relationship

$$\mathbf{F}_{n+\alpha} = \frac{\partial \varphi_{n+\alpha}}{\partial \mathbf{X}} = \alpha \mathbf{F}_n + (1 - \alpha) \mathbf{F}_{n+1} \quad (3.18)$$

3.3.5.3 Overall objective integration algorithm

First of all, an incrementally objective update formula for the hypoelastic constitutive equation (3.7) shall be constructed. Given the skew-symmetric spin tensor $\boldsymbol{\Omega}$ corresponding to the corotational rate used in the fomulation, consider the following initial value problem for the proper orthogonal rotation tensor $\boldsymbol{\Lambda}$:

$$\begin{cases} \dot{\boldsymbol{\Lambda}} = \boldsymbol{\Omega} \boldsymbol{\Lambda} \\ \boldsymbol{\Lambda}|_{t=0} = \mathbf{I} \end{cases} \quad (3.19)$$

Assuming for the time being that problem (3.19) can be solved appropriately and $\boldsymbol{\Lambda}$ is the rotation from the current configuration to the superposed spatial rigid-body-motion-unaffected configuration, the hypoelastic relation (3.7) is transformed into a rotation-neutralized description by multiplying it from the left and right with $\boldsymbol{\Lambda}^T$ and $\boldsymbol{\Lambda}$, respectively, leading to

$$\overset{\circ}{\boldsymbol{\tau}} = \mathcal{C} [\mathbf{d} - \mathbf{d}_p] \iff \boldsymbol{\Lambda}^T \overset{\circ}{\boldsymbol{\tau}} \boldsymbol{\Lambda} = \mathcal{C} [\boldsymbol{\Lambda}^T \mathbf{d} \boldsymbol{\Lambda} - \boldsymbol{\Lambda}^T \mathbf{d}_p \boldsymbol{\Lambda}] \quad (3.20)$$

In the latter relationship, the isotropy of $\mathcal{C}$ was exploited. For convenience, three new quantities are defined, namely $\bar{\boldsymbol{\tau}} := \boldsymbol{\Lambda}^T \boldsymbol{\tau} \boldsymbol{\Lambda}$, $\bar{\mathbf{d}} := \boldsymbol{\Lambda}^T \mathbf{d} \boldsymbol{\Lambda}$ and $\bar{\mathbf{d}}_p := \boldsymbol{\Lambda}^T \mathbf{d}_p \boldsymbol{\Lambda}$ which are called the rotated Kirchhoff stress, rotated rate of deformation and rotated rate of plastic deformation tensor, respectively. With these and noting that $\dot{\bar{\boldsymbol{\tau}}} \equiv \boldsymbol{\Lambda}^T \overset{\circ}{\boldsymbol{\tau}} \boldsymbol{\Lambda}$ (for a proof, see Appendix 3.7.2), the hypoelastic equation in the rotation-neutralized description may be stated more clearly as

$$\dot{\bar{\boldsymbol{\tau}}} = \mathcal{C} [\bar{\mathbf{d}} - \bar{\mathbf{d}}_p] \quad (3.21)$$

Expression (3.21) is indeed rigid-motion-insensitive (see Appendix 3.7.3) and is ready for being numerically integrated as usual by a standard time-stepping algorithm. Here, the gener-

alized midpoint rule will be applied which leads to the update formula

$$\bar{\boldsymbol{\tau}}_{n+1} = \bar{\boldsymbol{\tau}}_n + \mathcal{C} [\Delta t (\bar{\mathbf{d}}_{n+\alpha} - \bar{\mathbf{d}}_{p_{n+\alpha}})], \quad \alpha \in [0, 1] \quad (3.22)$$

for the rotated stress¹. Specific values for α lead to specific integration algorithms, e. g., $\alpha = 0$ for explicit Euler, $\alpha = 1/2$ for the mid-point rule and $\alpha = 1$ for implicit Euler.

Afterwards, the equation must be transformed back to the spatial description by multiplying it from the left and right with $\boldsymbol{\Lambda}$ and $\boldsymbol{\Lambda}^T$, respectively, which leads to

$$\boldsymbol{\tau}_{n+1} = \boldsymbol{\Lambda}_\Delta \boldsymbol{\tau}_n \boldsymbol{\Lambda}_\Delta^T + \boldsymbol{\Lambda}_\delta \mathcal{C} [\Delta t (\mathbf{d}_{n+\alpha} - \mathbf{d}_{p_{n+\alpha}})] \boldsymbol{\Lambda}_\delta^T \quad (3.23)$$

In the last expression, the isotropy of $\mathcal{C}$ was utilized and $\boldsymbol{\Lambda}_\Delta$, $\boldsymbol{\Lambda}_\delta$ are defined by

$$\boldsymbol{\Lambda}_\Delta := \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_n^T, \quad \boldsymbol{\Lambda}_\delta := \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_{n+\alpha}^T \quad (3.24)$$

which can be interpreted as incremental rotations from the n and $n+\alpha$ configurations to the $n+1$ configuration, respectively. By using relationship (3.12) and simple rearrangement of the terms the following formula is obtained

$$\boldsymbol{\tau}_{n+1} = (\boldsymbol{\Lambda}_\Delta \boldsymbol{\tau}_n \boldsymbol{\Lambda}_\Delta^T + \boldsymbol{\Lambda}_\delta \mathcal{C} [\Delta t \mathbf{d}_{n+\alpha}] \boldsymbol{\Lambda}_\delta^T) - \Delta\gamma \boldsymbol{\Lambda}_\delta \mathcal{C} \left[\frac{\partial \Phi}{\partial \boldsymbol{\tau}} \bigg|_{n+\alpha} \right] \boldsymbol{\Lambda}_\delta^T \quad (3.25)$$

where $\Delta\gamma := \Delta t \dot{\gamma}$.

The leftmost term inside the brackets can be interpreted as a trial stress

$$\boldsymbol{\tau}_{n+1}^{\text{trial}} := \boldsymbol{\Lambda}_\Delta \boldsymbol{\tau}_n \boldsymbol{\Lambda}_\Delta^T + \boldsymbol{\Lambda}_\delta \mathcal{C} [\Delta t \mathbf{d}_{n+\alpha}] \boldsymbol{\Lambda}_\delta^T \quad (3.26)$$

which is the actual stress in case of a purely hypoelastic step. Otherwise, a non-zero correction term $-\Delta\gamma \boldsymbol{\Lambda}_\delta \mathcal{C} \left[\frac{\partial \Phi}{\partial \boldsymbol{\tau}} \bigg|_{n+\alpha} \right] \boldsymbol{\Lambda}_\delta^T$ must be added to project the stress back to the yield surface. This suggests a two-step elastic predictor/plastic corrector solution strategy as in the infinitesimal strain case. It is general practice (see, e. g., Simo and Hughes [1998, p. 292]) to perform the corrector step in the current configuration ($\alpha = 1$) which leads finally to the update formula

$$\boldsymbol{\tau}_{n+1} = \boldsymbol{\tau}_{n+1}^{\text{trial}} - \Delta\gamma \mathcal{C} \left[\frac{\partial \Phi}{\partial \boldsymbol{\tau}} \bigg|_{n+1} \right] \quad (3.27)$$

since in this case $\boldsymbol{\Lambda}_\delta = \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_{n+1}^T = \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_{n+1}^{-1} = \mathbf{I}$.

¹The notation $(\bullet)_{n+\alpha}$ is used to denote the value of a quantity $(\bullet)$ at the discrete time step $n+\alpha$, $\alpha \in [0, 1]$.

Proceeding in the same manner also for the internal variables and taking into account the evolution equations (3.13), (3.14) of the model as well as the yield function (3.10), the return-mapping equations of the hypoelastic-based plasticity model can be summarized as

$$\begin{aligned}
 \boldsymbol{\tau}_{n+1} &= \boldsymbol{\tau}_{n+1}^{\text{trial}} - \Delta\gamma \mathbf{C} \left[\frac{\partial \Phi}{\partial \boldsymbol{\tau}} \Big|_{n+1} \right] \\
 \boldsymbol{\chi}_{n+1} &= \boldsymbol{\chi}_{n+1}^{\text{trial}} - \Delta\gamma \left(c \frac{\partial \Phi}{\partial \boldsymbol{\tau}} \Big|_{n+1} - \sqrt{\frac{3}{2}} b \boldsymbol{\chi}_{n+1} \right) \\
 \kappa_{n+1} &= \kappa_{n+1}^{\text{trial}} + \Delta\gamma \\
 \Phi(\boldsymbol{\tau}_{n+1}, \boldsymbol{\chi}_{n+1}, R_{n+1}) &= 0
 \end{aligned} \tag{3.28}$$

where the trial internal variables are defined by

$$\boldsymbol{\chi}_{n+1}^{\text{trial}} = \boldsymbol{\Lambda}_{\Delta} \boldsymbol{\chi}_n \boldsymbol{\Lambda}_{\Delta}^T, \quad \kappa_{n+1}^{\text{trial}} = \kappa_n \tag{3.29}$$

Similarly to the small strain case, the elastic predictor step firstly assumes a purely hypoelastic deformation in which the internal variables remain unchanged. This trial state is then tested for plastic admissibility by checking whether

$$\Phi(\boldsymbol{\tau}_{n+1}^{\text{trial}}, \boldsymbol{\chi}_{n+1}^{\text{trial}}, R_{n+1}^{\text{trial}}) \leq 0 \tag{3.30}$$

in which $R_{n+1}^{\text{trial}} = Q [1 - \exp(-\beta \kappa_{n+1}^{\text{trial}})]$. If this is the case, the new state is already found and all state variables are updated to $(\bullet)_{n+1} = (\bullet)_{n+1}^{\text{trial}}$. Otherwise, the return-mapping equations must be solved iteratively, e. g., by the Newton algorithm in every time step until the solution of (3.28) is found.

Examining the discretized scalar evolution equation for the isotropic hardening variable in (3.28), it is observed that κ_{n+1} is explicitly given in terms of $\kappa_{n+1}^{\text{trial}}$ and $\Delta\gamma$. Therefore, it can be eliminated as an unknown from the above return-mapping equations and needs to be updated only when the local iteration has already converged. In total, this leads to a system of 13 nonlinear scalar equations for 13 unknowns $\boldsymbol{\tau}_{n+1}$, $\boldsymbol{\chi}_{n+1}$ and $\Delta\gamma$.

3.3.5.4 Addendum 1: determination of the rotation tensors

For the computation of the trial stress (3.26) the numerical determination of the incremental rotation tensors $\boldsymbol{\Lambda}_{\Delta} = \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_n^T$ and $\boldsymbol{\Lambda}_{\delta} = \boldsymbol{\Lambda}_{n+1} \boldsymbol{\Lambda}_{n+\alpha}^T$ is required. The following generalized

exponential map midpoint rule is used for solving problem (3.19) numerically:

$$\begin{cases} \Lambda_{n+1} = \exp(\Delta t \Omega_{n+\alpha}) \Lambda_n \\ \Lambda_0 = \mathbf{I}, \quad \alpha \in [0, 1] \end{cases} \quad (3.31)$$

Since the tensor exponential function maps skew-symmetric tensors onto proper orthogonal tensors, it is ensured that Λ_{n+1} is indeed a rotation (see, e. g., Itskov [2009]).

It may be shown that algorithm (3.31) is consistent with problem (3.19) and second-order accurate for $\alpha = 1/2$ (see Simo and Vu-Quoc [1986]). In this case, also the computation of $\Lambda_{n+\frac{1}{2}}$ is simple (see Appendix 3.7.4), namely

$$\Lambda_{n+\frac{1}{2}} = \exp\left(\frac{1}{2} \Delta t \Omega_{n+\frac{1}{2}}\right) \Lambda_n \quad (3.32)$$

Concerning the actual computation of the tensor exponential function it should be noted that, for any skew-symmetric tensor $\hat{\omega}$, the following closed-form expression of the tensor exponential exists which is known as Rodrigues' formula:

$$\exp(\hat{\omega}) = \mathbf{I} + \frac{\sin(\|\omega\|)}{\|\omega\|} \hat{\omega} + \frac{1}{2} \left(\frac{\sin(\|\omega\|/2)}{\|\omega\|/2} \right)^2 \hat{\omega}^2 \quad (3.33)$$

where ω is the axial vector which is for all vectors x uniquely defined by

$$\hat{\omega}x = \omega \times x \quad (3.34)$$

Several parametrizations for (3.33) are known as, e. g., the quaternion parametrization which is optimal from a computational point of view (Simo and Vu-Quoc [1986]).

3.3.5.5 Addendum 2: approximation of the rate of deformation tensor

An algorithmic approximation of the rate of deformation tensor d may be found by transferring it to a convective representation, i. e., by a 'pull back' to the reference configuration. This leads to the identity (see Appendix 3.7.5)

$$\dot{\mathbf{C}} \equiv 2 \mathbf{F}^T d \mathbf{F} \quad (3.35)$$

where $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ is the right Cauchy-Green tensor. Since $\dot{\mathbf{C}}$ is defined on the reference configuration, it is unaltered by superposed spatial rigid body rotations and ready for being

numerically integrated by the generalized mid-point rule:

$$\mathbf{F}_{n+\alpha}^T \mathbf{d}_{n+\alpha} \mathbf{F}_{n+\alpha} = \frac{1}{2} \frac{\mathbf{C}_{n+1} - \mathbf{C}_n}{\Delta t}, \quad \alpha \in [0, 1] \quad (3.36)$$

This expression can be transformed back to the spatial description ('push-forward') by multiplying it from the left and right with $\mathbf{F}_{n+\alpha}^{-T}$ and $\mathbf{F}_{n+\alpha}^{-1}$, respectively, which finally gives

$$\mathbf{d}_{n+\alpha} = \frac{1}{2\Delta t} \mathbf{F}_{n+\alpha}^{-T} (\mathbf{C}_{n+1} - \mathbf{C}_n) \mathbf{F}_{n+\alpha}^{-1} \quad (3.37)$$

3.3.6 Hypoelastic-based plasticity in ABAQUS / Standard

For researchers and scientists working with ABAQUS / Standard, it might be interesting to gain better insight into how internal elastoplastic material models for standard J_2 metal elastoplasticity behave if geometric nonlinearities are taken into account, i. e., if NLGEOM=YES. This is also useful for gaining a better understanding of the working method of the user material subroutine interface (UMAT).

The point of departure is a standard hypoelastic-plasticity formulation based on the Kirchhoff stress and the Jaumann rate, namely

$$\overset{\circ}{\boldsymbol{\tau}} = \dot{\boldsymbol{\tau}} - \mathbf{w} \boldsymbol{\tau} + \boldsymbol{\tau} \mathbf{w} = \mathcal{C} [\mathbf{d} - \mathbf{d}_p] \quad (3.38)$$

At the outset, in the case of J_2 metal elastoplasticity ABAQUS / Standard assumes that elastic strains are negligibly small and that the elastic behavior is isotropic which justifies the use of $\mathcal{C}$. Furthermore, since no essential elastic volume changes are present and the material is additionally assumed to be plastically incompressible, the Kirchhoff and Cauchy stress are approximately the same, i. e., $\boldsymbol{\tau} \approx \boldsymbol{\sigma}$, which leads to the formulation

$$\overset{\circ}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{w} \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{w} = \mathcal{C} [\mathbf{d} - \mathbf{d}_p] \quad (3.39)$$

It is this model which is algorithmically implemented in ABAQUS / Standard. The numerical implementation is based on the famous incrementally objective algorithm according to Hughes and Winget [1980] which can be seen as a specialization of the algorithm discussed in Sect. 3.3.5². More specifically, to obtain the latter algorithm, the midpoint rule must be used ($\alpha = 1/2$) and the rotation of the material response part of the stress increment must be neglected by setting $\boldsymbol{\Lambda}_\delta := \mathbf{I}$. Moreover, the incremental rotation tensor $\boldsymbol{\Lambda}_\Delta$ is slightly different

²A numerical example confirming this assertion will be given in Sect. 3.5.4.

which finally leads to the update formula

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\Lambda}_\Delta \boldsymbol{\sigma}_n \boldsymbol{\Lambda}_\Delta^T + \mathcal{C} \left[\Delta t \mathbf{d}_{n+\frac{1}{2}} \right] - \Delta \gamma \mathcal{C} \left[\frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \Big|_{n+1} \right] \quad (3.40)$$

in which $\boldsymbol{\Lambda}_\Delta$ is defined as

$$\boldsymbol{\Lambda}_\Delta := \left(\mathbf{I} - \frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right)^{-1} \left(\mathbf{I} + \frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \quad (3.41)$$

The latter expression can be derived by using a first-order series truncation of the tensor exponential function in the update formula (3.31) (see Appendix 3.7.6).

Concerning the UMAT interface, it might seem reasonable that ABAQUS / Standard provides as input, e. g., the already rotated Cauchy stress $\boldsymbol{\Lambda}_\Delta \boldsymbol{\sigma}_n \boldsymbol{\Lambda}_\Delta^T$ so that the user does not have to take care of this when implementing a hypoelastic-based plasticity model in a similar fashion to the above described algorithm. Furthermore, as was mentioned also, e. g., by Stein and Sagar [2008], a user of the UMAT is required to specify the material Jacobian ddsdde as a tangent stiffness which is associated with the Jaumann rate of the Cauchy stress. An algorithm for the numerical approximation of the consistent tangent in ABAQUS / Standard was given by Sun et al. [2008] whose approach is based on Miehe [1996].

3.4 Hyperelastic-based plasticity model

3.4.1 Multiplicative split of the deformation gradient

In the following, a finite strain elastoplasticity model developed by Dettmer and Reese [2004] and further developed by Vladimirov et al. [2008] will be discussed. As most finite strain hyperelastic-based plasticity models, it is based on the fundamental hypothesis that the total deformation gradient $\mathbf{F}$ can be multiplicatively decomposed into elastic and plastic parts according to

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \quad (3.42)$$

where $\mathbf{F}_e$ and $\mathbf{F}_p$ are labeled the elastic and plastic part of the deformation gradient, respectively. Physically motivated by micromechanical observations (see, e. g., Asaro [1983]), the multiplicative decomposition was introduced and developed by a number of authors, among others Eckart [1948], Kröner [1959], Lee [1969], Lee and Liu [1967], Lubarda and Lee [1981] and Mandel [1972]. According to the theory, the existence of a (local) unstressed intermediate configuration defined by $\mathbf{F}_p$ is implicitly assumed. The intermediate configuration is local in

the sense that it belongs to the immediate vicinity of a material point and is obtained from the fully deformed configuration by a purely elastic relaxation (associated with the inverse of $\mathbf{F}_e$) of this vicinity only. In other words, the intermediate configuration concept is valid only in a pointwise sense: compatible unstressed configurations of arbitrary multiaxially loaded elastoplastic bodies do not exist in general.

In addition to the classical multiplicative decomposition of the deformation gradient (3.42), an additional multiplicative split of the plastic part of the deformation gradient into elastic and inelastic parts is assumed in the discussed model, namely

$$\mathbf{F}_p = \mathbf{F}_{pe} \mathbf{F}_{pi} \quad (3.43)$$

The latter split is used in order to model nonlinear kinematic hardening of Armstrong-Frederick type and is physically motivated (see, e. g., Lion [2000]). Analogously to the intermediate plastic configuration resulting from the multiplicative split of the total deformation gradient, decomposition (3.43) introduces the so-called intermediate configuration of kinematic hardening (see Fig. 3.1).

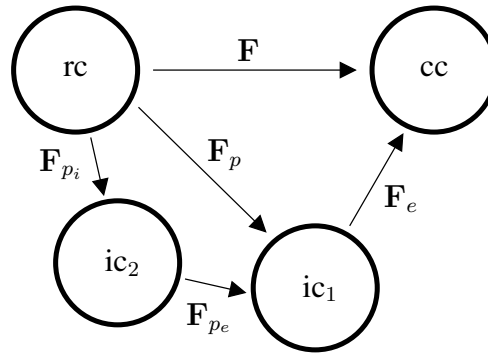


Figure 3.1: Configurations: rc - reference configuration, cc - current configuration, ic₁ - intermediate plastic configuration, ic₂ - intermediate configuration of kinematic hardening

3.4.2 Constitutive relationships and thermodynamical consistency

Hyperelastic-based constitutive models possess an underlying free energy potential. Based on the principle of material objectivity and the concept of material isomorphism, the Helmholtz free energy per unit undeformed volume is assumed to have the form

$$\psi = \psi_e(\mathbf{C}_e) + \psi_{\text{kin}}(\mathbf{C}_{pe}) + \psi_{\text{iso}}(\kappa) \quad (3.44)$$

where $\mathbf{C}_{p_e} = \mathbf{F}_{p_e}^T \mathbf{F}_{p_e} = \mathbf{F}_{p_i}^{-T} \mathbf{C}_p \mathbf{F}_{p_i}^{-1}$ is the elastic part of the plastic right Cauchy-Green tensor. The term ψ_e is related to the stored elastic energy and represents the macroscopic elastic material properties, whereas the other two terms in (3.43) are energies connected to the hardening of the material. More precisely, ψ_{kin} corresponds to the elastic energy stored in dislocation fields due to kinematic hardening and ψ_{iso} is connected to the stored amount of energy due to isotropic hardening. As usual, κ denotes the accumulated plastic strain.

By utilizing the isothermal version of the Clausius-Duhem inequality describing the second law of thermodynamics

$$-\dot{\psi} + \mathbf{S} \cdot \frac{1}{2} \dot{\mathbf{C}} \geq 0 \quad (3.45)$$

and assuming additionally that $\psi_e(\mathbf{C}_e)$ and $\psi_{\text{kin}}(\mathbf{C}_{p_e})$ are isotropic functions of $\mathbf{C}_e$ and $\mathbf{C}_{p_e}$, respectively, the following relation for the second Piola-Kirchhoff stress tensor can be obtained

$$\mathbf{S} = 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-T} \quad (3.46)$$

Furthermore, the plastic flow rule is derived as

$$\mathbf{d}_p = \dot{\gamma} \frac{\partial \Phi}{\partial \mathbf{M}} = \dot{\gamma} \sqrt{\frac{3}{2}} \frac{\mathbf{M}^D - \boldsymbol{\chi}^D}{\|\mathbf{M}^D - \boldsymbol{\chi}^D\|} \quad (3.47)$$

and the evolution equations for kinematic and isotropic hardening are

$$\mathbf{d}_{p_i} = \dot{\gamma} \sqrt{\frac{3}{2}} \frac{b}{c} \mathbf{M}_{\text{kin}}^D, \quad \dot{\kappa} = \dot{\gamma} \quad (3.48)$$

respectively. In the latter expressions, $\mathbf{d}_p$ denotes the symmetric part of the plastic velocity gradient $\mathbf{l}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}$ and, analogously, $\mathbf{d}_{p_i}$ is the symmetric part of $\mathbf{l}_{p_i} := \dot{\mathbf{F}}_{p_i} \mathbf{F}_{p_i}^{-1}$. Once more, a yield function

$$\Phi = \sqrt{\frac{3}{2}} \|\mathbf{M}^D - \boldsymbol{\chi}^D\| - (\sigma_y + R) \quad (3.49)$$

of von Mises type is assumed where R is defined by expression (3.11). The quantities

$$\mathbf{M} = 2 \mathbf{C}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e}, \quad \mathbf{M}_{\text{kin}} = 2 \mathbf{C}_{p_e} \frac{\partial \psi_{\text{kin}}}{\partial \mathbf{C}_{p_e}} \quad (3.50)$$

represent symmetric stress tensors of Mandel-type and

$$\boldsymbol{\chi} = 2 \mathbf{F}_{p_e} \frac{\partial \psi_{\text{kin}}}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_e}^T \quad (3.51)$$

is the back stress in the intermediate configuration. Finally, for a complete description of the model the usual Kuhn-Tucker conditions have to be taken into account.

Although the derivation of the material model is conveniently carried out in the intermediate configuration, the numerical implementation is based on the reference configuration. By a tensorial ‘pull-back’ of the tensors $\mathbf{M}$, $\mathbf{M}_{\text{kin}}$ and χ and by utilization of the relationship $\dot{\mathbf{C}}_p = 2 \mathbf{F}_p^T \mathbf{d}_p \mathbf{F}_p$, an alternative representation of the constitutive model in the reference configuration can be derived. The involved quantities are given below:

- Stress tensors

$$\mathbf{S} = 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-T}, \quad \mathbf{X} = 2 \mathbf{F}_{p_i}^{-1} \frac{\partial \psi_{\text{kin}}}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_i}^{-T}, \quad \mathbf{Y} = \mathbf{C} \mathbf{S} - \mathbf{C}_p \mathbf{X}, \quad \mathbf{Y}_{\text{kin}} = \mathbf{C}_p \mathbf{X}$$

- Evolution equations

$$\dot{\mathbf{C}}_p = 2 \dot{\gamma} \sqrt{\frac{3}{2}} \frac{\mathbf{Y}^D \mathbf{C}_p}{\sqrt{\mathbf{Y}^D \cdot (\mathbf{Y}^D)^T}}, \quad \dot{\mathbf{C}}_{p_i} = 2 \dot{\gamma} \sqrt{\frac{3}{2}} \frac{b}{c} \mathbf{Y}_{\text{kin}}^D \mathbf{C}_{p_i}, \quad \dot{\kappa} = \dot{\gamma}$$

- Yield function

$$\Phi = \sqrt{\frac{3}{2}} \sqrt{\mathbf{Y}^D \cdot (\mathbf{Y}^D)^T} - (\sigma_y + R)$$

- Kuhn-Tucker conditions

$$\Phi \leq 0, \quad \dot{\gamma} \geq 0, \quad \Phi \dot{\gamma} = 0$$

In the latter expressions, $\mathbf{X}$ is the back stress tensor in the reference configuration and $\mathbf{Y}$ and $\mathbf{Y}_{\text{kin}}$ are stress-like quantities which are unsymmetric. The internal variables of the model are $\mathbf{C}_p = \mathbf{F}_p^T \mathbf{F}_p$, $\mathbf{C}_{p_i} = \mathbf{F}_{p_i}^T \mathbf{F}_{p_i}$ and κ which describe the evolution of plastic deformation as well as kinematic and isotropic hardening, respectively.

It should be noted that the expressions for the stresses are dependent on the particular form of the Helmholtz free energy which has not been specified yet. In the numerical examples to be discussed later, the following energies belonging to a Neo-Hookean material with nonlinear isotropic hardening of Voce type (Voce [1955]) and nonlinear kinematic hardening of

Armstrong-Frederick type (Armstrong and Frederick [1966]) will be used:

$$\psi_e = \frac{\mu}{2} (\text{tr } \mathbf{C}_e - 3) - \mu \ln \left(\sqrt{\det \mathbf{C}_e} \right) + \frac{\lambda}{4} \left(\det \mathbf{C}_e - 1 - 2 \ln \left(\sqrt{\det \mathbf{C}_e} \right) \right) \quad (3.52)$$

$$\psi_{\text{kin}} = \frac{c}{4} (\text{tr } \mathbf{C}_{pe} - 3) - \frac{c}{2} \ln \left(\sqrt{\det \mathbf{C}_{pe}} \right) \quad (3.53)$$

$$\psi_{\text{iso}} = Q \left(\kappa + \frac{e^{-\beta \kappa}}{\beta} \right) \quad (3.54)$$

Having defined the latter expressions, the constitutive relations for the second Piola-Kirchhoff stress $\mathbf{S}$ and the back stress $\mathbf{X}$ finally read:

$$\mathbf{S} = \mu (\mathbf{C}_p^{-1} - \mathbf{C}^{-1}) + \frac{\lambda}{2} (\det \mathbf{C} (\det \mathbf{C}_p)^{-1} - 1) \mathbf{C}^{-1} \quad (3.55)$$

$$\mathbf{X} = \frac{c}{2} (\mathbf{C}_{pi}^{-1} - \mathbf{C}_p^{-1}) \quad (3.56)$$

Remark 1. The question may arise as to the specific relationship between the kinematic hardening formulation of the hypoelastic-based model described in Sect. 3.3 and the just-presented hyperelastic-based model. This problem was investigated thoroughly by Dettmer and Reese [2004]. The authors argued that both formulations represent finite strain extensions of the classical Armstrong-Frederick model for kinematic hardening, however, their theoretical concepts deviate noticeably from each other. Whereas the kinematic hardening formulation of the hypoelastic-based model is considered as a so-called ‘Chaboche-type’ model which can be derived by means of a dissipation potential and which uses the back stress as internal variable, the counterpart of the hyperelastic-based model is a continuum mechanical extension of the classical rheological model based on strain-like internal variables. Several structural examples were discussed in the latter reference. Despite the remarkable theoretical differences, both formulations led - even in the case of large deformations - to similar numerical results which were surprisingly close to the ones of the corresponding small strain model by Armstrong and Frederick [1966].

3.4.3 Algorithmic implementation

In the work by Vladimirov et al. [2008], the algorithmic implementation of the above described hyperelastic-based plasticity model was discussed in detail. Two modified backward Euler schemes which preserve plastic incompressibility were compared to a type of the exponential map algorithm which preserves plastic volume and the symmetry of the internal variables.

The latter integration algorithm exploits the spectral decomposition to evaluate the existing tensor-valued exponential functions in closed-form. It was shown that the integration scheme based on this exponential map leads to improved results in terms of accuracy, performance and robustness for increasing step sizes. A short summary of the exponential map implementation will be presented next³.

The starting point for the developments is that the plastic flow rule given above is rewritten as

$$\dot{\mathbf{C}}_p = \dot{\gamma} \mathbf{f}(\mathbf{C}, \mathbf{C}_p, \mathbf{C}_{p_i}) = \dot{\gamma} \mathbf{g}(\mathbf{C}, \mathbf{C}_p, \mathbf{C}_{p_i}) \mathbf{C}_p \quad (3.57)$$

in which $\mathbf{f}$ is a second-order tensor defined by

$$\mathbf{f} := 2 \sqrt{\frac{3}{2}} \frac{\mathbf{Y}^D \mathbf{C}_p}{\sqrt{\mathbf{Y}^D \cdot (\mathbf{Y}^D)^T}} \quad (3.58)$$

and $\mathbf{g} = \mathbf{f} \mathbf{C}_p^{-1}$ holds. The tensor-valued function $\mathbf{f}$ is a symmetric quantity, since $\dot{\mathbf{C}}_p$ is also symmetric. However, the same is not true for $\mathbf{g}$, i. e., $\mathbf{g} \neq \mathbf{g}^T$. Therefore, utilizing the implicit exponential map algorithm

$$\mathbf{C}_p = \exp(\Delta\gamma \mathbf{g}) \mathbf{C}_{p_n} \quad (3.59)$$

to solve (3.57) numerically would demand the use of a truncated series representation of the exponential term since no closed-form expression is available in this case.

In order to avoid this, Reese and Christ [2008] and Vladimirov et al. [2008] proposed a modification of the integration scheme given in (3.59). Their considerations were inspired by a methodology originally developed by Dettmer and Reese [2004]. For using this approach, the latter equation must first be multiplied from the right by $\mathbf{C}_{p_n}^{-1} \mathbf{C}_p$ which leads to

$$\mathbf{C}_p \mathbf{C}_{p_n}^{-1} \mathbf{C}_p = \exp(\Delta\gamma \mathbf{g}) \mathbf{C}_p \quad (3.60)$$

Then, by exploiting the series representation and having in mind that the plastic right stretch tensor $\mathbf{U}_p = \sqrt{\mathbf{C}_p}$ as well as its inverse are symmetric tensors, the following expression can

³In what follows, any quantity is referred to the current time step $n+1$, if not explicitly denoted otherwise.

be derived

$$\begin{aligned}
\exp(\Delta\gamma \mathbf{g}) &= \mathbf{I} + \Delta\gamma \mathbf{g} + \frac{(\Delta\gamma)^2}{2} \mathbf{g}^2 + \dots \\
&= \mathbf{I} + \Delta\gamma \mathbf{f} \mathbf{C}_p^{-1} + \frac{(\Delta\gamma)^2}{2} (\mathbf{f} \mathbf{C}_p^{-1})^2 + \dots \\
&= \mathbf{U}_p \left(\mathbf{I} + \Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} + \frac{(\Delta\gamma)^2}{2} (\mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1})^2 + \dots \right) \mathbf{U}_p^{-1} \\
&= \mathbf{U}_p \exp(\Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1}
\end{aligned} \tag{3.61}$$

Since the product $\mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}$ represents a symmetric tensor, the exponential term can be evaluated in closed-form by means of the spectral decomposition. Therefore, by replacing $\exp(\Delta\gamma \mathbf{g})$ in (3.60) with the expression $\mathbf{U}_p \exp(\Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1}$, the final form of the update formula for the plastic flow is obtained⁴:

$$\mathbf{C}_p \mathbf{C}_{p_n}^{-1} \mathbf{C}_p = \mathbf{U}_p \exp(\Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p \Rightarrow \mathbf{C}_{p_n}^{-1} = \mathbf{U}_p^{-1} \exp(\Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1} \tag{3.62}$$

Proceeding in an analogous manner for the evolution equation of kinematic hardening, the corresponding algorithmic expression reads

$$\mathbf{C}_{p_i n}^{-1} = \mathbf{U}_{p_i}^{-1} \exp(\Delta\gamma \mathbf{U}_{p_i}^{-1} \mathbf{f}_{\text{kin}} \mathbf{U}_{p_i}^{-1}) \mathbf{U}_{p_i}^{-1} \tag{3.63}$$

where $\mathbf{f}_{\text{kin}} := 2\sqrt{\frac{3}{2}} \frac{b}{c} \mathbf{Y}_{\text{kin}}^D \mathbf{C}_{p_i}$ holds. The evolution equation of isotropic hardening (3.48) is discretized by means of the classical backward Euler integration algorithm

$$\kappa = \kappa_n + \Delta\gamma \tag{3.64}$$

In summary, the discretized evolution equations together with the requirement that the yield function must be zero (plastic step) are given below in a residuum format⁵:

$$\begin{aligned}
\mathbf{r}_1 &= -\mathbf{C}_{p_n}^{-1} + \mathbf{U}_p^{-1} \exp(\Delta\gamma \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1} = \mathbf{0} \\
\mathbf{r}_2 &= -\mathbf{C}_{p_i n}^{-1} + \mathbf{U}_{p_i}^{-1} \exp(\Delta\gamma \mathbf{U}_{p_i}^{-1} \mathbf{f}_{\text{kin}} \mathbf{U}_{p_i}^{-1}) \mathbf{U}_{p_i}^{-1} = \mathbf{0} \\
r_3 &= \Phi = 0
\end{aligned} \tag{3.65}$$

⁴Using a similar approach, Arghavani et al. [2010, 2011] proposed an alternative update formula for the plastic flow based on a logarithmic mapping.

⁵The discretized scalar evolution equation for isotropic hardening is not included in the equation system to be solved, since κ can be eliminated as an unknown and needs to be updated only when the local iteration has converged (see also the last paragraph of Sect. 3.3.5.3).

The symmetry of the internal variables leads to a resulting system of 13 nonlinear scalar equations for 13 unknowns. Typically, by using Newton's method a local iteration is performed in every time step until the root-mean-square value of the total residuum falls below a certain prescribed tolerance. The update variables during the iteration are $\mathbf{U}_p^{-1}$, $\mathbf{U}_{p_i}^{-1}$ and $\Delta\gamma$.

Remark 2. It is possible to incorporate the discussed model into a reduced integration eight-node solid-shell finite element formulation which can successfully be applied, e. g., in metal forming simulations (see Schwarze et al. [2011] and Vladimirov et al. [2011]). Furthermore, there exist also four-node shell element formulations which are applicable to general three-dimensional (3-D) thick and thin shell structures and make use of the multiplicative split of the deformation gradient (3.42) in order to model finite elastoplasticity (see, e. g., Eberlein and Wriggers [1999]).

3.5 Numerical examples

3.5.1 Adjustment of material parameters

Before the numerical calculations could be performed, it was necessary to ensure that the various material parameters of the hypoelastic- and hyperelastic-based model were compatible to each other. By inspecting the various equations of the models, a simple one-to-one correspondence between them could be revealed which was used throughout all computations.

For a numerical validation, a cyclic simple shear test of a single C3D8R finite element with unit dimensions, reduced integration and hourglass stabilization was performed in ABAQUS / Standard (see Fig. 3.2a) using both models and considering the aforementioned relationship between the parameters which were chosen as: $\mu = 72509.4$ [MPa], $\lambda = 140753.5$ [MPa], $\sigma_y = 325$ [MPa], $b = 25$ [-], $c = 5200$ [MPa], $\beta = 8$ [-] and $Q = 215$ [MPa]. Although it was expected that the behavior of the models could be brought into agreement for small strains (since they are theoretically identical in the small strain limit), it is interesting to note that they behave almost equally in this case also for finite strains. Indeed, the corresponding shear stress-strain plot shown in Fig. 3.2b confirms the relationship between the parameters, the curves are practically identical. However, such a good agreement cannot be expected in general for more complex situations.

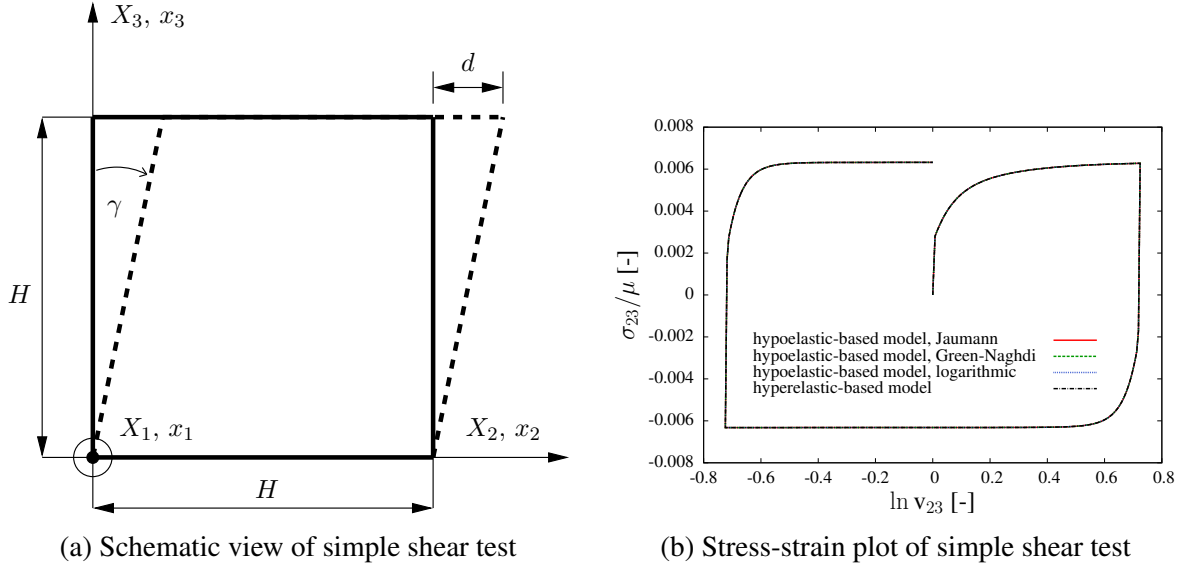


Figure 3.2: Parameter adjustment

3.5.2 Comparison of objective rates in hypoelastic-based models

In a first example, the influence of different objective rates in the hypoelastic-based constitutive model was investigated. Meyers et al. [2003] studied the influence of three corotational rates, namely the Jaumann, Green-Naghdi and logarithmic rate, on the elastic stress ratcheting response of a purely hypoelastic model (which is obtained from the model reviewed in Sect. 3.3 by neglecting plastic deformations, i. e., by setting $\mathbf{d}_p = \mathbf{0}$). For this, they used a strain cycle characterized by a single parameter φ . In this work, the very same problem was considered by subjecting a single C3D8R finite element with unit dimensions in ABAQUS / Standard to this circular closed-path deformation cycle. The algorithmic implementation was realized according to the objective integration scheme discussed in Sect. 3.3.5 for the purely hypoelastic case and by using the UMAT interface. The nodal displacements were prescribed by using the DISP user subroutine in ABAQUS / Standard. For the sake of completeness, also the behavior of a pure Neo-Hookean hyperelastic model was investigated which was used in Sect. 3.4 for the elastic response of the hyperelastic-based plasticity model. The material parameters were chosen as $\mu = 80000$ [MPa] and $\lambda = 119999.67$ [MPa].

The side view of a square element of edge length H within ABAQUS which is embedded in the Cartesian reference system X_i ($i = 1, 2, 3$) is schematically shown in Fig. 3.3. A strain cycle was imposed in which the four upper nodes were rotated along a circle of radius r , the four lower nodes were held fixed. Accordingly, the element was subjected to a combined lengthening in X_3 -direction and shear deformation, it always remained in a parallelogram

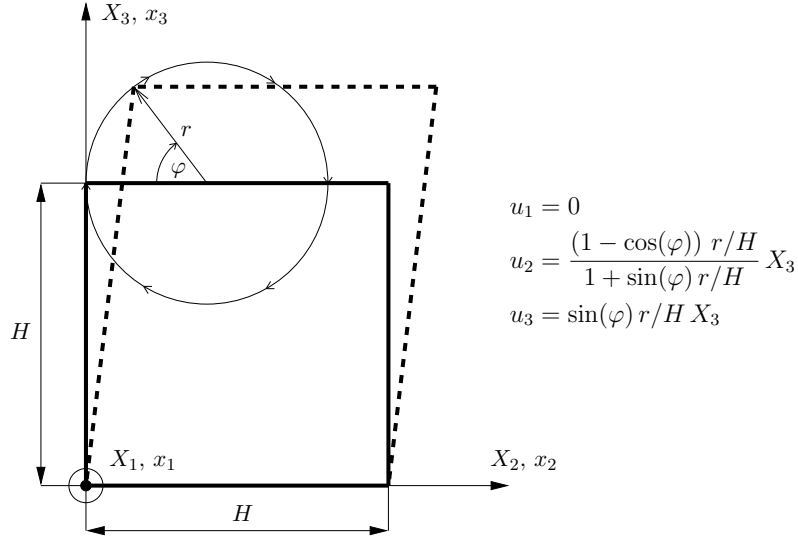
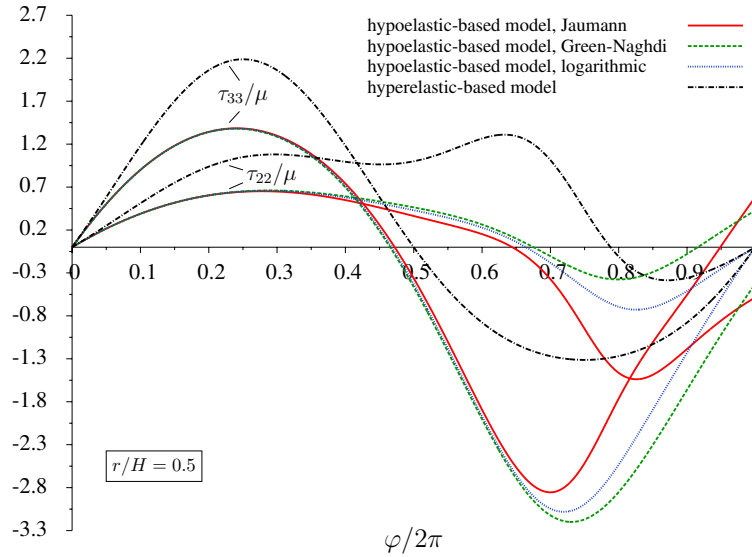


Figure 3.3: Schematic view of circular closed-path deformation

shape. Zero deformations were imposed in X_1 -direction. The corresponding displacements of the nodes are given in Fig. 3.3 and were calculated from the current positions given in Meyers et al. [2003] by the well-known formula $\mathbf{u} = \mathbf{x} - \mathbf{X}$. To allow for comparisons with the results given in the latter reference, a ratio of $r/H = 0.5$ was selected for the cyclic closed-path loading, i. e., relatively large elastic deformations were considered.

Fig. 3.4 shows the plots of the normal stresses τ_{22} and τ_{33} in a single cycle for both models and by using different corotational rates in the hypoelastic formulation. Since the results for

Figure 3.4: Circular deformation: Single cycle, normal stresses τ_{22} and τ_{33}

the stress component τ_{11} are almost equivalent to τ_{22} , they were not included in the graph. Remarkable differences can be observed for the respective corotational rates. Spurious residual stresses are detected already after a single cycle using either the Jaumann or Green-Naghdi rate in the hypoelastic formulation. Regarding the shear stress component τ_{23} , the situation is similar (see Fig. 3.5). Only by using the logarithmic rate and in the case of the hyperelastic

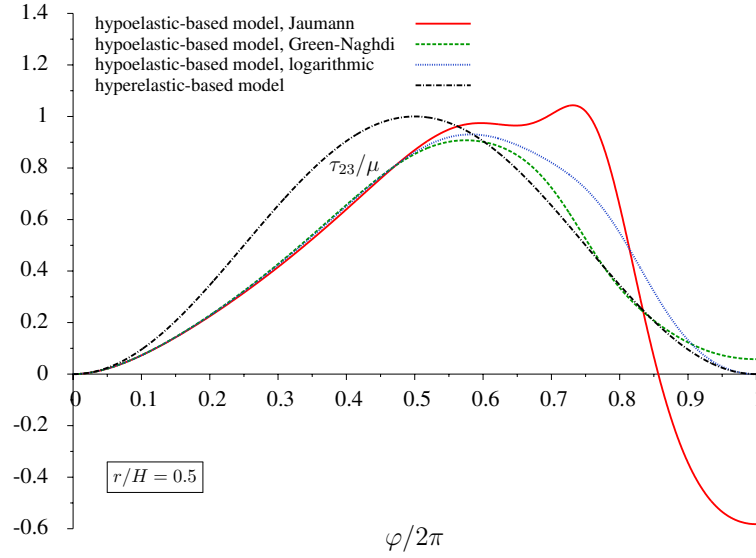


Figure 3.5: Circular deformation: Single cycle, shear stress τ_{23}

model, all stress components return back to zero. It should be noted that the differences between the hypoelastic and hyperelastic model are not surprising, they arise due to the different description of the elastic behavior and become clearly visible for large deformations.

Three major ‘zones’ may be detected and distinguished in Figs. 3.4 and 3.5. In accordance with the theory, for sufficiently small values of $\varphi/2\pi$ up to 0.05, all models behave essentially the same. This is the maximum order of magnitude reached by elastic strains in usual metal forming applications. For larger values of $\varphi/2\pi$ up to approximately 0.25, the results of all hypoelastic models are still virtually identical to each other, whereas they are different from the ones predicted by the hyperelastic model. Finally, if the elastic strains are even larger, the specific properties of the respective corotational rates come into effect and the limitations of ‘classical’ hypoelastic models based on the Jaumann or Green-Naghdi rate become readily apparent. In other words, the merit of the self-consistent Eulerian model based on the logarithmic rate or the hyperelastic model can be observed.

Fig. 3.6 shows the development of the Kirchhoff stress components for ten consecutive cycles using the logarithmic rate in the hypoelastic model. The stresses return to zero after each single cycle which is physically meaningful. No residual stresses remain.

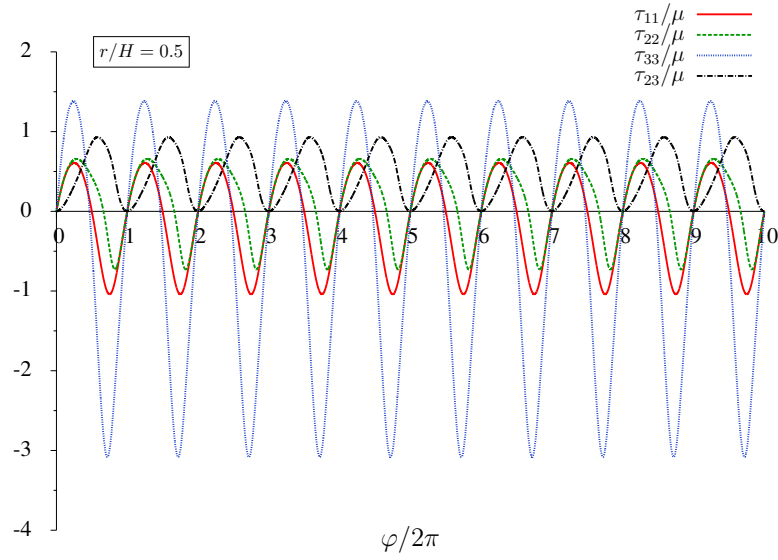


Figure 3.6: Circular deformation: Ten cycles, hypoelastic model using logarithmic rate

However, the situation changes for the other two rates. The results using the Green-Naghdi rate in the hypoelastic formulation are reported in Fig. 3.7. Except for the normal stress τ_{11} ,

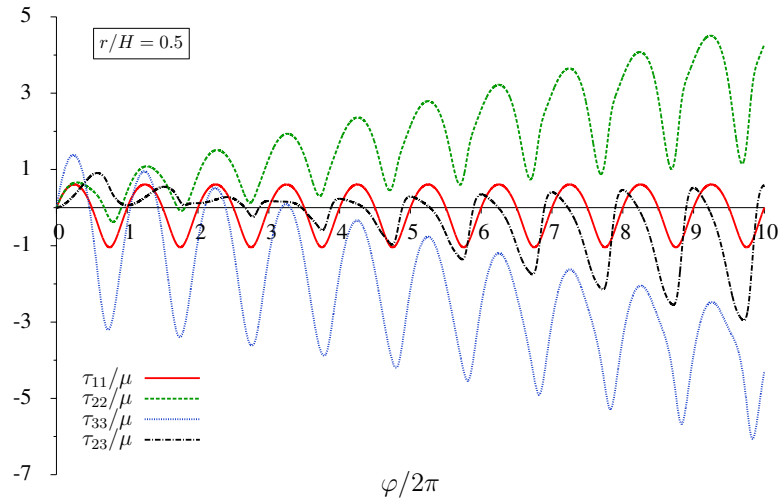


Figure 3.7: Circular deformation: Ten cycles, hypoelastic model using Green-Naghdi rate

all stresses start to drift away over the cycles and, moreover, change their magnitudes. In other words, considerable elastic stress ratcheting occurs. In case of the Jaumann rate, the development of the Kirchhoff stresses shows a rather physically implausible behavior after a few cycles (Fig. 3.8). The drift of the stress components τ_{22} , τ_{33} is oscillatory and the results for τ_{23} seem somewhat unpredictable. In both cases, undesirable residual stresses are present

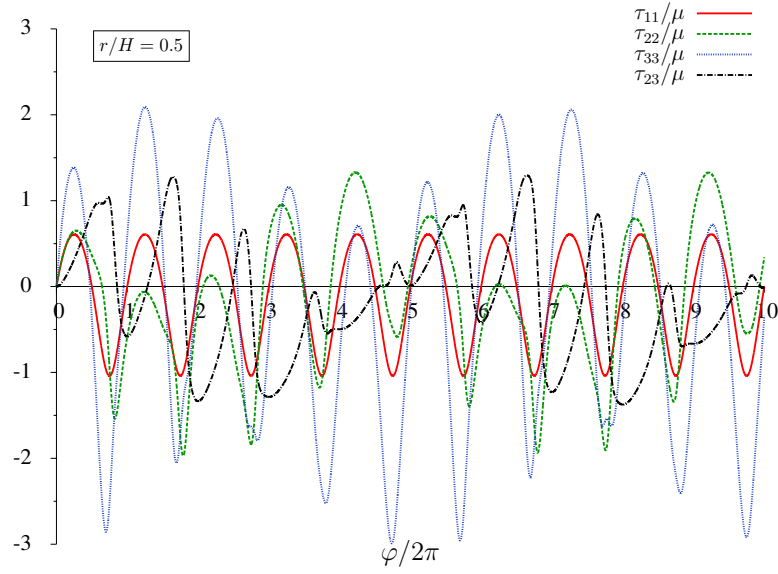


Figure 3.8: Circular deformation: Ten cycles, hypoelastic model using Jaumann rate

at the end of ten cycles.

The hyperelastic model produces equally good results as the hypoelastic model using the logarithmic rate (Fig. 3.9), no spurious residual stresses are observable at the end of any cycle. The results differ from each other in magnitude, for the same reasons as explained above.

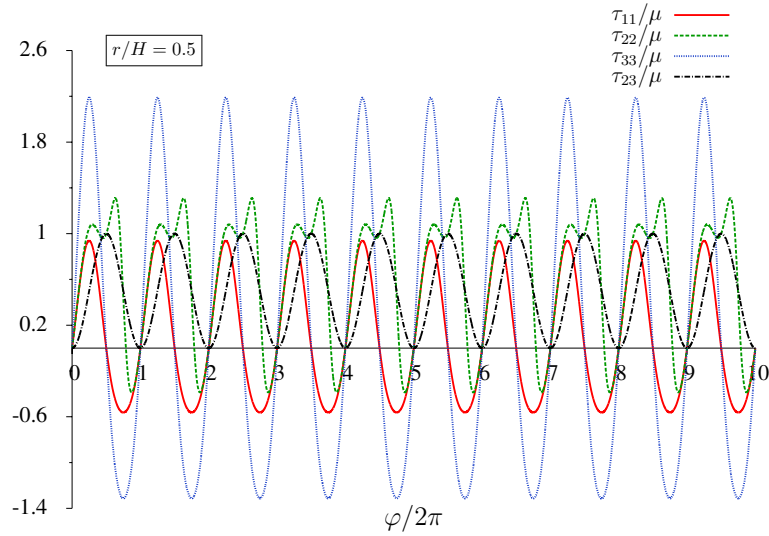


Figure 3.9: Circular deformation: Ten cycles, hyperelastic model

It should be remarked that the results for the hypoelastic model in the above example are in excellent agreement with those found by Meyers et al. [2003], although the latter authors did not mention what kind of integration algorithm or software they used to compute the results.

This gives a good indication that the self-implemented hypoelastic-based model indeed works properly as a UMAT subroutine within ABAQUS / Standard.

3.5.3 Comparison of incrementally objective algorithms for hypoelastic-based models

In Sect. 3.3.5 it was mentioned that the use of incrementally objective algorithms is necessary for the implementation of hypoelastic-based models. To confirm this also practically, the objectivity properties of the Hughes-Winget algorithm (Hughes and Winget [1980]) and the algorithm discussed in Sect. 3.3.5 were examined in this work by considering a specific test problem which was (in a slightly modified form) originally given by Seifert and Maier [2008]. In this test problem, a unit cube of 125 C3D8R elements (length x thickness x width = 5 x 5 x 5) in ABAQUS / Standard was subjected to two different prescribed motions by using the DISP subroutine. In both cases, a purely hypoelastic constitutive model for the Cauchy stress based on the Jaumann rate (i. e., $\overset{\circ}{\boldsymbol{\sigma}} = \mathcal{C}[\mathbf{d}]$) was taken into consideration with the material parameters specified as $\mu = 80000$ [MPa] and $\lambda = 119999.67$ [MPa]. Two different, self-implemented UMAT subroutines of the latter model were applied in the simulations either based upon the Hughes-Winget or the algorithm discussed in Sect. 3.3.5. For the sake of completeness, the same computations were carried out using an algorithmic implementation of a Neo-Hookean model which serves as the elastic foundation in the hyperelastic-based plasticity model reviewed in Sect. 3.4.

Case 1: deformation followed by pure rotation

The cube was deformed in a first step ($0 \leq t \leq 1$) in a pure shear-like manner such that the principal axes of stress and strain did not rotate and transversal contraction was prevented. Afterwards, in a second step ($1 < t \leq 2$) the cube was exposed to a rotation of 360° about its origin. In a continuum mechanics notation, the above described motion may be stated as:

- Step 1 (Deformation) $0 \leq t \leq 1$:

$$\mathbf{x} = \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} X_1 \\ X_2 + \dot{\gamma} X_3 \\ X_3 + \dot{\gamma} X_2 \end{Bmatrix} \quad (3.66)$$

- Step 2 (Pure rotation) $1 < t \leq 2$:

$$\mathbf{x} = \mathbf{Q}(t) \mathbf{x}|_{t=1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\dot{\theta}t) & -\sin(\dot{\theta}t) \\ 0 & \sin(\dot{\theta}t) & \cos(\dot{\theta}t) \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} \bigg|_{t=1} \quad (3.67)$$

Here, $\{X_i\}_{i=1,2,3}$ and $\{x_i\}_{i=1,2,3}$ denote the reference and current coordinates of the nodes, respectively. The corresponding displacements of the nodes were obtained by $\mathbf{u} = \mathbf{x} - \mathbf{X}$. The shear rate $\dot{\gamma}$ and the angular velocity $\dot{\theta}$ were specified as $\dot{\gamma} = 0.2$ [1/s] and $\dot{\theta} = 1.0$ [rad/s]. For illustration, the undeformed and the deformed cube (after a complete rotation) are shown in Fig. 3.10. All numerical results described in the following were obtained by using a constant step size $\Delta t = 0.1$ [s] in the calculations.

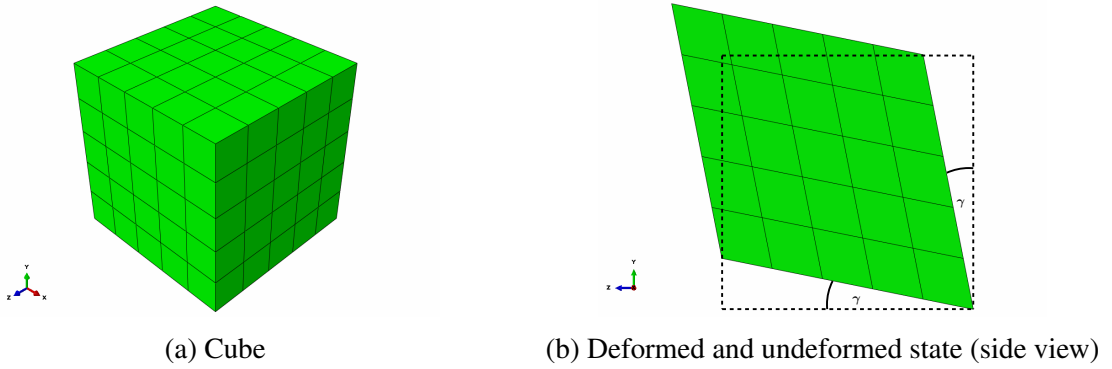


Figure 3.10: Deformation of cube

In Fig. 3.11 the results of this investigation are plotted for the hypoelastic model by using either an algorithmic implementation according to the one discussed in Sect. 3.3.5 or according to Hughes and Winget [1980]. Displayed are the components of the rotated Cauchy stress $\bar{\sigma} = \mathbf{Q}^T \boldsymbol{\sigma} \mathbf{Q}$ over the (pseudo-)time t at the integration point at the center of the cube. This is exactly the Cauchy stress perceived by an observer who rotates along with the cube. From fundamental physical considerations it seems clear that this stress should not change when the cube is only rotated and not deformed in the second step ($t > 1$). As a ‘reference’ solution to the problem, also the results are plotted which were calculated for the case of a vanishing rotation of the cube, i. e., $\dot{\theta} = 0$. It can be seen that both the Hughes-Winget algorithm and the algorithm shown in Sect. 3.3.5 deliver very good results in this case which match the reference solution (since the results are almost the same for both algorithms, they are only plotted once).

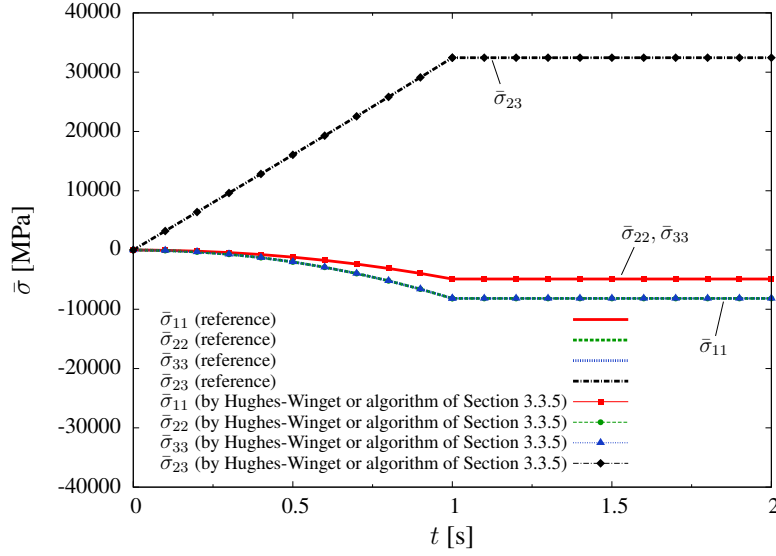


Figure 3.11: Case 1, hypoelastic model with Hughes-Winget or algorithm of Sect. 3.3.5

Only for illustration, it is also shown in Fig. 3.12 what happens if the issue of objectivity were not considered at all in the constitutive formulation and algorithm, i. e., if a model $\dot{\sigma} = \mathcal{C}[d]$ and a trivial incrementally non-objective algorithm were used instead. It can be seen that the stress components of $\bar{\sigma}$ are not constant for a pure rotation in this case. On the contrary, they vary in an oscillatory manner which is not physically meaningful.

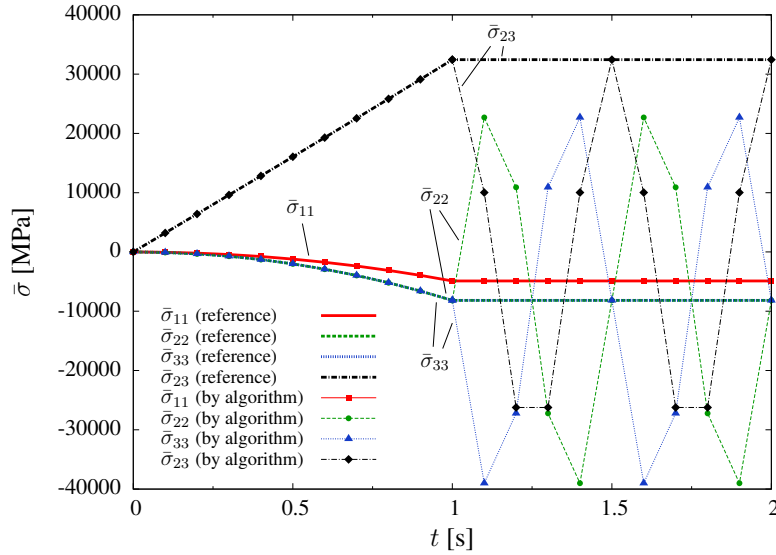


Figure 3.12: Case 1, model $\dot{\sigma} = \mathcal{C}[d]$ with incrementally non-objective algorithm

Fig. 3.13 shows the results for the algorithmically implemented Neo-Hookean hyperelastic model. The results are in perfect agreement with the reference solution which is obvious

since the objectivity is fulfilled on fundamental grounds by the formulation and the issue of incremental objectivity does not play any role. It may be worthwhile to note that, in contrast to the hypoelastic model, the Neo-Hookean hyperelastic model predicts a transversal stress σ_{11} which is larger in absolute value than σ_{22} and σ_{33} in this case.

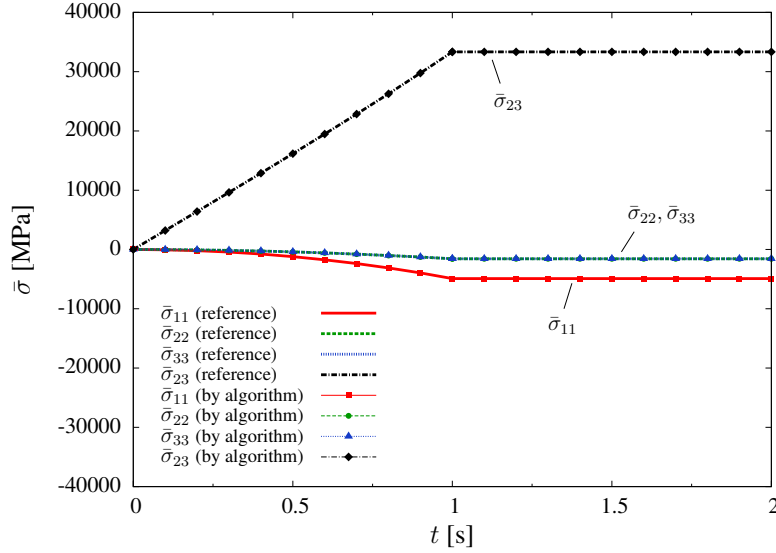


Figure 3.13: Case 1, hyperelastic model with corresponding algorithm

Case 2: deformation with superposed rotation

In the second example, both the deformation and rotation of the cube were superposed such that they took place simultaneously. The description of the motion is accordingly given by:

- Step (Deformation with superposed rotation) $0 \leq t \leq 1$:

$$\mathbf{x} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\dot{\theta}t) & -\sin(\dot{\theta}t) \\ 0 & \sin(\dot{\theta}t) & \cos(\dot{\theta}t) \end{bmatrix} \begin{Bmatrix} X_1 \\ X_2 + \dot{\gamma} X_3 \\ X_3 + \dot{\gamma} X_2 \end{Bmatrix} \quad (3.68)$$

Again, the shear rate and angular velocity were specified as $\dot{\gamma} = 0.2$ [1/s] and $\dot{\theta} = 1.0$ [rad/s], respectively, and a constant step size $\Delta t = 0.1$ [s] was used for the computations.

Figs. 3.14 - 3.16 illustrate the results obtained in the second example. The components of the rotated Cauchy stress $\bar{\sigma}$ are plotted over the (pseudo-)time t . Figs. 3.14 and 3.15 display the results of the hypoelastic model either implemented by using the procedure proposed by Hughes and Winget [1980] or according to the algorithm reviewed in Sect. 3.3.5. As before,

also the solutions which were calculated for the case of a vanishing rotation of the cube are illustrated as reference.

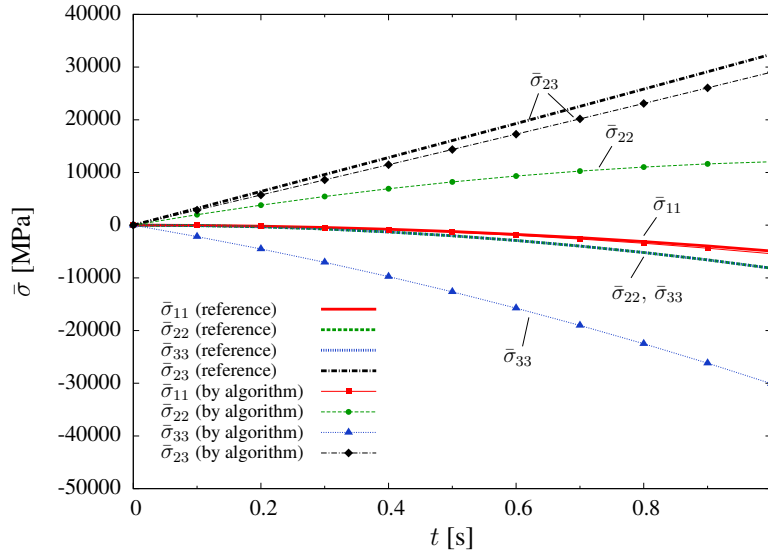


Figure 3.14: Case 2, hypoelastic model with Hughes-Winget algorithm

This time, remarkable differences between the predictions of both algorithms can be recognized. The Hughes-Winget algorithm behaves here worse than the algorithm discussed in Sect. 3.3.5 which may be explained by the fact that the former can be viewed as a simplified special case of the latter. Nevertheless, neither of the two algorithms delivers results which match the reference solutions. In contrast to this, the results of the algorithmic hyperelastic model (see Fig. 3.16) are very good, the reference solutions are matched perfectly. The reasons for this were explained already above.

Summarizing the results of both examples, it can be concluded that neither the Hughes-Winget nor the algorithm discussed in Sect. 3.3.5 do necessarily preserve the (incremental) objectivity of a hypoelastic-based model in a full sense for every kind of motion. This observation is in agreement with results found in the literature. It seems that Rashid [1993] was the first who distinguished between ‘weakly’ and ‘strongly’ objective algorithms. A weakly objective algorithm predicts exact solutions in cases of special input motions (such as pure stretch or pure rotation) but only approximative solutions in cases of more general motions. On the contrary, a strongly objective algorithm is also objective for superposed motions of both stretching and rotation. In this sense, the Hughes-Winget algorithm as well as the algorithm reviewed in Sect. 3.3.5 are only weakly objective. However, as mentioned also in the latter reference, the lack of strong objectivity becomes decreasingly influential when both the rotation and stretching parts of the deformation increments become smaller. This was verified

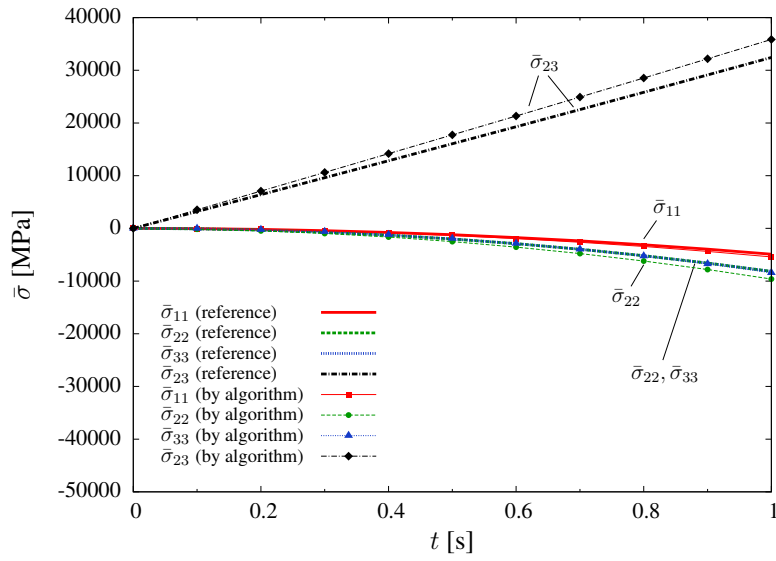


Figure 3.15: Case 2, hypoelastic model with algorithm according to Sect. 3.3.5

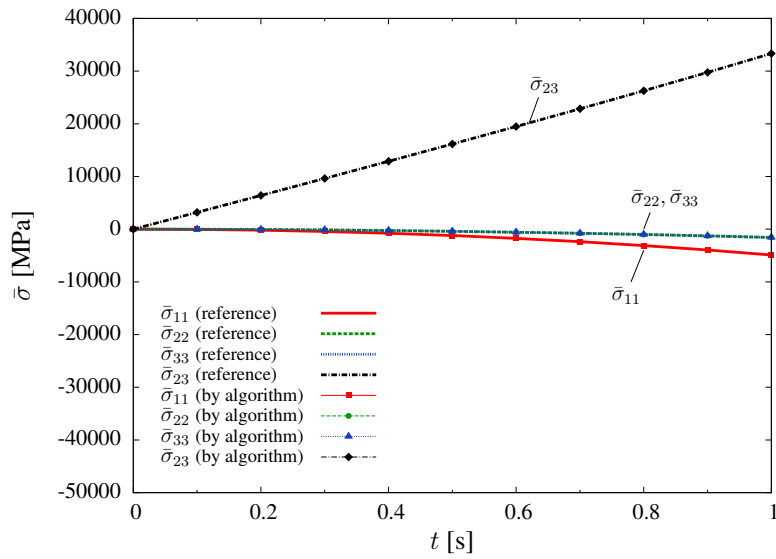


Figure 3.16: Case 2, hyperelastic model with corresponding algorithm

numerically in this study by decreasing the step size Δt in the calculations (results are not shown for brevity). In this case, the results predicted by the Hughes-Winget algorithm and the algorithm described in Sect. 3.3.5 converge gradually towards the reference solutions. This feature is especially important for many finite element applications, as, e. g., common metal forming simulations in which step sizes are usually small.

3.5.4 Comparison of ABAQUS / Standard built-in elastoplastic model with self-implemented hypoelastic-based plasticity model

In Sect. 3.3.6 it was discussed how usual built-in material models in ABAQUS / Standard (e. g., for standard J_2 metal elastoplasticity) behave if geometric nonlinearities are taken into account. It was mentioned that they rely upon a hypoelastic-based formulation in terms of the Cauchy stress and the Jaumann rate (see expression (3.39)) and that the numerical implementation is realized according to the objective integration algorithm proposed by Hughes and Winget [1980]. However, it seems worthwhile to have a practical confirmation of this statement.

Therefore, a simple but instructive example problem was considered in this work. More precisely, a large strain simple shear test (shown schematically in Fig. 3.2a) of a single C3D8R finite element with unit dimensions was performed within ABAQUS / Standard by using both the ABAQUS built-in elastoplastic model for large strains and a self-implemented hypoelastic-plastic model based on the Jaumann rate of the Cauchy stress. The latter model was implemented into two different UMAT subroutines by using either the algorithm according to Hughes and Winget [1980] or the algorithm discussed in Sect. 3.3.5. A material with linear kinematic hardening was assumed, the corresponding material parameters were specified as $\mu = 80000$ [MPa], $\lambda = 119999.67$ [MPa], $\sigma_y = 300$ [MPa], $b = 0$ [-], $c = 2000$ [MPa], $\beta = 0$ [-] and $Q = 0$ [MPa].

Fig. 3.17 shows the obtained results up to very large shear deformations $d = 20$ [mm] with both pretty small ($\Delta d = 0.002$ [mm]) and pretty large deformation increments ($\Delta d = 2$ [mm]) for the respective models and implementations. In accordance with the theory, the large shear deformations lead to the well-known oscillatory stress behavior which is typical for hypoelastic-based models of grade zero using the Jaumann rate (see, e. g., Dienes [1979]) and linear kinematic hardening (see, e. g., Lehmann [1972], Nagtegaal and De Jong [1982]). In the case of very small increments, the results of the ABAQUS built-in model and the implemented hypoelastic-based model look virtually the same, irrespective of the specific algorithm used to numerically integrate the model (smooth curves lying on top of each other). On the one hand, this practically confirms that ABAQUS / Standard indeed relies upon the hypoelastic-

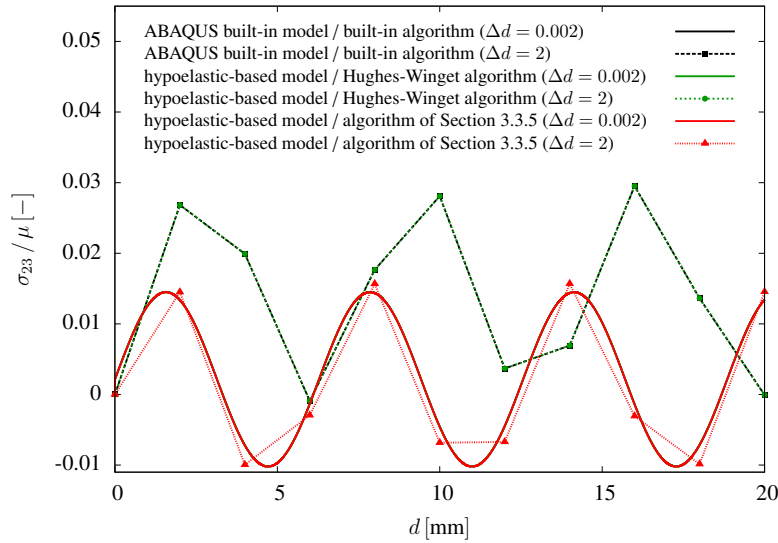


Figure 3.17: Results for large strain simple shear test

based model described above if geometric nonlinearities are taken into account. On the other hand, it demonstrates that the algorithm by Hughes and Winget [1980] and the one discussed in Sect. 3.3.5 merge into each other for sufficiently small increments.

For large increments, a direct comparison between the curves in Fig. 3.17 and the data of the results (see Table 3.1) reveals that the ABAQUS built-in model again behaves virtually the same as the self-implemented model based on the integration scheme by Hughes and Winget [1980], at least to the maximum accuracy that ABAQUS provides for the user (8 significant digits). It is, however, different from the solution predicted by the model based on

	$\sigma_{23} / \mu [-]$		
d [mm]	ABAQUS	Hughes-Winget algorithm	algorithm of Sect. 3.3.5
0	0.00000000E+00	0.00000000E+00	0.00000000E+00
2	2.68296935E-02	2.68296935E-02	1.44961439E-02
4	1.99161097E-02	1.99161097E-02	-9.94988717E-03
6	-9.03642154E-04	-9.03642154E-04	-2.94588157E-03
8	1.76689997E-02	1.76689997E-02	1.56689882E-02
10	2.80880723E-02	2.80880723E-02	-6.82805479E-03
12	3.68075026E-03	3.68075026E-03	-6.71877805E-03
14	6.92977756E-03	6.92977756E-03	1.56873148E-02
16	2.95176450E-02	2.95176450E-02	-3.07041104E-03
18	1.36194117E-02	1.36194117E-02	-9.86456778E-03
20	-6.54450487E-05	-6.54450487E-05	1.45478928E-02

Table 3.1: Large strain simple shear test, comparison of data ($\Delta d = 2$ [mm])

the algorithm discussed in Sect. 3.3.5. Additionally, it can be realized that the latter algorithm delivers more accurate results than the former one, since the predicted solution is clearly closer to the ‘reference’ curve found by using very small deformation increments. An explanation for this might be that the Hughes-Winget algorithm can be seen as a simplified special case of the algorithm discussed in Sect. 3.3.5.

It should be noted that, only if all requirements for the classical Hughes-Winget algorithm are met, such a good correlation between the ABAQUS built-in and the self-implemented model can be achieved. The degree of agreement is yet quite surprising and explains the assertions given in Sect. 3.3.6.

3.5.5 Comparison of hypo- and hyperelastic-based plasticity models with application to industrial forming processes

3.5.5.1 Elliptical closed-path deformation of a single element

A single C3D8R finite element in ABAQUS / Standard with unit dimensions was subjected to a repeated elliptical closed-path deformation in which the displacements of the nodes were prescribed as shown in Fig. 3.18. In a first instance, the material response was assumed to be

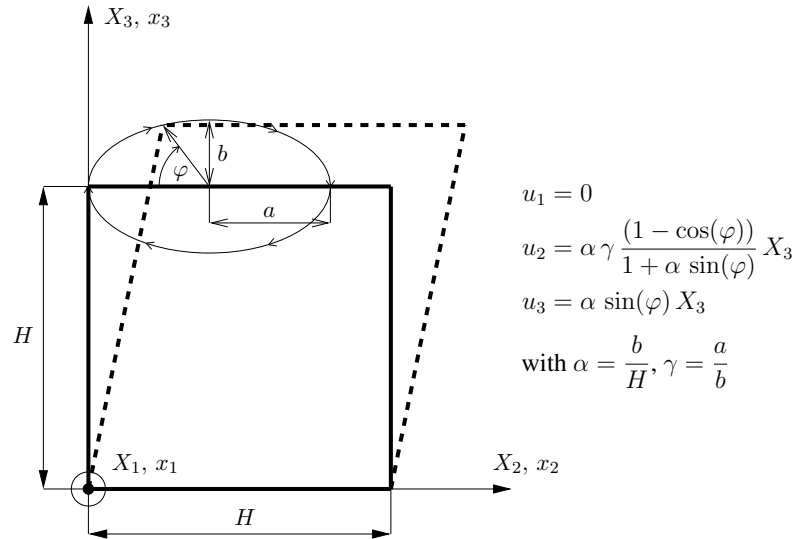


Figure 3.18: Schematic view of elliptical closed-path deformation

hypoelastic-plastic according to the model discussed in Sect. 3.3 based on the Kirchhoff stress. Either the Jaumann, Green-Naghdi or logarithmic rate were utilized in the formulation and the algorithmic implementation into a UMAT subroutine was realized by applying the algorithm described in Sect. 3.3.5. In a second instance, a hyperelastic-plastic material model according

to Sect. 3.4 was considered and implemented using the algorithm shown in Sect. 3.4.3. The material parameters were specified as: $\mu = 80000$ [MPa], $\lambda = 119999.67$ [MPa], $\sigma_y = 800$ [MPa], $b = 0$ [-], $c = 20000$ [MPa], $\beta = 0$ [-] and $Q = 0$ [MPa]. The parameters Q , β and b were set to zero such that an elastoplastic material with linear kinematic hardening was present and the ratios $\alpha = b/H$, $\gamma = a/b$ were set to 0.1 and 5, respectively. The idea for this example was given in Eshraghi [2009].

Fig. 3.19 shows the shear stress-strain responses of the element at the integration point for 50 subsequent elliptical cycles. In these plots, a remarkable dependency of the results of the

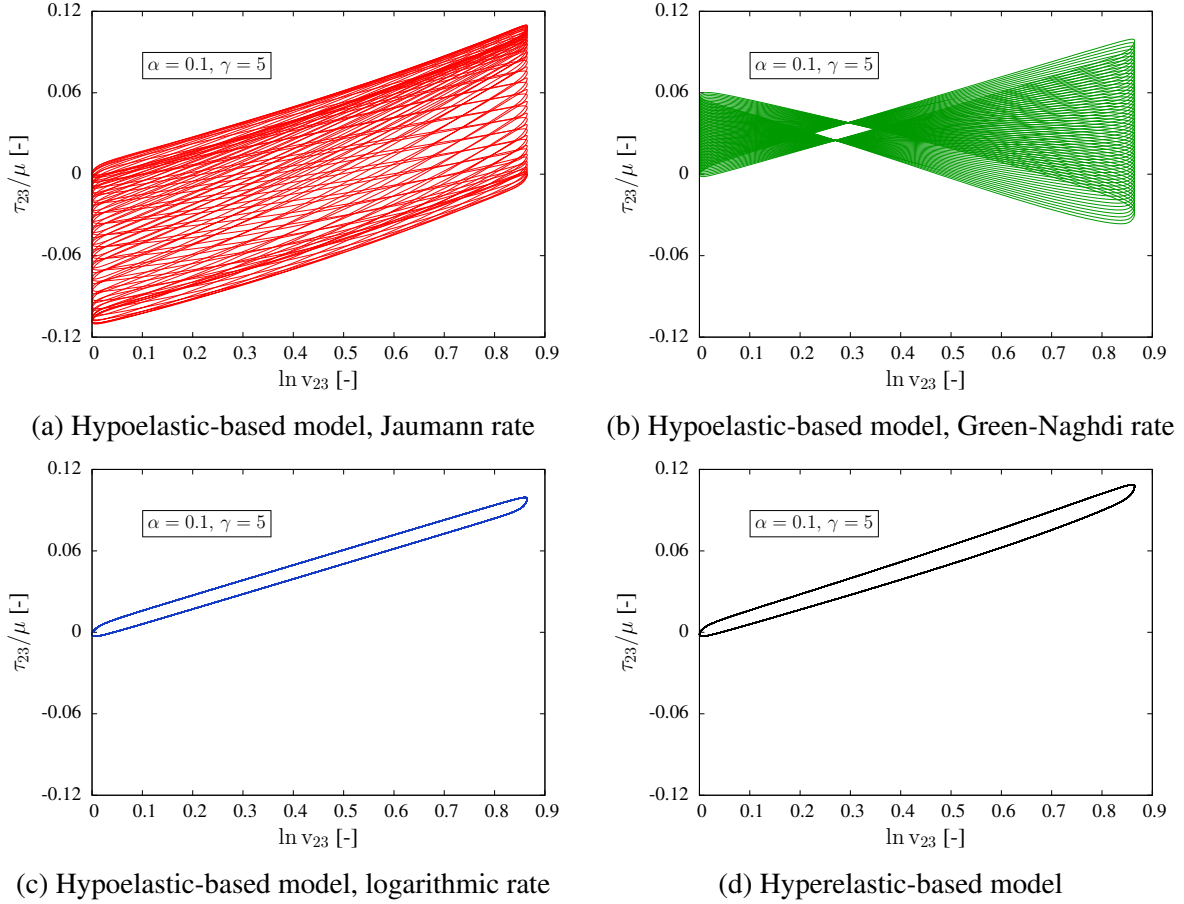


Figure 3.19: Stress-strain plots for 50 elliptical deformation cycles

hypoelastic-based model on the respective objective rate can be observed. In the case of the Jaumann rate, a distinct cyclic softening response can be observed, for the Green-Naghdi rate also rather unusual and unrealistic results are obtained. Only in the case of the logarithmic rate a physically meaningful stabilized stress-strain hysteresis loop can be observed for the hypoelastic-based model which emphasizes the physical soundness of the self-consistent Eulerian model. The problems in the other two cases arise due to the extreme simple shear defor-

mation in connection with the applied linear kinematic hardening model, an issue which was reported already by Nagtegaal and De Jong [1982]. The hyperelastic-based model leads as the self-consistent Eulerian model to reasonable results. The differences in the results between those two models are not surprising, both rely upon totally different kinematic assumptions which may become visible for large deformations.

It is interesting to remark that the internal hypoelastic-based plasticity model in ABAQUS for standard J_2 metal elastoplasticity produces similar results as shown in Fig. 3.19a. Only very slight differences appear since the built-in material model in ABAQUS / Standard is based on a Jaumann rate formulation of the Cauchy stress and the Hughes-Winget algorithm, as was mentioned in Sect. 3.3.6.

3.5.5.2 Cylindrical cup drawing of a sheet metal

A structural simulation of the cylindrical cup drawing process was performed with both the self-implemented hypoelastic- and hyperelastic-based plasticity models in ABAQUS / Standard. The objective was to determine whether there is really a noticeable influence of the chosen objective rate in more realistic situations, as, e. g., in the case of a metal forming process or not.

Deep drawing is an important process in the field of sheet metal forming. The basic tools for this process consist of a die, a blankholder and a punch which were modeled by rigid-body elements. In the process, the blank is mounted between the die and the blankholder and a downwards moving punch forms the blank into the die. A schematic view of the cylindrical cup drawing setup is shown in Fig. 3.20. The process parameters and the dimensions of the

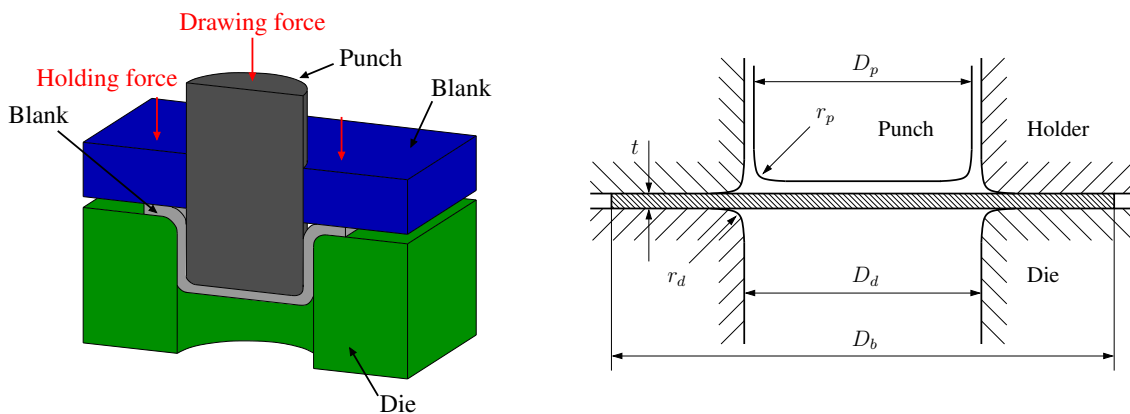


Figure 3.20: Schematic view of cylindrical cup drawing process

tools were taken from Vladimirov et al. [2010] and are given in Table 3.2. The blank itself was discretized by 2560 C3D8R brick elements (four elements were used in thickness direction).

Parameter / Data	Value	Dimension
Punch diameter D_p	50	[mm]
Punch profile radius r_p	5	[mm]
Die opening diameter D_d	52.8	[mm]
Die profile radius r_d	5	[mm]
Blank diameter D_b	100	[mm]
Sheet thickness t	1	[mm]
Coloumb's coefficient of friction	0.02	[-]
Blankholder force	5	[kN]

Table 3.2: Process parameters and tool data

By exploiting symmetry conditions, it was sufficient to model only a quarter of the blank. A combined nonlinear isotropic and kinematic hardening behavior was assumed, the material parameters were taken from Vladimirov et al. [2009] and specified as⁶: $\mu = 72509.4$ [MPa], $\lambda = 140753.5$ [MPa], $\sigma_y = 325$ [MPa], $b = 25$ [-], $c = 5200$ [MPa], $\beta = 8$ [-] and $Q = 215$ [MPa].

Fig. 3.21 shows the calculated punch force plotted over the punch displacement for the hyper- and hypoelastic-based plasticity model by using either the Jaumann, Green-Naghdi or logarithmic rate. All curves are virtually coincident. Fig. 3.22 shows a contour plot of the

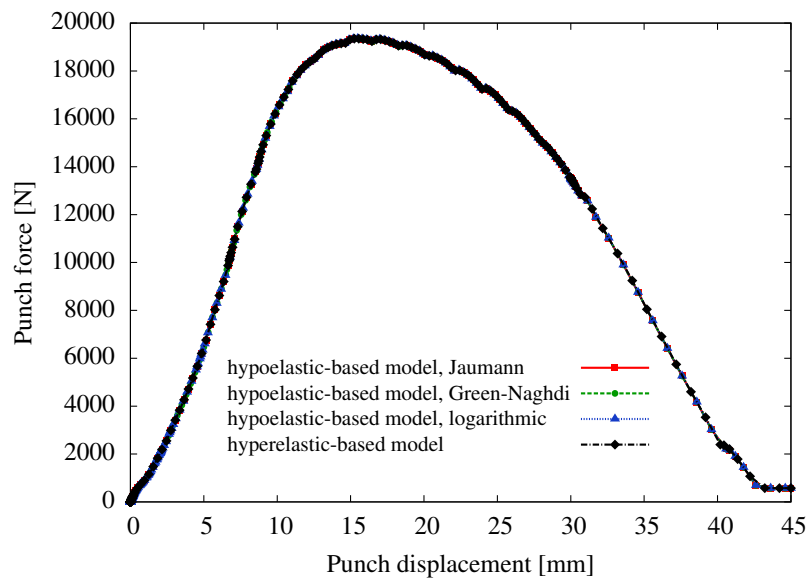


Figure 3.21: Punch force-punch displacement diagram

⁶For consistency, the actual values of b and c had to be doubled, since the free energy related to nonlinear kinematic hardening ψ_{kin} (3.53) defined in the current paper is two times the value of that used in the latter reference.

distribution of the accumulated plastic strain within the blank during and after the forming phase. For brevity, these results are only plotted once since they are essentially the same for the different models and all objective rates considered.

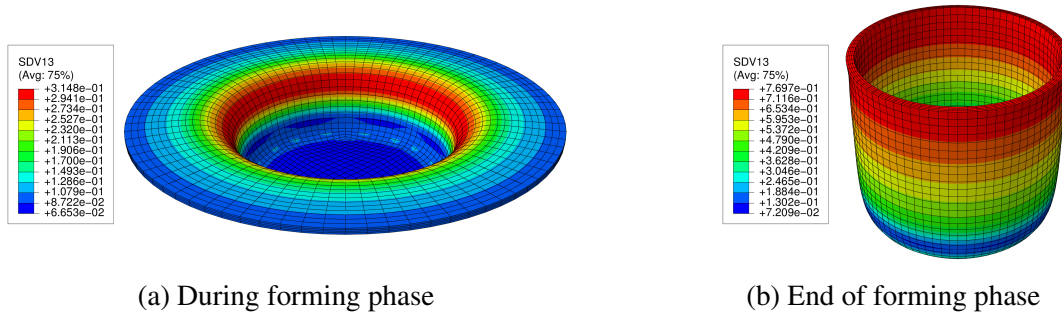


Figure 3.22: Cup drawing simulation: accumulated plastic strain in blank

The results show that in the simulation of a standard deep drawing process the particular choice of objective rate used in the hypoelastic-based model is of minor importance. This may be explained by the fact that, even though intensive shearing deformations occur in the flange of the cup, they are still not high enough to cause problems for the hypoelastic-based model and kinematic hardening does not play an important role since the loading is proportional. Moreover, it seems that the hypoelastic- and the hyperelastic-based model are able to produce equally good results in a numerical simulation of a deep drawing process. It should be mentioned that in real cup drawing experiments the formation of ‘cup ears’ can be observed, the reason for which lies in the anisotropy of the metal sheet that cannot be considered by the discussed isotropic material models. This topic is out of the scope of this work and is treated elsewhere (among many others, see, e. g., Barlat et al. [2005], Chung and Park [2013], Chung et al. [2005], Rabahallah et al. [2009], Tikhovskiy et al. [2007, 2008], Yoon et al. [1998, 2000, 2006] and Vladimirov et al. [2010, 2011]).

3.5.5.3 Draw bending of a sheet metal strip

In a third example, the self-implemented hypoelastic- and hyperelastic-based plasticity models were utilized in a draw bending simulation of a narrow sheet metal strip in ABAQUS / Standard. This test is attractive for the present study: it leads to a cyclic loading of the sheet since the latter is subjected to tension, bending and unbending during the process. Accordingly, the Bauschinger effect takes place and the influence of kinematic hardening is of major importance (see, e. g., Zhao and Lee [2001]). First references in the field where the draw bending test was applied to investigate springback behavior of sheet metals are given, e. g., by Kuwabara et al. [1995, 1996], Takahashi et al. [1996].

A schematic representation of the setup and the loading sequence of the considered 90° draw bending test is shown in Fig. 3.23. Two hydraulically actuated clamp jaws (not shown

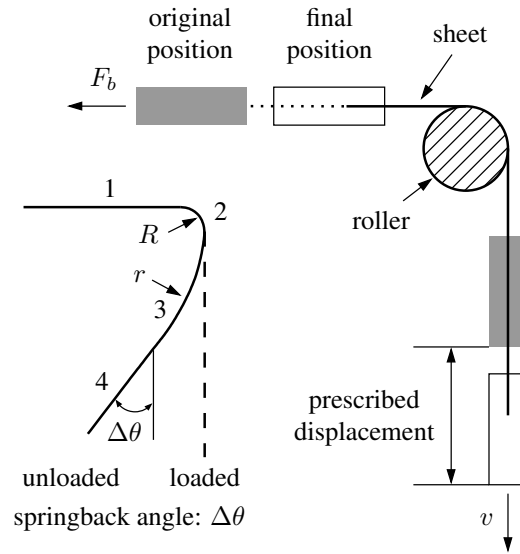


Figure 3.23: Schematic view of 90° draw bending process (idea from Li et al. [2002])

but indicated in the upper left and lower right part of the figure) are oriented perpendicular to each other and a rotating cylinder at the intersection of their action lines simulates a tooling radius over which the sheet metal is drawn. One actuator supplies a constant back force F_b whereas the other moves the strip at a constant speed v . During the process, the sheet metal strip is held fixed between the two clamp jaws and is being bent and drawn over a lubricated roller up to a prescribed drawing distance. Afterwards, it is unloaded and removed from the machinery such that the springback of the strip can be observed.

In Fig. 3.23, a loaded and unloaded steel sheet specimen are schematically illustrated. Within the unloaded strip, four regions of deformation can be distinguished (Li et al. [2002]). Regions 1 and 4 undergo pure stretching only and are usually of minor interest in springback analyses. Region 2 is characterized by a relaxed radius R which is originally equal to the radius of the roller. Region 3 experiences sequential bending/unbending with superposed stretching and is characterized by radius r . As can be seen, the change of the specimen is dominated by the bend-unbend area of the strip. This springback phenomenon is called ‘side-wall curl’ and is responsible for the curvature of the sheet. Near the roller, the change of shape due to simple bending is much smaller.

In the simulation, a converged mesh of 9600 C3D8R brick elements (length x thickness x width = 300 x 8 x 4) with reduced integration and hourglass stabilization was used for the sheet metal strip, the roller was modeled as rigid-body. Since a lubricated roller was assumed

in the process, the contact between the sheet and the roller was defined to be frictionless. The corresponding material parameters were specified as in Sect. 3.5.5.2. The radius of the roller and the thickness of the sheet were considered as $R = 10$ mm and $t = 1$ mm.

Fig. 3.24 shows a contour plot of the distribution of the accumulated plastic strain within the sheet metal strip during and after the drawing phase when springback has occurred. For brevity, the results are only plotted once since they are essentially the same for the different models and all objective rates considered.

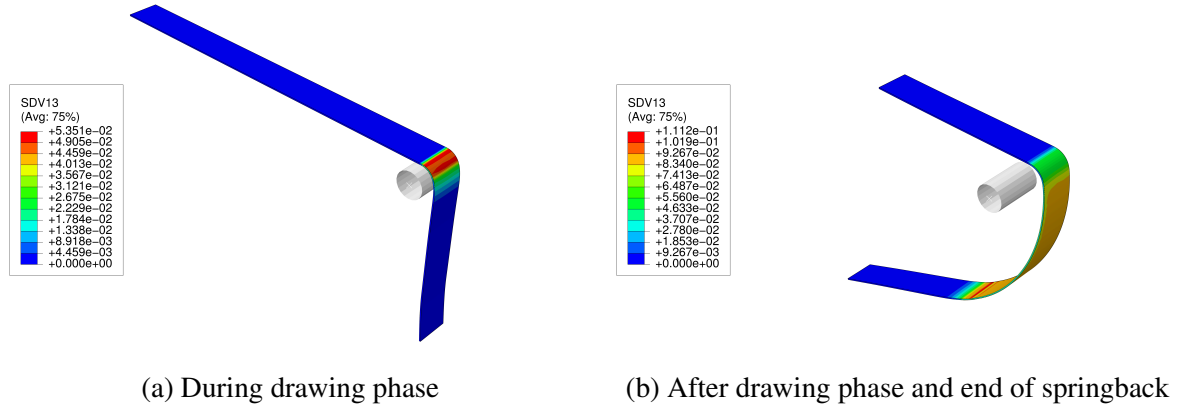


Figure 3.24: Draw bending simulation: accumulated plastic strain in sheet metal strip

Fig. 3.25 shows the predicted sheet strip profiles after springback by using either the hypoelastic-based model with the Jaumann, Green-Naghdi or logarithmic rate or the hyperelastic-based model in the simulation.

The results of the hypoelastic-based model once again do not depend on the respective objective rate used in the formulation which is to some extent surprising since the sheet was subjected to severe cyclic loading to which hypoelastic-based models are known to be sensitive. However, obviously the shear deformations are still too small to really have a remarkable influence. As in the cup drawing example, there are furthermore no noticeable differences between the results of the hypoelastic- and hyperelastic-based plasticity model.

3.5.5.4 Thermoforming of a polymer sheet

The last example in this study was concerned with the simulation of a thermoforming process of a polymer sheet. Thermoforming is a very common process which has found many applications in a wide range of industrial fields, e. g., in the automotive, medical or cosmetics industry. In this process, a thermoplastic polymer sheet is first clamped at its outer boundary and pre-heated up to a specified temperature after which it is brought into contact with and

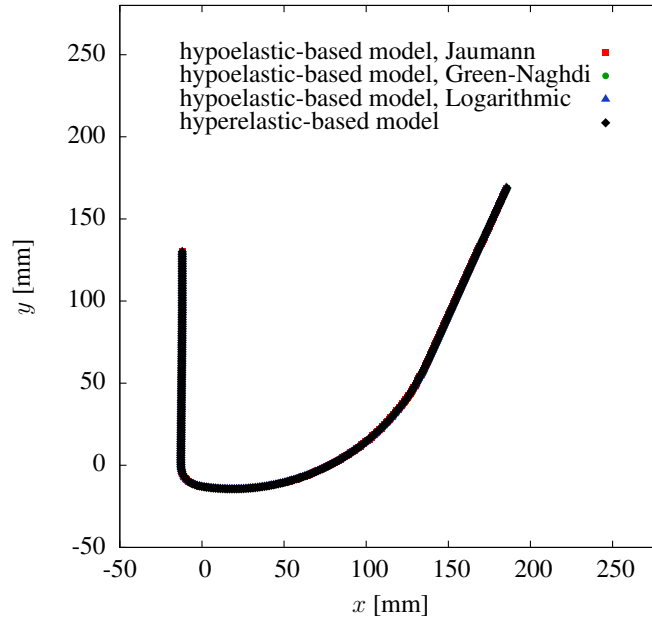


Figure 3.25: Strip profile after springback

drawn by an upwards-moving mould. With the help of a vacuum system, the trapped air is sucked out such that the sheet is adjusted to the contour of the mould and finally formed into its desired shape. For a schematic view of the process, see Fig. 3.26. The mentioned process was particularly interesting for the current study since it represents a real structural example in which the material (i. e, the polymer sheet) undergoes considerable elastic deformations.

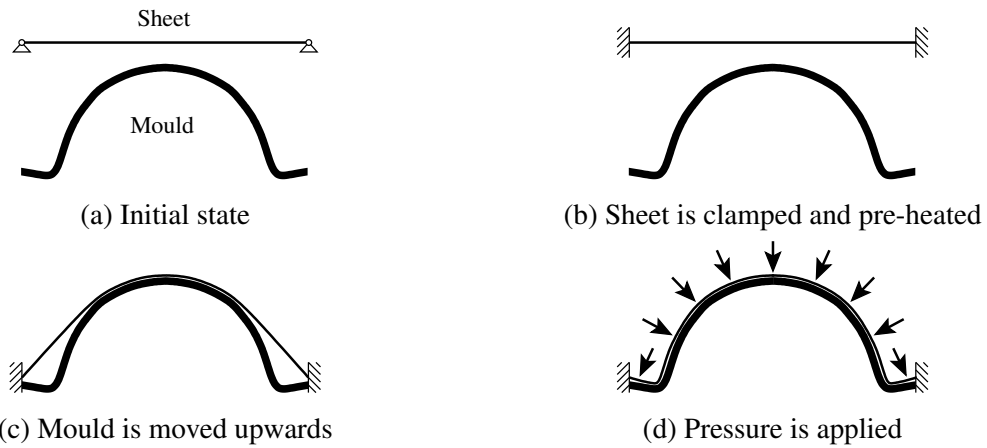


Figure 3.26: Schematic view of thermoforming process (idea from Jiang et al. [2003])

The process was simulated in ABAQUS / Standard according to the description given above and by using either the self-implemented hypoelastic-based or hyperelastic-based plasticity

model. A circular sheet was clamped at the nodes along its perimeter and put into contact with a rigid mould that was moved upwards up to a prescribed distance. Due to symmetry conditions, only a quarter of the sheet needed to be considered. A relatively fine mesh of approximately 12000 C3D8R brick elements with reduced integration and hourglass stabilization was used to model the polymer sheet (two elements were used in thickness direction). The effect of the vacuum was modeled in the simulation by applying a distributed load on the outer surface of the sheet which resulted in a close adhesion of the latter at the pre-defined shape of the mould. It should be remarked that a pure mechanical simulation was performed which should be considered as a strong simplification of the real process conditions. However, the main goal of the investigation was rather to evaluate the qualitative influence of the respective elastic response of the material model (hypoelastic-based or hyperelastic-based) in a structural example involving significant elastic strains than to give a thoroughly accurate prediction of the real process results.

The material parameters for the simulation were taken from Igl and Osswald [1992] who performed a one-dimensional finite element simulation of a thermoforming process. The corresponding authors developed an empirical elastoplastic material model with linear isotropic hardening to describe a specific polypropylene material and obtained reasonable results. The models used for the current example were therefore also restricted to the case of linear isotropic hardening⁷ (kinematic hardening should be negligible since no cyclic loading of the sheet is present in the process). In detail, the material properties were specified as⁸ $\mu = 2.5$ [MPa], $\lambda = 10.0$ [MPa], $\sigma_y = 0.7362$ [MPa] and $H = 3.2083$ [MPa].

Fig. 3.27 shows a contour plot of the distribution of the accumulated plastic strain within the polymer sheet during and after the forming phase when the vacuum has been applied. Since the results for the respective models and all objective rates considered do not differ substantially from each other, the results are only plotted once.

In Fig. 3.28, a stress-strain diagram of the element in the center of the sheet is plotted before the vacuum pressure was applied. In case of the hyperelastic-based model, the border of the elastic range lies at approximately 5.6 % of true strain. Irrespective of the specific rate considered in the formulation, the elastic border in the case of the hypoelastic-based model lies at 5.8 %. Up to approximately 30 % of strain, the stress response is the same for both models and all objective rates considered in the hypoelastic-based model. From there on, the

⁷Linear isotropic hardening can be obtained for both models by simply exchanging R in (3.11) by $R = H\kappa$ where H is the isotropic hardening modulus.

⁸Since a one-dimensional simulation was performed by Igl and Osswald [1992], no value was given for the Poisson ratio ν of the material. For the current example, the value was guessed as $\nu = 0.4$ which seems to be a reasonable choice for polymers.

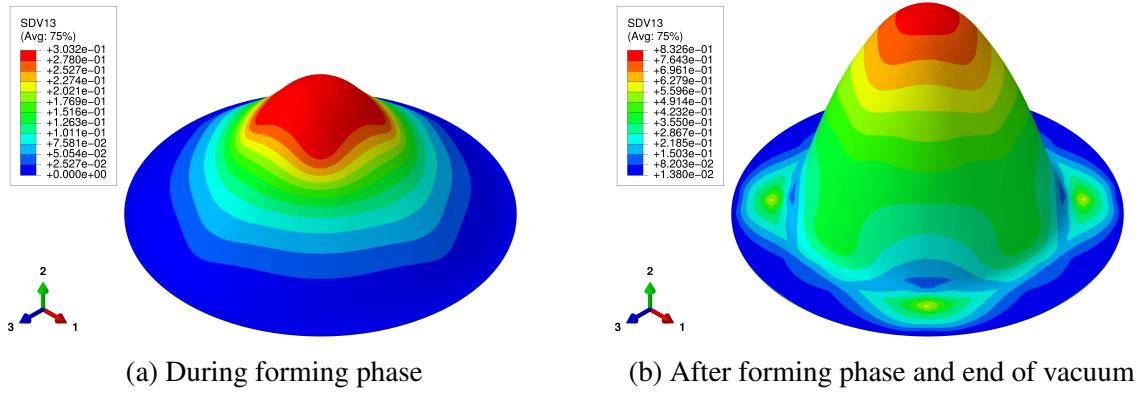


Figure 3.27: Thermoforming simulation: accumulated plastic strain in polymer sheet

stress-strain curve of the hyperelastic-based model develops slightly differently and shows a little larger straining of the element at the end of the forming step. The corresponding mould force-mould displacement diagram displayed in Fig. 3.29 does not, however, noticeably reflect this observation: all results are essentially the same.

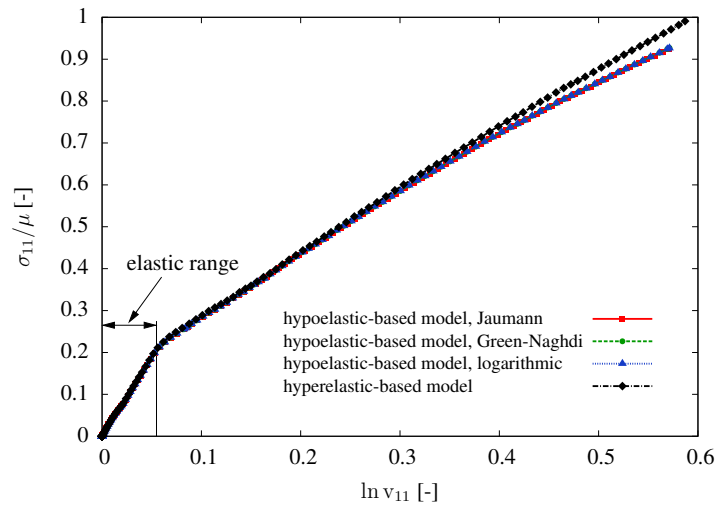


Figure 3.28: Stress-strain diagram of the element in the center of the sheet

In a similar example, Chatti [2010] investigated also the von Mises stress distribution along the radius from the center to the outer side of the blank at the end of the simulation. The author noticed a quantitatively higher stress distribution in case of the hyperelastic-based model than in case of the hypoelastic-based model. A somehow similar observation can be made for the current example (see Fig. 3.30), however, the differences are less pronounced and become negligible for elements near the boundary. In contrast to the results given by Chatti [2010], Fig. 3.30 also shows a sudden increase of the stress in the direct neighbourhood of the

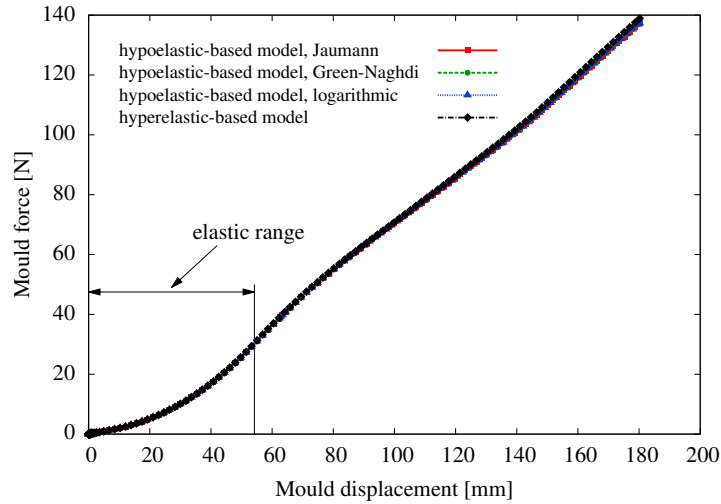


Figure 3.29: Mould force-mould displacement diagram

boundary which seems reasonable due to the clamping of the sheet.

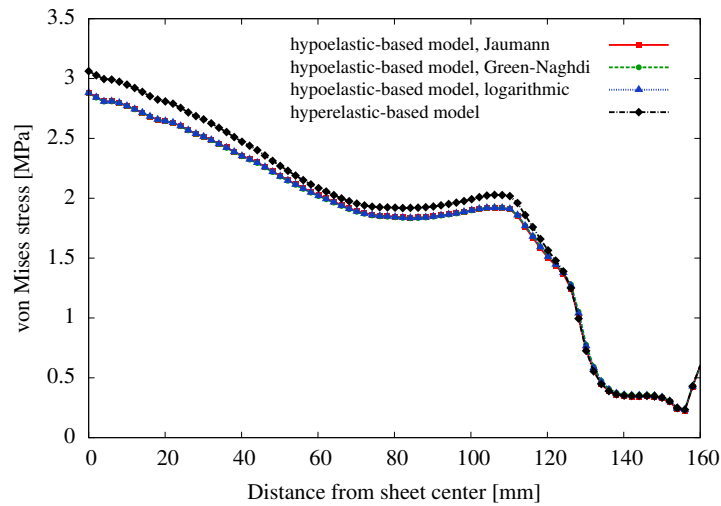


Figure 3.30: von Mises stress distribution along the radius of the sheet

In summary, the just described thermoforming example illustrates that the results for the discussed hypoelastic- and hyperelastic-based model can indeed differ in a structural simulation (even though these differences are still quite small). However, the authors believe that the reason for the differences in the results more likely arise due to the distinct description of the elastic response for large strains (Neo-Hookean elasticity in case of the hyperelastic-based model vs. Hencky-type elasticity in case of the hypoelastic-based model) than due to the inherently different kinematic description of elastoplasticity (multiplicative split of $\mathbf{F}$ vs. additive split of $\mathbf{d}$).

3.6 Conclusions

In the present work, both hypo- and hyperelastic-based approaches for modeling elastoplastic materials at finite strains were discussed. Whereas the former approach relies upon an additive decomposition of the rate of deformation tensor into elastic and plastic parts and a hypoelastic constitutive law involving a suitable objective stress rate, the latter assumes a multiplicative elastic-plastic split of the deformation gradient and postulates a hyperelastic law for the stress. The respective capabilities of both models were directly compared with each other in numerical simulations on the Gauss point and on the structural level.

Hypoelastic-based models are usually not based on an underlying free energy potential. For this reason, depending on the specific objective rate used in the formulation, dissipation of energy may occur in closed ‘elastic’ deformation cycles and lead to unexpected and undesirable results. This was demonstrated in this study by subjecting a single finite element to different repeating closed-path deformation cycles. Considerable elastic stress ratcheting was observed by using either the Jaumann or Green-Naghdi corotational rates in the formulation.

On the contrary, it was also clearly verified in this work that the self-consistent Eulerian model developed mainly by Bruhns and coauthors based on the Kirchhoff stress and logarithmic stress rate does not suffer from these problems. In accordance with the theory, it produced physically reasonable results in all numerical examples involving even large elastic strains. With the development of the self-consistent Eulerian model, the major issues of hypoelastic-based material models, namely elastic dissipation and non-uniqueness of the theory with respect to the choice of the objective rate, could be eliminated.

A practical difficulty connected to the application of hypoelastic-based models lies in their algorithmic implementation which requires the usage of incrementally objective algorithms. In this work, a well-known algorithm on the basis of a rotationally neutralized description of the problem was reviewed and discussed. It was demonstrated that the famous Hughes-Winget algorithm (which is, e. g., used by ABAQUS / Standard for internal models of J_2 metal elastoplasticity) can be viewed as a special case of this more general approach. However, in a specific test problem involving either a separated or superimposed motion of deformation and pure rotation of a material body, it was demonstrated that both algorithms are only ‘weakly’ objective in the sense defined by Rashid [1993].

The aforementioned problems do not arise for hyperelastic-based models. Due to the assumption of an underlying free energy potential, truly reversible elastic material behavior can be predicted in the absence of plastic flow. Moreover, the restrictions imposed by the principle of material frame-indifference are already considered in the constitutive formulation, the

question of incremental objectivity does not naturally arise. The specific model discussed in this work is based on an additional split of the plastic deformation gradient into elastic and inelastic parts in order to model nonlinear kinematic hardening. Its physically reasonable behavior was demonstrated numerically in a further single element closed-path deformation test and, as expected, the results did not show any spurious dissipation phenomena.

Despite all these fundamental differences between the models, it is interesting enough that the simulations of a cup drawing and draw bending process as more realistic examples delivered nearly congruent results not only for the specific hyperelastic-based and the self-consistent Eulerian model but also for the two ‘classical’ hypoelastic-based models involving the Jaumann and Green-Naghdi rates. This suggests that the problem of elastic dissipation is obviously of minor importance in usual applications of sheet metal forming which justifies also the use and success of ‘classical’ hypoelastic-based plasticity models, e. g., in combination with commercial finite element codes as ABAQUS / Standard. Finally, even the simulation of a thermoforming process of a polymer sheet which undergoes considerable elastic strains led only to slight differences in the results between the considered models.

3.7 Appendix

3.7.1

With $m \leq 3$ defined as the number of distinct eigenvalues, $\mathbf{b} = \mathbf{F} \mathbf{F}^T$ can be written as

$$\mathbf{b} = \sum_{i=1}^m b_i \mathbf{b}_i \quad (3.69)$$

where the symmetric tensors $\{\mathbf{b}_i\}$ are called the eigenprojections of $\mathbf{b}$. The latter can be expressed by

$$\mathbf{b}_i = \begin{cases} \sum_{j=1, j \neq i}^m \frac{\mathbf{b} - b_i \mathbf{I}}{b_i - b_j} & \text{if } m > 1 \\ \mathbf{I} & \text{if } m = 1 \end{cases} \quad (3.70)$$

in closed-form.

3.7.2

By the product rule of differentiation, simple rearranging and (3.19) it follows

$$\begin{aligned}
 \dot{\bar{\tau}} &= \overline{\dot{\Lambda}^T \tau \Lambda} = \dot{\Lambda}^T \tau \Lambda + \Lambda^T \dot{\tau} \Lambda + \Lambda^T \tau \dot{\Lambda} \\
 &= \Lambda^T \left(\dot{\tau} + \Lambda \dot{\Lambda}^T \tau + \tau \dot{\Lambda} \Lambda^T \right) \Lambda \\
 &= \Lambda^T (\dot{\tau} - \Omega \tau + \tau \Omega) \Lambda \\
 &= \Lambda^T \overset{\circ}{\tau} \Lambda
 \end{aligned} \tag{3.71}$$

3.7.3

To show this, it is sufficient to prove that $\dot{\bar{\tau}}$ as well as $\bar{\mathbf{d}}_p$ and $\bar{\mathbf{d}}$ are invariant under a change of frame $\mathcal{O} \rightarrow \mathcal{O}^+$:

$$\begin{aligned}
 \dot{\bar{\tau}} &\rightarrow (\dot{\bar{\tau}})^+ = (\Lambda^T)^+ \left(\overset{\circ}{\tau} \right)^+ (\Lambda)^+ \\
 &= (\Lambda^T Q^T) \left(Q \overset{\circ}{\tau} Q^T \right) (Q \Lambda) \\
 &= \Lambda^T \underbrace{Q^T Q}_{=I} \overset{\circ}{\tau} \underbrace{Q^T Q}_{=I} \Lambda \\
 &= \Lambda^T \overset{\circ}{\tau} \Lambda = \dot{\bar{\tau}}
 \end{aligned} \tag{3.72}$$

The invariance of $\bar{\mathbf{d}}$ and $\bar{\mathbf{d}}_p$ can be shown analogously.

3.7.4

Let $\hat{\Lambda}$ be a proper orthogonal tensor defined such that

$$\left. \begin{aligned} \Lambda_{n+\frac{1}{2}} &= \hat{\Lambda} \Lambda_n \\ \Lambda_{n+1} &= \hat{\Lambda} \Lambda_{n+\frac{1}{2}} \end{aligned} \right\} \Rightarrow \Lambda_{n+1} = \hat{\Lambda}^2 \Lambda_n \tag{3.73}$$

Furthermore, by noting that the tensor $(\Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}})/2$ commutes with itself, it can be found that

$$\begin{aligned}
 \boldsymbol{\Lambda}_{n+1} &= \exp \left(\Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \boldsymbol{\Lambda}_n \\
 &= \exp \left(\frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} + \frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \boldsymbol{\Lambda}_n \\
 &= \exp \left(\frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \exp \left(\frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \boldsymbol{\Lambda}_n \\
 &= \left[\exp \left(\frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \right]^2 \boldsymbol{\Lambda}_n
 \end{aligned} \tag{3.74}$$

Comparing (3.73) with (3.74), it can be concluded that

$$\hat{\boldsymbol{\Lambda}} = \exp \left(\frac{1}{2} \Delta t \boldsymbol{\Omega}_{n+\frac{1}{2}} \right) \tag{3.75}$$

3.7.5

Time differentiation of $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and usage of $\mathbf{l} = \dot{\mathbf{F}} \mathbf{F}^{-1}$ delivers

$$\begin{aligned}
 \dot{\mathbf{C}} &= \dot{\mathbf{F}}^T \mathbf{F} + \mathbf{F}^T \dot{\mathbf{F}} \\
 &= \mathbf{F}^T \left(\mathbf{F}^{-T} \dot{\mathbf{F}}^T + \dot{\mathbf{F}} \mathbf{F}^{-1} \right) \mathbf{F} \\
 &= \mathbf{F}^T (\mathbf{l}^T + \mathbf{l}) \mathbf{F} \\
 &= 2 \mathbf{F}^T \mathbf{d} \mathbf{F}.
 \end{aligned} \tag{3.76}$$

3.7.6

Considering the definition of the tensor exponential function and using its properties (see, e. g., Itskov [2009]), it follows:

$$\begin{aligned}
 \mathbf{\Lambda}_{n+1} &= \exp \left(\Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \mathbf{\Lambda}_n \\
 \iff \mathbf{\Lambda}_{n+1} \mathbf{\Lambda}_n^T &= \exp \left(\Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \\
 &= \exp \left(\frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} + \frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \\
 &= \exp \left(\frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \exp \left(\frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \\
 &= \left[\exp \left(-\frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \right]^{-1} \exp \left(\frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \\
 &\approx \left(\mathbf{I} - \frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right)^{-1} \left(\mathbf{I} + \frac{1}{2} \Delta t \mathbf{w}_{n+\frac{1}{2}} \right) \\
 &=: \mathbf{\Lambda}_\Delta
 \end{aligned} \tag{3.77}$$

4 | Article 3:

Gradient-extended ‘two-surface’ damage-plasticity: micromorphic formulation and numerical aspects

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T. Brepols reviewed the relevant existing literature, developed the ‘two-surface’ gradient-extended damage-plasticity model and implemented it into the academic finite element software FEAP (as an own element subroutine using a corresponding interface in the software). It was his idea to apply the Fischer-Burmeister approach in the context of the algorithmic implementation of the model. Furthermore, he set up and performed all simulations, interpreted the results and wrote the article. S. Wulfinghoff had the idea to use the micromorphic approach of Forest [2009] for the gradient-extension of the model. Moreover, he and S. Reese gave conceptual advice, contributed to the discussion of the results, read the article and gave valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

4.1 Abstract

A regularized gradient-extended damage-plasticity model is discussed which is based on a micromorphic approach in the spirit of Forest [2009]. Damage and plasticity are treated as independent but strongly coupled dissipative phenomena by means of a ‘two-surface’ formulation, i. e., by using separate yield and damage functions as well as appropriate loading/unloading conditions. By means of two independent dissipation potentials for plasticity and damage, thermodynamically consistent evolution equations are derived. The model accounts for non-linear plastic as well as damage hardening. The models’ implementation at the local Gauss-point level, both using a local active-set search strategy known from multisurface plasticity and a recent approach based on a reformulation of the model equations by means of the Fischer-Burmeister complementarity function, is discussed in detail. It is shown how the model can be implemented into finite elements and the four algorithmically consistent tangent operators are presented which are necessary to obtain quadratic convergence in a global Newton scheme. Various numerical benchmark tests performed in the study nicely indicate the model’s ability to deliver mesh-independent results in coupled damage-plasticity finite element simulations.

4.2 Introduction

4.2.1 Modeling of damage and fracture

The modeling of fracture phenomena in solid structures is and has always been an important topic in the field of computational mechanics. Nowadays, the increasing availability of computing power allows scientists and engineers to perform simulations of ever more complex crack initiation and crack propagation phenomena under realistic conditions which is of major concern in various scientific disciplines (among many others, see, e. g., Duda et al. [2015], Geers et al. [1998], Hütter et al. [2013], Linse et al. [2012], Mediavilla et al. [2006], Miehe, Hofacker and Welschinger [2010], Miehe, Welschinger and Hofacker [2010], Miehe, Aldakheel and Raina [2016], Mozaffari and Voyiadjis [2016], Naderi et al. [2016], Seabra et al. [2013], Simone et al. [2003]). As a direct consequence, a growing demand of powerful and reliable material models which are capable of representing material failure is also noticeable within the community.

Concerning ductile materials, void nucleation, growth and coalescence have for long been identified as predominant physical mechanisms causing and preceding failure (see, e. g., Hancock and Mackenzie [1976], McClintock [1968], Rice and Tracey [1969]), however, research is still very active and ongoing in this area (Hosokawa et al. [2013], Landron et al. [2013],

Tekoğlu et al. [2015]). A detailed modeling of the above mentioned individual phenomena proves to be complicated and is often not necessary, especially if only their overall impact on the material's behavior is of interest. For this reason, starting with the pioneering works of Kachanov [1958] and Rabotnov [1963] the discipline of Continuum Damage Mechanics (CDM) emerged, accounting for the mentioned effects in an averaged sense by incorporating additional internal 'damage' variables into a standard continuum mechanics description. These variables usually degrade the stiffness, strength and/or other properties of the material in one way or the other, leading to softening behavior which typically occurs in conjunction with strain hardening of the material. If the former effects finally prevail in a certain region of the structure, a localization process can be initiated which typically acts as a direct precursor to complete material failure in this location.

Depending on the complexity of the model, damage can be represented by (possibly multiple) tensor-valued variables of higher-order, with a single scalar variable being the simplest case usually sufficient for situations in which the above mentioned material defects occur approximately in an isotropic manner (Gurson [1977], Lemaitre [1985a], Lemaitre and Chaboche [1990], Tvergaard and Needleman [1984]). Usually, the damage variables take on values between zero for a virgin and unity¹ for a fully damaged material which has lost all its load-bearing capacity (in at least a certain direction), respectively. Damage as a measure of average material degradation becomes an internal variable which needs to be computed either incrementally or explicitly as a function of other appropriate variables. One of the advantages of CDM models is that, formally, the modeling of crack initiation and propagation remains entirely at the level of the constitutive formulation such that CDM models can be easily incorporated into standard nonlinear finite element codes.

Unfortunately, finite element computations involving material softening (may it be, e. g., softening plasticity or damage) can suffer from strongly mesh-dependent results, rendering the latter often useless for subsequent qualitative or quantitative analyses (Bažant et al. [1984], de Borst et al. [1993] and other references therein). As such, CDM models are also affected by this problem. On the one hand, one observes that the predicted damage zone shrinks upon mesh refinement since damage tends to localize in a zone of measure zero. Consequently, mesh-convergence cannot be obtained for finite mesh sizes and the computed dissipated energy during the localization process becomes smaller and smaller, leading in the limit (i. e., for an hypothetically infinitely fine mesh) to the occurrence of a crack whose formation requires no energy. Such a model behavior is clearly physically unlikely and undesirable. On the other

¹What 'unity' means in case of a higher-order tensorial damage variable is a matter of definition and depends on the specific formulation, see, e. g., Lemaitre and Desmorat [2005].

hand, a crack’s initial location and its subsequent propagation may also be influenced by the specific structure of the mesh and the element-types used (Cervera and Chiumenti [2006], Grassl and Jirásek [2004], Jirásek and Grassl [2008]). Therefore, physically reasonable finite element simulations of localization and fracture processes using local CDM models can usually not be achieved. It is crucial to understand that these problems are not related to the finite element method but to the material formulation itself: prior to the onset of strain localization, the so-called acoustic tensor becomes singular which renders the underlying boundary value problem ill-posed (see, e. g., Bažant and Belytschko [1985], Lasry and Belytschko [1988], de Borst et al. [2012], Jirásek and Bažant [2001]). In a quasi-static context, one commonly speaks of the ‘loss of ellipticity’ of the governing equations.

To overcome the above mentioned shortcomings, several methodologies were developed which, in one way or the other, introduce additional terms into the model that prevent the damage zone from shrinking towards a zone of measure zero, frequently also called ‘localization limiters’. Among the most efficient and conceptually sound approaches are those based on the incorporation of spatial interaction terms that automatically introduce an internal material length into the formulation, e. g., CDM models that define damage as a function of a spatial integral of a variable (integral-type formulations) or of a variable which exhibits gradient-effects (gradient-type formulations). Physical arguments supporting the hypothesis of the nonlocal character of damage were given, e. g., by Bažant [1991]. Both variants are loosely called ‘nonlocal’ approaches, even though only the former type truly abandons the classical principle of local action. Here, the nonlocal variable is defined as a certain weighted average of a corresponding local quantity over a neighborhood at a point (de Sciarra [2012], Grassl et al. [2014], Leblond et al. [1994], Pijaudier-Cabot and Bažant [1987], Nguyen et al. [2015], Tvergaard and Needleman [1995]). The internal material length is explicitly given by means of the size of the averaging zone. However, even though integral-type formulations allow for the highest degree of flexibility regarding the specific type of averaging, their implementation into nonlinear finite element codes is usually not straightforward. Besides other difficulties, special considerations are necessary to, e. g., carry out a consistent linearization (Jirásek and Patzák [2002]).

On the other side, gradient-type formulations maintain the principle of local action and are typically easier to implement. One often distinguishes additionally between ‘explicit’ and ‘implicit’ gradient-extended models. Explicit models directly introduce higher-order gradient terms of already existing local quantities into the constitutive framework (see Aifantis [1984], de Borst and Mühlhaus [1992], Fleck and Hutchinson [2001], Martínez-Pañeda and Niordson [2016], Mühlhaus and Aifantis [1991], Reddy et al. [2008] for examples in the framework of

gradient plasticity or Comi and Driemeier [1998], Comi [1999] for examples in the framework of gradient damage, respectively). In contrast, implicit models assume the existence of a new nonlocal variable and make use of a further partial differential equation (PDE) for it, mostly of Helmholtz-type, the origin and structure of which are sometimes motivated differently in various works. Anyway, the decisive feature is here that a related local quantity acts as a source term in the PDE. The internal material length is implicitly defined through a parameter controlling the influence of the gradient term in the PDE. Actually, one then deals with a coupled problem in which both the displacement and the nonlocal variable become global unknowns of the system. In a finite element context, this means that one or more degrees of freedoms are additionally present at the respective nodes of the mesh, depending on the specific order of the nonlocal variable. In the implicit context, examples of gradient plasticity models were developed by Anand et al. [2012], Engelen et al. [2002], Geers [2004] and Wulfinghoff et al. [2013, 2015], among many others. Gradient damage models for quasi-brittle or brittle-like materials were, e. g., proposed by Dimitrijevic and Hackl [2008], Frémond and Nedjar [1996], Peerlings et al. [1995], Peerlings et al. [1996], Peerlings et al. [1998], Pham et al. [2011] and Pham and Marigo [2012]. Models coupling local plasticity to gradient damage were discussed, e. g., by Alessi et al. [2015], Aslan, Quilici and Forest [2011], de Borst et al. [1999], Nedjar [2001] and Reusch et al. [2003a], whereas Aslan, Cordero, Gaubert and Forest [2011], Dimitrijevic and Hackl [2011] and Saanouni and Hamed [2013] introduced separate internal material lengths and limiters for both plasticity and damage.

4.2.2 Aim and scope of the present work

The present work discusses a gradient-extended and fully coupled isotropic damage-plasticity model based on the micromorphic approach as proposed by Forest [2009]. Damage is assumed to be the variable which exhibits gradient effects. The model relies upon a ‘two-surface’ formulation in which damage and plasticity are treated as independent physical mechanisms by considering both a yield and damage function as well as appropriate loading/unloading conditions. A strong coupling between the two phenomena is enforced via the constitutive assumption of total energy equivalence (Saanouni et al. [1994]). The model accounts for (possibly non-associative) nonlinear plastic isotropic and kinematic hardening as well as damage hardening by using two separate dissipation potentials from which the evolution equations of the model are derived in a thermodynamically consistent manner.

The model in the present study has several features in common with the formulation of Saa-

nouni and Hamed [2013] in which damage is also extended by the micromorphic approach.² The latter authors used a ‘single-surface’ formulation in which only a yield surface is present and damage is included by means of a ‘Lemaitre-type’ plastic dissipation potential (Lemaitre [1985a]). The present work differs in the sense that a two-surface formulation for plasticity and damage is used which makes the model applicable also in situations in which the material exhibits a quasi-brittle, brittle or possibly mixed ductile-brittle-like damage behavior. In such a case, a single-surface formulation could turn out to be a limiting factor (Chaboche [2003]). Clearly, the presence of two independent sets of loading/unloading conditions for plasticity and damage complicates the numerical treatment. Therefore, special attention is devoted also to two inherently different strategies to numerically integrate the model equations: on the one hand, a local active-set search strategy is considered which is similar to algorithms known from multisurface plasticity, and, on the other hand, a more recent reformulation of the original problem in terms of the so-called Fischer-Burmeister complementarity function is presented. To the authors’ knowledge, the latter strategy has not yet been applied or described in the context of two-surface damage-plasticity formulations. Furthermore, an algorithmically consistent linearization of the two-surface gradient-extended damage-plasticity model is carried out in order to obtain quadratic convergence in Newton iterations at both the global finite element and local Gauss-point level. Explicit expressions for a computation of the consistent tangent operators (four in total) are given and are general enough to account for other particular forms of, e. g., the yield and damage functions or evolution equations of the model. To the authors’ best knowledge, this issue has – in the present context – not been addressed in the literature in such a detail, yet.

The paper is structured as follows: Sect. 4.3 gives a detailed overview of the constitutive modeling. The general micromorphic approach is shortly reviewed and the principle of total energy is explained which is responsible for the coupling of plasticity and damage. The specific Helmholtz free energy and dissipation potentials of the model are defined from which the state relations and evolution equations are derived in accordance with the second principle of thermodynamics. Furthermore, the strong and weak forms of the equations to be solved are presented as well as a linearized weak form which is suitable for being implemented into finite elements. The algorithmic treatment is then thoroughly discussed in Sect. 4.4 beginning with the derivation of the general finite element equations. Next, a backward Euler discretization of the evolution equations is carried out and two different solution strategies are presented

²Theoretically, the authors presented a model in which the damage, isotropic and kinematic hardening variables are all supposed to carry micromorphic effects, resulting in three PDEs which need to be solved in addition to the balance of linear momentum. However, in their numerical examples, the authors restricted themselves to the usage of a model in which only the damage variable exhibits micromorphic effects.

to solve the local equation system. Furthermore, it is shown how the consistent tangent operators can be computed. Section 4.5 is then devoted to several numerical benchmark tests which prove the model's ability to serve as a tool for predicting mesh-independent results during crack initiation and crack propagation phases in coupled damage-plasticity finite element simulations. Finally, a conclusion is given in Sect. 4.6.

4.2.3 Notational conventions

A direct tensor notation is preferred throughout the text. Scalars and scalar-valued functions are represented by light-face italic characters of either case, e. g., A or a . First-order tensors and tensor-valued functions are denoted by bold-face italic letters of either case, e. g., $\mathbf{B}$ or $\mathbf{b}$. Second-order tensors and tensor-valued functions are usually written as bold-face roman characters of either case, e. g., $\mathbf{C}$ or $\mathbf{c}$. However, if greek symbols are used to denote second-order tensors, the latter are written in italic style, as, e. g., $\boldsymbol{\sigma}$ or $\boldsymbol{\varepsilon}$. Uppercase calligraphic bold-face letters in italic style are used to represent fourth-order tensors, e. g., $\mathcal{D}$.

The symmetric part of a second-order tensor $\mathbf{C}$ is designated by $\mathbf{C}^s := (\mathbf{C} + \mathbf{C}^T)/2$ where $\mathbf{C}^T$ means its transpose. The deviatoric part of a second-order tensor is abbreviated as $\mathbf{C}' := \mathbf{C} - \frac{1}{3}\text{tr}(\mathbf{C})\mathbf{I}$ in which $\mathbf{I}$ is the second-order identity tensor and $\text{tr}(\mathbf{C})$ the trace of $\mathbf{C}$. A single contraction of a second-order tensor $\mathbf{C}$ from the right with a first-order tensor $\mathbf{d}$ (which might also be considered as a linear mapping of $\mathbf{d}$ by $\mathbf{C}$) is written as $\mathbf{C}[\mathbf{d}]$. A double contraction of a fourth-order tensor $\mathcal{D}$ from the right with a second-order tensor $\mathbf{C}$ (which might also be considered as a linear mapping of $\mathbf{C}$ by $\mathcal{D}$) is denoted as $\mathcal{D}[\mathbf{C}]$. The scalar and dyadic products of two first-order tensors $\mathbf{a}$ and $\mathbf{b}$ are written as $\mathbf{a} \cdot \mathbf{b}$ and $\mathbf{a} \otimes \mathbf{b}$, respectively. Analogous conventions hold for second-order tensors. Finally, a double contraction between two fourth-order tensors $\mathcal{D}$ and $\mathcal{E}$ is denoted as $\mathcal{D} : \mathcal{E}$.

4.3 Constitutive modeling

4.3.1 Gradient-extension based on the micromorphic approach

The regularized two-surface damage-plasticity gradient-enhanced material model discussed in this work is a special instant of the general class of micromorphic media as introduced by Forest [2009]. The micromorphic approach may be regarded as a systematic procedure for constructing higher-order gradient materials which make use of additional internal (micromorphic) degrees of freedom in the formulation, also called 'microvariables'. The difference

with respect to internal variables is that these degrees of freedom do explicitly appear in further generalized balance equations which have to be solved in addition to the classical balance equations, as, e. g., the balance of linear momentum in the purely mechanical case. The microvariables are coupled to certain strain-like internal variables of the model by introducing a direct dependence of the underlying free energy on the difference between the just mentioned quantities. One appealing property of the micromorphic approach is the fact that many well-established higher-order gradient models in the literature can be derived from it, see, e. g., Forest [2009, 2016], Forest et al. [2011].³

Applying the general micromorphic approach to the special case of a geometrically linear, quasi-static and purely mechanical framework with a single micromorphic variable $\bar{\phi}$, it is necessary first to define the expression for the virtual work which consists of internal and external contributions, here denoted as g_{int} and g_{ext} , respectively:⁴

$$g_{\text{int}} = \int_{\Omega} \boldsymbol{\sigma} \cdot \nabla^s \delta \mathbf{u} \, d\Omega + \underbrace{\int_{\Omega} (a_i \delta \bar{\phi} + \mathbf{b}_i \cdot \nabla \delta \bar{\phi}) \, d\Omega}_{\text{micromorphic extension}} \quad (4.1)$$

$$g_{\text{ext}} = \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} \, d\Omega + \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma + \underbrace{\int_{\Omega} (a_e \delta \bar{\phi} + \mathbf{b}_e \cdot \nabla \delta \bar{\phi}) \, d\Omega + \int_{\Gamma_c} a_c \delta \bar{\phi} \, d\Gamma}_{\text{micromorphic extension}} \quad (4.2)$$

In the above, $\boldsymbol{\sigma}$ denotes the Cauchy stress, $\mathbf{u}$ is the displacement and a_i , $\mathbf{b}_i$ are considered as internal forces which are associated to the micromorphic variable $\bar{\phi}$ and its gradient $\nabla \bar{\phi}$ acting within body Ω . Conventional body forces are represented by $\mathbf{f}$ whereas a_e and $\mathbf{b}_e$ account for generalized volume forces. Moreover, $\mathbf{t}$ and a_c denote conventional and generalized tractions, respectively, acting on parts Γ_t and Γ_c of the outer surface of the body where tractions and generalized tractions are prescribed (Neumann boundary conditions). Finally, $\delta \mathbf{u}$ and $\delta \bar{\phi}$ are arbitrary test functions of the displacement field $\mathbf{u}$ and the micromorphic field $\bar{\phi}$, constructed such that $\delta \mathbf{u} = \mathbf{0}$ on Γ_u and $\delta \bar{\phi} = 0$ on $\Gamma_{\bar{\phi}}$, i. e., on parts of the outer surface of the body where the displacements and the micromorphic variable are prescribed (Dirichlet boundary conditions).

Now, applying the principle of virtual work (PVW), the usual balance equation of linear momentum and a generalized balance equation for the micromorphic variable are obtained

³For the convenience of the reader, a short presentation of the general micromorphic approach is given in Appendix 4.7.1.

⁴In line with the notational convention given in Sect. 4.2.3, operator $\nabla^s(\bullet) = \frac{1}{2} (\nabla(\bullet) + \nabla(\bullet)^T)$ denotes the symmetric gradient of a quantity $(\bullet)$.

with corresponding boundary conditions:⁵

$$\text{PVW : } g_{\text{int}} \stackrel{!}{=} g_{\text{ext}} \implies \left\{ \begin{array}{l} \text{linear momentum balance:} \\ \quad \text{div}(\boldsymbol{\sigma}) + \mathbf{f} = \mathbf{0} \quad \text{in } \Omega \\ \quad \mathbf{t} = \boldsymbol{\sigma}[\mathbf{n}] \quad \text{on } \Gamma_t \\ \quad \mathbf{u} = \hat{\mathbf{u}} \quad \text{on } \Gamma_u \\ \\ \text{micromorphic balance equation:} \\ \quad \text{div}(\mathbf{b}_i - \mathbf{b}_e) - a_i + a_e = 0 \quad \text{in } \Omega \\ \quad a_c = (\mathbf{b}_i - \mathbf{b}_e) \cdot \mathbf{n} \quad \text{on } \Gamma_c \\ \quad \bar{\phi} = \hat{\phi} \quad \text{on } \Gamma_{\bar{\phi}} \end{array} \right. \quad (4.3)$$

In the above, $\mathbf{n}$ represents suitable outward unit normals at the boundaries Γ_t and Γ_c and $\hat{\mathbf{u}}$ and $\hat{\phi}$ are prescribed values of the displacement and the micromorphic variable on the Dirichlet parts of the boundary Γ_u and $\Gamma_{\bar{\phi}}$, respectively. As will be shown later, the expression for the micromorphic balance equation and its boundary conditions can be further simplified if additional assumptions are made.

4.3.2 Energy equivalence and effective variables

The present model is formulated in the framework of irreversible thermodynamics (see, e. g., Germain et al. [1983], Halphen and Nguyen [1975], Lemaitre and Chaboche [1990], Truesdell and Noll [1965]). Moreover, it is based on the concept of effective stress, originally introduced by Kachanov [1958] and Rabotnov [1963], and exploits main ideas known from the hypotheses of elastic energy equivalence (Cordebois and Sidoroff [1982]) and total energy equivalence (Chow and Lu [1992], Saanouni et al. [1994]). Focusing on a geometrically linear theory in the present work, the total strain $\boldsymbol{\varepsilon} := \nabla^s(\mathbf{u})$ is assumed to be additively separable into an elastic part $\boldsymbol{\varepsilon}_e$ and a plastic part $\boldsymbol{\varepsilon}_p$, i. e., $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$.

As common for most continuum damage models, an internal damage variable D is introduced which measures the degree of material degradation at a certain point in an averaged sense. With regard to the present framework of isotropic damage, this variable is assumed to be a scalar quantity. For a virgin (i. e., undamaged) material, D is defined to be zero whereas it takes on a critical value D_{cr} in case of a completely defective state. With regard to the micromorphic character of the model (see Sect. 4.3.1), the damage variable is selected to exhibit gradient effects. Therefore, an associated (scalar) quantity $\bar{D}$ is defined which acts as the ‘micromorphic’ damage variable and extends the basic set of degrees of freedom of the model.

⁵Mathematical details of the derivation are given in Appendix 4.7.2.

Following irreversible thermodynamics and the method of local state (see, e. g., Chaboche [2003], Germain et al. [1983]), all thermomechanical processes existing in the material are characterized by means of individual couples $(\mathbf{a}_i, \mathbf{A}_i)$ where index i denotes the set of the various processes available. Quantity $\mathbf{A}_i$ is a stress-like state variable associated with a corresponding strain-like state variable $\mathbf{a}_i$, both can be tensors of arbitrary order according to the physical phenomena they represent.

In a damaged configuration, i. e., in a damaged state of the material, the damage-plasticity model discussed in this study is characterized in every material point by a set of pairs $\{(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}), (\mathbf{X}_p, \boldsymbol{\beta}_p), (\xi_p, q_p), (D, Y), (\xi_d, q_d), (\bar{D}, a_i), (\nabla \bar{D}, \mathbf{b}_i)\}$. The individual pairs $(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma})$, $(\mathbf{X}_p, \boldsymbol{\beta}_p)$ and (ξ_p, q_p) describe the state of plastic flow, kinematic and isotropic plastic hardening, whereas (D, Y) and (ξ_d, q_d) characterize the state of damage and damage hardening, respectively. The last two pairs $(\bar{D}, a_i)$ and $(\nabla \bar{D}, \mathbf{b}_i)$ are related to the micromorphic damage and its first gradient, respectively.

In a similar spirit as the hypotheses of elastic energy equivalence (Cordebois and Sidoroff [1982]) and total energy equivalence (Chow and Lu [1992], Saanouni et al. [1994]), the present model assumes the existence of an additional (fictitious) undamaged configuration characterized by a corresponding set of effective variables $\{(\tilde{\boldsymbol{\varepsilon}}_e, \tilde{\boldsymbol{\sigma}}), (\tilde{\mathbf{X}}_p, \tilde{\boldsymbol{\beta}}_p), (\tilde{\xi}_p, \tilde{q}_p)\}$ which is defined such that the elastic and plastic energies of both configurations are equivalent to each other, respectively.⁶

In the special case of a purely quadratic energy (which fits the requirements of the small strain isotropic damage framework considered in this study), the aforementioned assumptions lead naturally to the following relations for the elastic and plastic energies due to kinematic and isotropic hardening:

$$\frac{1}{2} \boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon}_e = \frac{1}{2} \tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\varepsilon}}_e \quad (\text{elastic energy}) \quad (4.4)$$

$$\frac{1}{2} \boldsymbol{\beta}_p \cdot \mathbf{X}_p = \frac{1}{2} \tilde{\boldsymbol{\beta}}_p \cdot \tilde{\mathbf{X}}_p \quad (\text{plastic energy, kinematic hardening}) \quad (4.5)$$

$$\frac{1}{2} q_p \xi_p = \frac{1}{2} \tilde{q}_p \tilde{\xi}_p \quad (\text{plastic energy, isotropic hardening}) \quad (4.6)$$

The latter relations must be fulfilled for all pairs $(\tilde{\boldsymbol{\varepsilon}}_e, \tilde{\boldsymbol{\sigma}})$, $(\tilde{\mathbf{X}}_p, \tilde{\boldsymbol{\beta}}_p)$ and $(\tilde{\xi}_p, \tilde{q}_p)$ belonging to the fictitious undamaged configuration. A valid solution which automatically fulfills (4.4) -

⁶Note that the fictitious configuration is assumed free of damage, i. e., no ‘effective damage variables’ $(\bar{D}, \bar{Y})$, $(\tilde{\xi}_d, \tilde{q}_d)$, $(\bar{D}, \bar{a}_i)$ or $(\nabla \bar{D}, \bar{\mathbf{b}}_i)$ exist in the formulation.

(4.6) is directly given by

$$\tilde{\sigma} := \frac{\sigma}{f_{\text{dam}}(D)}, \quad \tilde{\epsilon}_e := f_{\text{dam}}(D) \epsilon_e \quad (4.7)$$

$$\tilde{\beta}_p := \frac{\beta_p}{f_{\text{dam}}(D)}, \quad \tilde{\mathbf{X}}_p := f_{\text{dam}}(D) \mathbf{X}_p \quad (4.8)$$

$$\tilde{q}_p := \frac{q_p}{f_{\text{dam}}(D)}, \quad \tilde{\xi}_p := f_{\text{dam}}(D) \xi_p \quad (4.9)$$

where $f_{\text{dam}}(D)$ is an at least twice-differentiable positive and decreasing (but otherwise arbitrary) scalar-valued phenomenological function which is defined to be unity for a virgin material ($D = 0$) and approaches zero, if damage attains a predefined critical value ($D = D_{\text{cr}}$).

4.3.3 State potential in terms of the Helmholtz free energy

In order to derive the state relations of the model, a state potential in terms of the Helmholtz free energy ψ is defined which is here assumed to be a convex and purely quadratic function of the strain-like state variables of the material.⁷ The free energy is additively separable into elastic (ψ_e), plastic (ψ_p) and damage hardening parts (ψ_d), as well as a part related to micromorphic damage ($\psi_{\bar{d}}$):

$$\psi(\epsilon_e, \mathbf{X}_p, \xi_p, D, \xi_d, \bar{D}, \nabla \bar{D}) = \psi_e(\epsilon_e, D) + \psi_p(\mathbf{X}_p, \xi_p, D) + \psi_d(\xi_d) + \psi_{\bar{d}}(D, \bar{D}, \nabla \bar{D}) \quad (4.10)$$

According to the assumptions given in Sect. 4.3.2, the elastic and plastic energy contributions can be expressed in terms of the effective variables, i. e., $\psi_e(\epsilon_e, D) \equiv \psi_e(\tilde{\epsilon}_e)$ and $\psi_p(\mathbf{X}_p, \xi_p, D) \equiv \psi_p(\tilde{\mathbf{X}}_p, \tilde{\xi}_p)$. In detail, the specific expressions for the individual contributions to the energy are defined as follows:

- elastic part of the free energy:

$$\begin{aligned} \psi_e(\tilde{\epsilon}_e) &:= \frac{1}{2} \tilde{\epsilon}_e \cdot \mathcal{C}[\tilde{\epsilon}_e] \\ &= \frac{1}{2} f_{\text{dam}}^2(D) \epsilon_e \cdot \mathcal{C}[\epsilon_e] =: \psi_e(\epsilon_e, D) \end{aligned} \quad (4.11)$$

Here, $\mathcal{C} := \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \mathcal{I}$ denotes the isotropic fourth-order elasticity tensor in which λ, μ are the Lamé parameters and $\mathcal{I}$ is the fourth-order symmetric identity tensor.

⁷This particular choice meets all the requirements of the small strain isotropic damage model considered in this study. However, more complex forms of the energy would certainly be possible, if desired.

- plastic part of the free energy:

$$\begin{aligned}\psi_p(\tilde{\mathbf{X}}_p, \tilde{\xi}_p) &:= \frac{1}{2} a \tilde{\mathbf{X}}_p \cdot \tilde{\mathbf{X}}_p + \frac{1}{2} e \tilde{\xi}_p^2 \\ &= \frac{1}{2} f_{\text{dam}}^2(D) a \mathbf{X}_p \cdot \mathbf{X}_p + \frac{1}{2} f_{\text{dam}}^2(D) e \xi_p^2 =: \psi_p(\mathbf{X}_p, \xi_p, D)\end{aligned}\quad (4.12)$$

Both plastic kinematic and isotropic hardening with corresponding material parameters a and e are considered, respectively.

- damage hardening part of the free energy:

$$\psi_d(\xi_d) := \frac{1}{2} r \xi_d^2 \quad (4.13)$$

The damage hardening variable ξ_d measures damage accumulation and plays a similar role as the isotropic hardening variable ξ_p in plasticity (Cordebois and Sidoroff [1982]).⁸ The constant r is the corresponding damage hardening material parameter.

- micromorphic damage part of the free energy:

$$\psi_{\bar{d}}(D, \bar{D}, \nabla \bar{D}) := \frac{1}{2} H (D - \bar{D})^2 + \frac{1}{2} A \nabla \bar{D} \cdot \nabla \bar{D} \quad (4.14)$$

This quadratic form of the micromorphic energy part represents the simplest micromorphic extension imaginable. The first contribution can be considered as an energetic term penalizing the difference between the local and the micromorphic damage variable. The second contribution is an energy term belonging to the gradient of the micromorphic damage variable which quantifies the amount of influence of the gradient. The parameters H and A are often referred to as the ‘micromorphic moduli’ of the model and can be considered as additional material parameters. Via A , an internal material length is implicitly introduced into the formulation.

⁸It is also possible to consider a translation of the damage surface during the loading process by means of an additional (tensorial) internal variable akin to kinematic hardening in plasticity (see, e. g., Voyiadjis and Thiagarajan [1996]). However, in the present case of scalar isotropic damage, a single damage hardening variable is sufficient.

4.3.4 Derivation of state relations based on the Clausius-Duhem inequality

Following general thermodynamical considerations, the second-law of thermodynamics must be fulfilled and is therefore exploited to derive the state relations of the model. To this end, the Clausius-Duhem inequality is considered which reads in its isothermal local form (Forest [2009]):

$$-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} + \underbrace{a_i \dot{\bar{D}} + \mathbf{b}_i \cdot \nabla \dot{\bar{D}}}_{\text{micromorphic extension}} \stackrel{!}{\geq} 0 \quad (4.15)$$

As indicated above, it can be shown that the micromorphic extension leads naturally to two additional terms in the Clausius-Duhem inequality which account for the contributions of the micromorphic damage and its first gradient to the second-law.

Using the chain rule of differentiation and considering the elastoplastic-split of the strain rate tensor $\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_e + \dot{\boldsymbol{\varepsilon}}_p$, inequality (4.15) can be reformulated as

$$\begin{aligned} & \left(\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(a_i - \frac{\partial \psi}{\partial \bar{D}} \right) \dot{\bar{D}} + \left(\mathbf{b}_i - \frac{\partial \psi}{\partial \nabla \bar{D}} \right) \cdot \nabla \dot{\bar{D}} + \\ & + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \cdot \dot{\boldsymbol{\varepsilon}}_p - \frac{\partial \psi}{\partial \bar{D}} \dot{\bar{D}} - \frac{\partial \psi}{\partial \mathbf{X}_p} \cdot \dot{\mathbf{X}}_p - \frac{\partial \psi}{\partial \xi_p} \dot{\xi}_p - \frac{\partial \psi}{\partial \xi_d} \dot{\xi}_d \geq 0 \end{aligned} \quad (4.16)$$

The latter expression must hold for arbitrary thermomechanical processes. A common (but certainly not necessary) choice is to intentionally set the expressions in the brackets to zero. By doing this and considering expressions (4.10) - (4.14), the state relations of the model follow automatically as

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} = f_{\text{dam}}^2(D) \mathcal{C}[\boldsymbol{\varepsilon}_e], \quad a_i = \frac{\partial \psi}{\partial \bar{D}} = -H(D - \bar{D}), \quad \mathbf{b}_i = \frac{\partial \psi}{\partial \nabla \bar{D}} = A \nabla \bar{D} \quad (4.17)$$

It is still necessary to ensure the validity of the remaining part of the dissipation inequality which can more conveniently be written as

$$\begin{aligned} & \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}_p - \underbrace{\frac{\partial \psi}{\partial \bar{D}} \dot{\bar{D}}}_{:=Y} - \underbrace{\frac{\partial \psi}{\partial \mathbf{X}_p} \cdot \dot{\mathbf{X}}_p}_{:=\beta_p} - \underbrace{\frac{\partial \psi}{\partial \xi_p} \dot{\xi}_p}_{:=q_p} - \underbrace{\frac{\partial \psi}{\partial \xi_d} \dot{\xi}_d}_{:=q_d} \geq 0 \\ \iff & \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}}_p + Y \dot{\bar{D}} - \beta_p \cdot \dot{\mathbf{X}}_p - q_p \dot{\xi}_p - q_d \dot{\xi}_d \geq 0 \end{aligned} \quad (4.18)$$

The above abbreviations have been introduced for notational convenience. These quantities

are the thermodynamic conjugate forces of the model which are computed as

$$Y = -\frac{\partial \psi}{\partial D} = -f_{\text{dam}}(D) \frac{df_{\text{dam}}(D)}{dD} (\boldsymbol{\varepsilon}_e \cdot \mathbf{C}[\boldsymbol{\varepsilon}_e] + a \mathbf{X}_p \cdot \mathbf{X}_p + e \xi_p^2) - H(D - \bar{D}) \quad (4.19)$$

$$\beta_p = \frac{\partial \psi}{\partial \mathbf{X}_p} = f_{\text{dam}}^2(D) a \mathbf{X}_p \quad (4.20)$$

$$q_p = \frac{\partial \psi}{\partial \xi_p} = f_{\text{dam}}^2(D) e \xi_p \quad (4.21)$$

$$q_d = \frac{\partial \psi}{\partial \xi_d} = r \xi_d \quad (4.22)$$

As can be seen from Eq. (4.19), Y is the only thermodynamic conjugate force which is directly influenced by the micromorphic damage variable through the term $-H(D - \bar{D})$. By utilizing this quantity in the definition of the damage loading function, a ‘nonlocal’ character is introduced into the constitutive equations at the Gauss-point level as will be explained in Sect. 4.3.5. Moreover, the expression for Y (often loosely referred to as the ‘energy release rate’) naturally contains not only elastic but also plastic contributions. As was pointed out by several authors, a purely elastic energy release rate might be regarded as too restrictive from a physical point of view (see, e. g., Chaboche [2003], Chow and Wang [1987], Ju [1989], Kachanov [1993], Saanouni et al. [1994]).

4.3.5 Two-surface damage-plasticity formulation

4.3.5.1 Thermodynamical framework

The present model is based on a two-surface formulation where plasticity and damage are treated as distinct dissipative mechanisms which may influence each other but occur also independently. In general, this allows for a high degree of flexibility and applicability of the model.

Formally, the model is inspired by the nowadays well-established framework of ‘generalized standard materials’ (see, e. g., Germain et al. [1983], Hackl [1997], Halphen and Nguyen [1975], Mielke [2006]) in which, in its original version, two potentials are utilized to define a material: (i) the state potential expressed in terms of the state variables sufficient to describe all reversible processes within the material (here the Helmholtz free energy defined in Sect. 4.3.3) and (ii) a single dissipation potential which characterizes all irreversible phenomena. Briefly speaking, if the latter potential can be formulated as a convex function of the thermodynamic conjugate forces which is zero-valued at the origin, evolution equations can be derived accord-

ing to a ‘generalized normality rule’ that a priori fulfill thermodynamic consistency. Further details are omitted here for brevity but can be found, e. g., in the latter references.

Since the mentioned framework using a single dissipation potential can still be too restrictive in certain situations, the concept was further extended to account also for several independent dissipation potentials that describe different processes (see, e. g., Chaboche [1997, 2003]). As will be described in the following, such an approach is adopted in the present work to model plasticity and damage as independent dissipative phenomena.

4.3.5.2 Plasticity modeling

Regarding plasticity, a standard deviatoric von Mises-type yield function is considered in this study⁹ taking into account combined kinematic and isotropic hardening. Coupling between plasticity and damage is introduced into the formulation by expressing the yield function in terms of the effective variables defined in Sect. 4.3.2, i. e.,

$$\begin{aligned}\Phi_p(\tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\beta}}_p, \tilde{q}_p) &= \sqrt{\frac{3}{2}} \left\| \tilde{\boldsymbol{\sigma}}' - \tilde{\boldsymbol{\beta}}_p' \right\| - (\sigma_0 + \tilde{q}_p) \\ &= \sqrt{\frac{3}{2}} \left\| \frac{\boldsymbol{\sigma}'}{f_{\text{dam}}(D)} - \frac{\boldsymbol{\beta}_p'}{f_{\text{dam}}(D)} \right\| - \left(\sigma_0 + \frac{q_p}{f_{\text{dam}}(D)} \right) = \Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) \leq 0\end{aligned}\quad (4.23)$$

Kinematic and isotropic plastic hardening are represented by $\boldsymbol{\beta}_p$ and q_p , respectively, and the initial yield stress is given by the material parameter σ_0 .

In order to model both nonlinear kinematic and isotropic hardening (to account, e. g., for saturated hardening states) and to derive plastic evolution equations which a priori fulfill the remaining dissipation inequality (4.18), the following plastic dissipation potential Ψ_p (again expressed in terms of the effective variables) is defined:

$$\begin{aligned}\Psi_p(\tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\beta}}_p, \tilde{q}_p) &= (\Phi_p + \sigma_0) + \frac{b}{2a} \tilde{\boldsymbol{\beta}}_p' \cdot \tilde{\boldsymbol{\beta}}_p' + \frac{f}{2e} \tilde{q}_p^2 \\ &= (\Phi_p + \sigma_0) + \frac{b}{2a} \frac{\boldsymbol{\beta}_p' \cdot \boldsymbol{\beta}_p'}{f_{\text{dam}}^2(D)} + \frac{f}{2e} \frac{q_p^2}{f_{\text{dam}}^2(D)} = \Psi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D)\end{aligned}\quad (4.24)$$

Here, b and f denote additional plastic material parameters. As required by the theory of generalized standard materials briefly explained in Sect. 4.3.5.1, the potential is a non-negative convex function of its arguments $\tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\beta}}_p, \tilde{q}_p$ (or, equivalently, $\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D$) and zero-valued at the origin, i. e., $\Psi_p(0, 0, 0) = 0$ (or, equivalently, $\Psi_p(0, 0, 0, 0) = 0$).

⁹The modeling of more advanced and complex plastic behavior would certainly be possible by merely adjusting the yield function accordingly.

With Ψ_p at hand, the plastic evolution equations of the model are derived according to the generalized normality rule (Chaboche [2003]) as

$$\dot{\epsilon}_p = \dot{\lambda}_p \frac{\partial \Psi_p}{\partial \boldsymbol{\sigma}}, \quad \dot{\mathbf{X}}_p = -\dot{\lambda}_p \frac{\partial \Psi_p}{\partial \boldsymbol{\beta}_p}, \quad \dot{\xi}_p = -\dot{\lambda}_p \frac{\partial \Psi_p}{\partial q_p} \quad (4.25)$$

Apparently, the structure of Ψ_p leads to non-associative hardening, whereas plastic flow is fully associative, viz.,

$$\dot{\epsilon}_p = \dot{\lambda}_p \frac{\partial \Psi_p}{\partial \boldsymbol{\sigma}} = \dot{\lambda}_p \frac{\partial \Phi_p}{\partial \boldsymbol{\sigma}} = \dot{\lambda}_p \mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, D) \quad (4.26)$$

$$\dot{\mathbf{X}}_p = -\dot{\lambda}_p \frac{\partial \Psi_p}{\partial \boldsymbol{\beta}_p} = -\dot{\lambda}_p \left(\frac{\partial \Phi_p}{\partial \boldsymbol{\beta}_p} + \frac{b}{a} \frac{\boldsymbol{\beta}_p'}{f_{\text{dam}}^2(D)} \right) = -\dot{\lambda}_p \left(-\mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, D) + \frac{b}{a} \frac{\boldsymbol{\beta}_p'}{f_{\text{dam}}^2(D)} \right) \quad (4.27)$$

$$\dot{\xi}_p = -\dot{\lambda}_p \frac{\partial \Psi_p}{\partial q_p} = -\dot{\lambda}_p \left(\frac{\partial \Phi_p}{\partial q_p} + \frac{f}{e} \frac{q_p}{f_{\text{dam}}^2(D)} \right) = -\dot{\lambda}_p \left(-\frac{1}{f_{\text{dam}}(D)} + \frac{f}{e} \frac{q_p}{f_{\text{dam}}^2(D)} \right) \quad (4.28)$$

In the above, $\mathbf{N}$ denotes the flow direction

$$\mathbf{N} := \frac{\partial \Phi_p}{\partial \boldsymbol{\sigma}} = \sqrt{\frac{3}{2}} \frac{1}{f_{\text{dam}}(D)} \frac{\tilde{\boldsymbol{\sigma}}' - \tilde{\boldsymbol{\beta}}_p'}{\|\tilde{\boldsymbol{\sigma}}' - \tilde{\boldsymbol{\beta}}_p'\|} \quad (4.29)$$

Finally, the loading / unloading conditions for plasticity are defined in the usual manner by demanding

$$\dot{\lambda}_p \geq 0, \quad \Phi_p \leq 0, \quad \dot{\lambda}_p \Phi_p = 0 \quad (4.30)$$

Remark 1. The accumulated plastic strain κ (also referred to as the von Mises equivalent or effective plastic strain) can be computed in view of Eq. (4.26) via the rate evolution equation

$$\dot{\kappa} = \sqrt{\frac{2}{3}} \dot{\epsilon}_p \cdot \dot{\epsilon}_p = \sqrt{\frac{2}{3}} \|\dot{\epsilon}_p\| = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} \quad (4.31)$$

4.3.5.3 Damage modeling

Proceeding with the damage behavior of the model, a damage loading function is defined as

$$\Phi_d(Y, q_d) = Y - (Y_0 + q_d) \leq 0 \quad (4.32)$$

where the structural analogy to the description of plastic yield is clearly visible.¹⁰ Damage hardening is represented by quantity q_d and the onset of damage is defined by the damage threshold Y_0 which serves as an additional material parameter of the model. In order to a priori fulfill thermodynamic consistency and model nonlinear damage hardening (able to represent, e. g., saturated damage hardening states), the following damage dissipation potential is postulated:

$$\Psi_d(Y, q_d) = (\Phi_d + Y_0) + \frac{s}{2r} q_d^2 \quad (4.33)$$

Here, s denotes an additional damage material parameter. Again, the potential is a non-negative convex function of its arguments Y , q_d and zero-valued at the origin, i. e., $\Psi_d(0, 0) = 0$.

According to the generalized normality rule and using Ψ_d , the following damage evolution equations are derived

$$\dot{D} = \dot{\lambda}_d \frac{\partial \Psi_d}{\partial Y}, \quad \dot{\xi}_d = -\dot{\lambda}_d \frac{\partial \Psi_d}{\partial q_d} \quad (4.34)$$

As can be seen, the evolution of the damage variable D is fully associative, whereas the evolution of damage hardening is non-associative:

$$\dot{D} = \dot{\lambda}_d \frac{\partial \Psi_d}{\partial Y} = \dot{\lambda}_d \frac{\partial \Phi_d}{\partial Y} = \dot{\lambda}_d \quad (4.35)$$

$$\dot{\xi}_d = -\dot{\lambda}_d \frac{\partial \Psi_d}{\partial q_d} = -\dot{\lambda}_d \left(\frac{\partial \Phi_d}{\partial q_d} + \frac{s}{r} q_d \right) = -\dot{\lambda}_d \left(-1 + \frac{s}{r} q_d \right) \quad (4.36)$$

The loading / unloading conditions for damage are defined by

$$\dot{\lambda}_d \geq 0, \quad \Phi_d \leq 0, \quad \dot{\lambda}_d \Phi_d = 0 \quad (4.37)$$

As was mentioned at the end of Sect. 4.3.4, ‘nonlocality’ of the model is achieved at the local Gauss-point level by expressing the damage loading function Φ_d in terms of the thermodynamic conjugate force to damage Y which itself is directly influenced by the micromorphic damage variable $\bar{D}$.

In total, the material model possesses 12 material parameters: λ , μ , σ_0 , a , b , e , f , Y_0 , r , s , H and A . Except for the penalty constant H which directly affects the penalizing term in expression (4.14) and which may in this work rather be considered as a numerical parameter

¹⁰If desired, the model could certainly be extended for more advanced or even multiple damage loading functions accounting for independent damage mechanisms, as was done, e. g., by Aslan, Cordero, Gaubert and Forest [2011], Aslan, Quilici and Forest [2011].

controlling the degree of interaction between the local and micromorphic damage variable, all other parameters should be determined via suitable experiments (a topic which is out of the scope of the present work).

4.3.6 Weak form of the problem and its linearization

The micromorphic balance equation in (4.3) was derived for a rather general case and can be further simplified in the present study which deals with a micromorphic damage-plasticity model. By neglecting generalized contact and external forces (i. e., $a_c = a_e = 0$, $\mathbf{b}_e = \mathbf{0}$), choosing the damage variable D as the quantity which induces gradient effects (i. e., $\phi = D$ and $\bar{\phi} = \bar{D}$, see Appendix 4.7.1), setting $\Gamma_c \equiv \Gamma$, $\Gamma_{\bar{\phi}} \equiv \emptyset$ and considering expressions (4.17)₂ and (4.17)₃ for a_i and $\mathbf{b}_i$, respectively, the micromorphic balance equation can be written as

$$\begin{aligned} H(D - \bar{D}) + A \operatorname{div}(\nabla \bar{D}) &= 0 \quad \text{in } \Omega \\ 0 &= \nabla \bar{D} \cdot \mathbf{n} \quad \text{on } \Gamma \end{aligned} \quad (4.38)$$

The weak form of the problem is then obtained in the usual way by multiplying the partial differential equations (linear momentum balance and micromorphic balance equation) by appropriate vectorial and scalar test functions $\delta \mathbf{u}$ and $\delta \bar{D}$, respectively, and integrating over the domain Ω . By further considering Gauss’ theorem and taking into account the boundary conditions, the weak form of the problem follows as:

$$g(\mathbf{u}, \bar{D}, \delta \mathbf{u}) := \int_{\Omega} (\boldsymbol{\sigma} \cdot \nabla^s \delta \mathbf{u} - \mathbf{f} \cdot \delta \mathbf{u}) \, d\Omega - \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma = 0 \quad \forall \delta \mathbf{u} \quad (4.39)$$

$$h(\mathbf{u}, \bar{D}, \delta \bar{D}) := \int_{\Omega} (H(D - \bar{D}) \delta \bar{D} - A \nabla \bar{D} \cdot \nabla \delta \bar{D}) \, d\Omega = 0 \quad \forall \delta \bar{D} \quad (4.40)$$

Since the weak form is generally nonlinear, a linearization of expressions (4.39) - (4.40) with respect to the unknowns $\mathbf{u}$ and $\bar{D}$ is carried out, leading to the following set of equations which need to be solved iteratively for the increments $\Delta \mathbf{u}$ and $\Delta \bar{D}$:¹¹

$$\begin{aligned} \int_{\Omega} \nabla^s \delta \mathbf{u} \cdot \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} [\nabla^s(\Delta \mathbf{u})] \right) \, d\Omega + \int_{\Omega} \nabla^s \delta \mathbf{u} \cdot \left(\frac{\partial \boldsymbol{\sigma}}{\partial \bar{D}} \Delta \bar{D} \right) \, d\Omega = \\ - \left(\int_{\Omega} \nabla^s \delta \mathbf{u} \cdot \boldsymbol{\sigma} \, d\Omega - \int_{\Omega} \delta \mathbf{u} \cdot \mathbf{f} \, d\Omega - \int_{\Gamma_t} \delta \mathbf{u} \cdot \mathbf{t} \, d\Gamma \right) \quad \forall \delta \mathbf{u} \end{aligned} \quad (4.41)$$

¹¹The interested reader can find details about the linearization in Appendix 4.7.3.

$$\begin{aligned} \int_{\Omega} \delta \bar{D} H \frac{\partial D}{\partial \varepsilon} \cdot \nabla^s(\Delta \mathbf{u}) \, d\Omega + \int_{\Omega} \delta \bar{D} H \left(\frac{\partial D}{\partial \bar{D}} - 1 \right) \Delta \bar{D} \, d\Omega - \int_{\Omega} A \nabla \delta \bar{D} \cdot \nabla(\Delta \bar{D}) \, d\Omega = \\ - \left(\int_{\Omega} \delta \bar{D} H (D - \bar{D}) \, d\Omega - \int_{\Omega} A \nabla \delta \bar{D} \cdot \nabla \bar{D} \, d\Omega \right) \quad \forall \delta \bar{D} \quad (4.42) \end{aligned}$$

In order to preserve the quadratic convergence of the global Newton-Raphson scheme, the material sensitivities $\partial \boldsymbol{\sigma} / \partial \varepsilon$, $\partial \boldsymbol{\sigma} / \partial \bar{D}$, $\partial D / \partial \varepsilon$ and $\partial D / \partial \bar{D}$ should be computed consistently, i. e., in accordance with the specific numerical algorithm used to integrate the constitutive equations (see, e. g., Simo and Taylor [1985]). This topic will be further discussed in Sect. 4.4.5.

4.4 Algorithmic implementation

4.4.1 Finite element discretization of global equations

In the present section, the finite element approximation of the linearized weak form and the necessary matrix notation will be developed. First of all, the domain of interest Ω is discretized by means of n_{el} finite elements Ω^e according to¹²

$$\Omega \approx \bigcup_{e=1}^{n_{\text{el}}} \Omega^e \quad (4.43)$$

With this, both integrals in the linearized weak form (4.41) - (4.42) defined over Ω can be expressed as sums of integrals over individual element domains Ω^e . Then, finite element approximations of the displacement field $\mathbf{u}(\mathbf{x})$, the micromorphic damage field $\bar{D}(\mathbf{x})$ and the test functions on a typical finite element are introduced as

$$\begin{aligned} \mathbf{u}(\mathbf{x}) \approx \mathbf{u}^e(\mathbf{x}) = \mathbf{N}_u^e(\mathbf{x}) \mathbf{u}^e \quad \delta \mathbf{u}(\mathbf{x}) \approx \delta \mathbf{u}^e(\mathbf{x}) = \mathbf{N}_u^e(\mathbf{x}) \delta \mathbf{u}^e \\ \bar{D}(\mathbf{x}) \approx \bar{D}^e(\mathbf{x}) = \mathbf{N}_{\bar{D}}^e(\mathbf{x}) \bar{D}^e \quad \delta \bar{D}(\mathbf{x}) \approx \delta \bar{D}^e(\mathbf{x}) = \mathbf{N}_{\bar{D}}^e(\mathbf{x}) \delta \bar{D}^e \end{aligned} \quad \mathbf{x} \in \Omega^e \quad (4.44)$$

where $\mathbf{u}^e$ and $\bar{D}^e$ are the respective element nodal values (column vectors) and $\mathbf{N}_u^e$ and $\mathbf{N}_{\bar{D}}^e$ are corresponding element shape functions (matrices). Likewise, necessary spatial derivatives are computed as

$$\begin{aligned} \nabla^s \mathbf{u}(\mathbf{x}) \approx \nabla^s \mathbf{u}^e(\mathbf{x}) = \mathbf{B}_u^e(\mathbf{x}) \mathbf{u}^e \quad \nabla^s \delta \mathbf{u}(\mathbf{x}) \approx \nabla^s \delta \mathbf{u}^e(\mathbf{x}) = \mathbf{B}_u^e(\mathbf{x}) \delta \mathbf{u}^e \\ \nabla \bar{D}(\mathbf{x}) \approx \nabla \bar{D}^e(\mathbf{x}) = \mathbf{B}_{\bar{D}}^e(\mathbf{x}) \bar{D}^e \quad \nabla \delta \bar{D}(\mathbf{x}) \approx \nabla \delta \bar{D}^e(\mathbf{x}) = \mathbf{B}_{\bar{D}}^e(\mathbf{x}) \delta \bar{D}^e \end{aligned} \quad \mathbf{x} \in \Omega^e \quad (4.45)$$

¹²Here and in the following, a superscript e is used to indicate that a quantity pertains to element e .

where $\mathbf{B}_u^e(\mathbf{x}) := \nabla^s \mathbf{N}_u^e(\mathbf{x})$ and $\mathbf{B}_{\bar{D}}^e(\mathbf{x}) := \nabla \mathbf{N}_{\bar{D}}^e(\mathbf{x})$ are matrices of element shape function derivatives.

Clearly, the specific shape of the vectors and matrices defined above depends strongly on the considered space dimension, element type and number of nodes belonging to the displacement and micromorphic damage variable (which may differ from each other, if desired). However, apart from that, these quantities maintain their usual format as commonly known from the field of conventional finite element analysis and as presented in many standard textbooks on this topic (see, e. g., Hughes [1987]).

Introducing $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ as vectors in Voigt notation of the stress and strain tensor, respectively, and inserting the above shown finite element approximations into the linearized weak form (4.41) - (4.42), leads to the following expressions:

$$\begin{aligned} \sum_{e=1}^{n_{el}} \delta \mathbf{u}^{eT} \left\{ \underbrace{\int_{\Omega^e} \mathbf{B}_u^{eT} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} \right)^e \mathbf{B}_u^e d\Omega}_{:= \mathbf{k}_{uu}^e} \Delta \mathbf{u}^e + \underbrace{\int_{\Omega^e} \mathbf{B}_u^{eT} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \bar{D}} \right)^e \mathbf{N}_{\bar{D}}^e d\Omega}_{:= \mathbf{k}_{u\bar{D}}^e} \Delta \bar{D}^e \right\} = \\ - \sum_{e=1}^{n_{el}} \delta \mathbf{u}^{eT} \left\{ \underbrace{\int_{\Omega^e} \mathbf{B}_u^{eT} \boldsymbol{\sigma}^e d\Omega - \int_{\Omega^e} \mathbf{N}_u^{eT} \mathbf{f} d\Omega - \int_{\Gamma_t^e} \mathbf{N}_u^{eT} \mathbf{t} d\Gamma}_{:= \mathbf{r}_u^e} \right\} \quad (4.46) \end{aligned}$$

$$\begin{aligned} \sum_{e=1}^{n_{el}} \delta \bar{D}^{eT} \left\{ \underbrace{\int_{\Omega^e} H \mathbf{N}_{\bar{D}}^{eT} \left(\frac{\partial D}{\partial \boldsymbol{\varepsilon}} \right)^{eT} \mathbf{B}_u^e d\Omega}_{:= \mathbf{k}_{\bar{D}u}^e} \Delta \mathbf{u}^e + \right. \\ \left. + \underbrace{\left(\int_{\Omega^e} H \left(\left(\frac{\partial D}{\partial \bar{D}} \right)^e - 1 \right) \mathbf{N}_{\bar{D}}^{eT} \mathbf{N}_{\bar{D}}^e d\Omega - \int_{\Omega^e} A \mathbf{B}_{\bar{D}}^{eT} \mathbf{B}_{\bar{D}}^e d\Omega \right)}_{:= \mathbf{k}_{\bar{D}\bar{D}}^e} \Delta \bar{D}^e \right\} = \\ - \sum_{e=1}^{n_{el}} \delta \bar{D}^{eT} \left\{ \underbrace{\int_{\Omega^e} H \mathbf{N}_{\bar{D}}^{eT} (D^e - \mathbf{N}_{\bar{D}}^e \bar{D}^e) d\Omega - \int_{\Omega^e} A \mathbf{B}_{\bar{D}}^{eT} \mathbf{B}_{\bar{D}}^e \bar{D}^e d\Omega}_{:= \mathbf{r}_{\bar{D}}^e} \right\} \quad (4.47) \end{aligned}$$

where $\mathbf{k}_{uu}^e$, $\mathbf{k}_{u\bar{D}}^e$, $\mathbf{k}_{\bar{D}u}^e$, $\mathbf{k}_{\bar{D}\bar{D}}^e$, $\mathbf{r}_u^e$, $\mathbf{r}_{\bar{D}}^e$ are used as abbreviations for certain parts of the element stiffness matrix and the element residual vector, respectively. Furthermore, $\Delta \mathbf{u}^e$ and $\Delta \bar{D}^e$ denote the element nodal increments in the displacements and micromorphic damage variable, respectively.

By assembling the individual element contributions in the usual way, taking into account the boundary conditions and further considering the arbitrariness of $\delta \mathbf{u}$ and $\delta \bar{D}$, the following

set of global finite element equations is finally obtained

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\bar{D}} \\ \mathbf{K}_{\bar{D}u} & \mathbf{K}_{\bar{D}\bar{D}} \end{bmatrix} \begin{Bmatrix} \Delta \mathbf{u} \\ \Delta \bar{D} \end{Bmatrix} = - \begin{Bmatrix} \mathbf{R}_u \\ \mathbf{R}_{\bar{D}} \end{Bmatrix} \quad (4.48)$$

where

$$\begin{aligned} \mathbf{K}_{uu} &= \mathbf{A}_{e=1}^{n_{el}}(\mathbf{k}_{uu}^e), \quad \mathbf{K}_{u\bar{D}} = \mathbf{A}_{e=1}^{n_{el}}(\mathbf{k}_{u\bar{D}}^e), \quad \mathbf{K}_{\bar{D}u} = \mathbf{A}_{e=1}^{n_{el}}(\mathbf{k}_{\bar{D}u}^e), \quad \mathbf{K}_{\bar{D}\bar{D}} = \mathbf{A}_{e=1}^{n_{el}}(\mathbf{k}_{\bar{D}\bar{D}}^e), \\ \mathbf{R}_u &= \mathbf{A}_{e=1}^{n_{el}}(\mathbf{r}_u^e), \quad \mathbf{R}_{\bar{D}} = \mathbf{A}_{e=1}^{n_{el}}(\mathbf{r}_{\bar{D}}^e) \end{aligned} \quad (4.49)$$

are the assembled global parts of the stiffness matrix and the residual vector, respectively. In the latter expressions, $\mathbf{A}_{e=1}^{n_{el}}(\bullet)$ denotes the classical finite element assembly operator. Equation system (4.48) needs to be solved iteratively for the global nodal increments $\Delta \mathbf{u}$ and $\Delta \bar{D}$ until convergence is achieved.

4.4.2 Backward Euler discretization of equations at the Gauss-point level

A fully implicit backward Euler scheme is used to discretize the ordinary differential equations of the model in time. Taking into account the evolution equations (4.26) - (4.28) and (4.35) - (4.36) of the present model, this leads to the following set of algebraic equations at the local Gauss-point level:¹³

$$\varepsilon_p = \varepsilon_{p_n} + \Delta \lambda_p \mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) \quad (4.50)$$

$$\mathbf{X}_p = \mathbf{X}_{p_n} - \Delta \lambda_p \left(-\mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) + \frac{b}{a} \frac{\boldsymbol{\beta}_p'}{f_{\text{dam}}^2(D)} \right) \quad (4.51)$$

$$\xi_p = \xi_{p_n} - \Delta \lambda_p \left(-\frac{1}{f_{\text{dam}}(D)} + \frac{f}{e} \frac{q_p}{f_{\text{dam}}^2(D)} \right) \quad (4.52)$$

$$D = D_n + \Delta \lambda_d \quad (4.53)$$

$$\xi_d = \xi_{d_n} - \Delta \lambda_d \left(-1 + \frac{s}{r} q_d \right) \quad (4.54)$$

For a given strain ε and micromorphic damage variable $\bar{D}$, the unknowns to be determined are ε_p , $\mathbf{X}_p$, ξ_p , D , ξ_d , $\Delta \lambda_p$, $\Delta \lambda_d$, where $\Delta \lambda_p = \Delta t \dot{\lambda}_p$ and $\Delta \lambda_d = \Delta t \dot{\lambda}_d$ denote the incremental plastic and damage multipliers, respectively. The stress-like quantities $\boldsymbol{\sigma}$, $\boldsymbol{\beta}_p$, q_p , Y and q_d at time t_{n+1} are computed according to the formulas given in Sect. 4.3.4. The above equations

¹³In what follows, any quantity is referred to the current time step $n+1$, if not explicitly denoted otherwise.

are additionally subject to the time-discrete form of the loading / unloading conditions (4.30) and (4.37) which leads to several distinct cases as will be described next.

Remark 2. During the iteration process at the Gauss-point level, the variables $\mathbf{X}_p$, ξ_p , D , ξ_d do not need to be treated as additional unknowns in the above equation system but can be expressed in terms of the quantities ε_p , $\Delta\lambda_p$, $\Delta\lambda_d$ according to the formulas

$$\begin{aligned}\mathbf{X}_p &= \frac{\mathbf{X}_{p_n} + (\varepsilon_p - \varepsilon_{p_n})}{1 + b \Delta\lambda_p} \\ \xi_p &= \frac{\xi_{p_n} + f_{\text{dam}}^{-1}(D_n + \Delta\lambda_d) \Delta\lambda_p}{1 + f \Delta\lambda_p} \\ D &= D_n + \Delta\lambda_d \\ \xi_d &= \frac{\xi_{d_n} + \Delta\lambda_d}{1 + s \Delta\lambda_d}\end{aligned}\tag{4.55}$$

4.4.3 Possible solutions of the incremental problem

The presence of the constraints (4.30) and (4.37) leads in total to the following four mutually exclusive cases which can occur during a typical (time-)step:

1. *Elastic loading / unloading or neutral loading:*

Both the incremental plastic and damage multipliers are zero, i. e.,

$$\Delta\lambda_p = \Delta\lambda_d = 0\tag{4.56}$$

and, additionally, the constraints

$$\Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) \leq 0, \quad \Phi_d(Y, q_d) \leq 0\tag{4.57}$$

are satisfied. In this case, no plastic flow or damage occurs within the interval $[t_n, t_{n+1}]$. In fact, no evolution of internal variables takes place at all, resulting in a purely elastic (or neutral) step.

2. *Plastic loading:*

The incremental plastic multiplier is strictly positive but the damage multiplier is zero, i. e.,

$$\Delta\lambda_p > 0, \quad \Delta\lambda_d = 0\tag{4.58}$$

and the constraints are given as

$$\Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) = 0, \quad \Phi_d(Y, q_d) \leq 0 \quad (4.59)$$

In this case, plastic evolution takes place within the interval $[t_n, t_{n+1}]$ at a constant state of damage, i. e., $\Delta\lambda_d = 0$, $D = D_n$ and $\xi_d = \xi_{d_n}$. As such, the solution is implicitly defined by Eqs. (4.50) - (4.52) in combination with $\Phi_p = 0$.

3. Elastic-damage loading:

The incremental plastic multiplier is zero but the damage multiplier is strictly positive, i. e.,

$$\Delta\lambda_p = 0, \quad \Delta\lambda_d > 0 \quad (4.60)$$

and the constraints are given as

$$\Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) \leq 0, \quad \Phi_d(Y, q_d) = 0 \quad (4.61)$$

In this case, damage evolution takes place within the interval $[t_n, t_{n+1}]$ but the plastic variables remain constant, i. e., $\Delta\lambda_p = 0$, $\boldsymbol{\varepsilon}_p = \boldsymbol{\varepsilon}_{p_n}$, $\mathbf{X}_p = \mathbf{X}_{p_n}$ and $\xi_p = \xi_{p_n}$. Therefore, the actual state can be computed by solving Eqs. (4.53) - (4.54) in combination with $\Phi_d = 0$.

4. Elastoplastic-damage loading:

In this case, both the incremental plastic and damage multipliers are strictly positive, i. e.,

$$\Delta\lambda_p > 0, \quad \Delta\lambda_d > 0 \quad (4.62)$$

and the constraints are given as

$$\Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) = 0, \quad \Phi_d(Y, q_d) = 0 \quad (4.63)$$

Both plastic and damage evolution takes place within the interval $[t_n, t_{n+1}]$ and the solution is implicitly defined by the fully coupled equation system (4.50) - (4.54) in combination with $\Phi_p = \Phi_d = 0$.

Having Remark 2 in mind, the actual equations which need to be solved in case of an elastoplastic-damage step (case 4) are given below in a residuum format:¹⁴

$$\begin{aligned} \mathbf{r}_1 &= \boldsymbol{\varepsilon}_p - \boldsymbol{\varepsilon}_{p_n} - \Delta\lambda_p \mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) = \mathbf{0} \\ r_2 &= \Phi_p(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) = 0 \\ r_3 &= \Phi_d(Y, q_d) = 0 \end{aligned} \quad (4.64)$$

Owing to the symmetry of the internal variables, the symmetric tensor $\mathbf{r}_1$ can be represented in Voigt form as a six-dimensional array, resulting in a system of eight nonlinear scalar equations in total. The latter have to be solved iteratively, e. g., by means of Newton’s method. For this, a preceding linearization of the equations in (4.64) has to be carried out (for constant values of $\boldsymbol{\varepsilon}$ and $\bar{D}$). In every time step, the iteration is performed until the root-mean-square value of the total residuum becomes smaller than a prescribed tolerance. The internal variables which need to be updated during the iteration are $\boldsymbol{\varepsilon}_p$, $\Delta\lambda_p$ and $\Delta\lambda_d$.

4.4.4 Algorithmic treatment at the Gauss-point level

Due to the above described four different cases which can occur during a typical time step, a suitable algorithmic strategy must be adopted in order to find the actual solution of the incremental problem at the Gauss-point level. Two different monolithic approaches are used in the study which will be explained in the following.

4.4.4.1 Predictor-corrector algorithm using an active set search strategy

The structure of the incremental elastoplastic-damage problem suggests a two-step predictor-corrector solution strategy which is similar to the classical return-mapping algorithms known from usual single-surface elastoplasticity without damage. First of all, a trial elastic solution (corresponding to case 1 described above) is computed and checked for plastic and damage admissibility. If this is indeed the case, the trial solution is accepted as the actual solution and the algorithm terminates.

However, in case that the trial solution is not admissible, a further corrector step is necessary to find the solution. The additional complexity in comparison to classical single-surface elastoplasticity models lies now in the question which system of equations has actually to be solved (either case 2, 3 or 4 described above). In other words, it is not known a priori

¹⁴The corresponding residuals in case of plastic loading (case 2) or elastic-damage loading (case 3) are obtained by deleting either r_3 or $\mathbf{r}_1$ and r_2 in (4.64), respectively.

which constraints $\Phi_\alpha = 0$ ($\alpha \in \{p, d\}$) are ultimately active, i. e., the set of active constraints $\mathbb{J}_{\text{act}} := \{\alpha \in \{p, d\} \mid \Phi_\alpha = 0\}$ becomes itself an unknown of the problem.

An analogous situation arises in the case of multisurface-plasticity where several plastic yield functions are employed in the formulation and can be active at the same time (among others, see Simo et al. [1988], Duriez et al. [2013]) or in crystal plasticity in the context of identifying active slip systems (among others, see Anand and Kothari [1996], Borja and Wren [1993], Schröder and Miehe [1997], Borja and Rahmani [2014]). Solution strategies for these problems can be found, e. g., in the latter references and be adopted for the problem at hand. In the present study, the working procedure for solving the correct equations belonging to the actual active set $\mathbb{J}_{\text{act}}$ in case of a corrector step follows the classical work of Simo et al. [1988] and can be described as follows:

- (1) Define the trial active set as

$$\mathbb{J}_{\text{act}}^{\text{trial}} := \{\alpha \in \{p, d\} \mid \Phi_\alpha^{\text{trial}} > 0\} \quad (4.65)$$

where $\Phi_\alpha^{\text{trial}}$ ($\alpha \in \{p, d\}$) is the plastic yield or damage loading function computed based on the trial values for the internal variables corresponding to the elastic predictor case. Set the counter $k = 0$ and $\mathbb{J}_{\text{act}}^{(0)} = \mathbb{J}_{\text{act}}^{\text{trial}}$.

- (2) Depending on the currently active constraints $\mathbb{J}_{\text{act}}^{(k)}$, solve the corresponding equations to obtain the stresses, plastic strains, internal variables and incremental multipliers $\Delta\lambda_\alpha$ where $\alpha \in \mathbb{J}_{\text{act}}^{(k)}$.
- (3) Check the sign of $\Delta\lambda_\alpha$. If $\Delta\lambda_\alpha < 0$ for any $\alpha \in \mathbb{J}_{\text{act}}^{(k)}$, drop α from the set of active constraints $\mathbb{J}_{\text{act}}^{(k)}$, set $k = k + 1$ and go to step (2). Otherwise, $\mathbb{J}_{\text{act}} \equiv \mathbb{J}_{\text{act}}^{(k)}$, i. e., the solution has been found and the algorithm terminates.

The crucial difference in comparison to classical return-mapping algorithms in single-surface elastoplasticity is an additional outer loop which needs to be performed over the set of active constraints. As mentioned above, this additional complexity is due to the fact that the trial set of active constraints $\mathbb{J}_{\text{act}}^{\text{trial}}$ does not necessarily correspond to the actual set of active constraints $\mathbb{J}_{\text{act}}$.

Remark 3. Theoretically, a situation is conceivable in which the set of trial active constraints $\mathbb{J}_{\text{act}}^{\text{trial}}$ suggests a plastic step (alternatively: elastic-damage step) but, after computing the new state variables in step (2), the damage constraint condition (alternatively: the plastic constraint

condition) is not fulfilled, i. e., $\Phi_d > 0$ (alternatively: $\Phi_p > 0$), even though $\Delta\lambda_d = 0$ (alternatively: $\Delta\lambda_p = 0$). This is a mere consequence of the influence of plastic evolution on the damage-driving force Y which is crucial for Φ_d (alternatively: the influence of damage evolution on the effective variables $\tilde{\sigma}, \tilde{\beta}_p, \tilde{q}_p$ which are crucial for Φ_p). Clearly, such a solution would violate the loading / unloading conditions (4.37) (alternatively: (4.30)) and should be rejected. Therefore, an additional check of the fulfillment of the constraint conditions in step (3) seems advisable before the algorithm actually terminates. In the present study, the strategy employed in such a case would be to solve the full elastoplastic-damage problem, instead of solving only the plastic problem (alternatively: the elastic-damage problem). However, practical experience obtained in all numerical examples of the present study suggests that such a situation is apparently unlikely to occur.

4.4.4.2 Algorithm based on the Fischer-Burmeister complementarity function

The implementation of the predictor-corrector algorithm in combination with the active set search strategy is cumbersome due to the necessary case differentiation as described in Sect. 4.4.3. In the authors’ opinion, the implementation effort is still bearable in the present context where only two constraint functions need to be considered. However, the complexity of active set search strategies usually significantly increases with the number of available constraints and the question arises as to whether other algorithms exist which are more convenient to implement.

Indeed, alternative solution strategies were proposed in the literature, as, e. g., those which are based on a reformulation of the original inequality-constrained problem as a corresponding unconstrained problem in terms of the so-called Fischer-Burmeister complementarity function (Fischer [1992, 1995a,b]). Such an approach was successfully utilized by Schmidt-Baldassari [2003] in the context of crystal plasticity in order to avoid a complex active set search strategy to satisfy several sets of Kuhn-Tucker conditions. Later, Ashrafi et al. [2016], Auricchio et al. [2014], Bartel and Hackl [2009, 2010], Bartel et al. [2011] and Scalet et al. [2015] applied the Fischer-Burmeister approach in models for shape-memory alloys. Furthermore, Kiefer et al. [2012] presented and compared two algorithms for the numerical treatment of magnetic shape-memory alloys, one based on a classical active set search strategy and the other based on the just mentioned reformulation in terms of the Fischer-Burmeister complementarity function. By means of several benchmark tests, they concluded that the latter algorithm in their particular case was numerically more efficient.

The scalar-valued Fischer-Burmeister complementarity function $\phi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is con-

structed as

$$\phi(a, b) := a + b - \sqrt{a^2 + b^2}, \quad a, b \in \mathbb{R} \quad (4.66)$$

and possesses the property that

$$\phi(a, b) = 0 \iff a \geq 0, b \geq 0, ab = 0 \quad (4.67)$$

Accordingly, the set of equality and inequality constraints (4.67) can be rewritten as a single equality constraint. Now observe that the following statements are equivalent to each other:

$$\phi(\Delta\lambda_p, -\Phi_p) = 0 \iff \Delta\lambda_p \geq 0, \Phi_p \leq 0, \Delta\lambda_p \Phi_p = 0 \quad (4.68)$$

$$\phi(\Delta\lambda_d, -\Phi_d) = 0 \iff \Delta\lambda_d \geq 0, \Phi_d \leq 0, \Delta\lambda_d \Phi_d = 0 \quad (4.69)$$

In other words, using the Fischer-Burmeister complementarity function a fulfillment of the two sets of time-discrete loading / unloading conditions for plasticity and damage can be achieved by solving two equations which is certainly easier from a conceptual point of view. In summary, by replacing residuals r_2 and r_3 in (4.64) one ends up with the following set of equations, viz.,

$$\begin{aligned} \mathbf{r}_1 &= \boldsymbol{\varepsilon}_p - \boldsymbol{\varepsilon}_{p_n} - \Delta\lambda_p \mathbf{N}(\boldsymbol{\sigma}, \boldsymbol{\beta}_p, q_p, D) = \mathbf{0} \\ r_2 &= \Delta\lambda_p - \Phi_p - \sqrt{\Delta\lambda_p^2 + \Phi_p^2} = 0 \\ r_3 &= \Delta\lambda_d - \Phi_d - \sqrt{\Delta\lambda_d^2 + \Phi_d^2} = 0 \end{aligned} \quad (4.70)$$

which need to be solved iteratively, e. g., by means of Newton's method. In contrast to the algorithm based on the active set search strategy, always the same equation system (4.70) is solved regardless of whether the step is actually elastic, plastic and involves damage or not. Any case differentiation is rigorously avoided which is appealing from an algorithmic point of view.

However, the very same argument could be interpreted negatively: even in case of a purely elastic-damage step, a system of eight nonlinear scalar equations needs to be solved in contrast to a single equation in case of the 'classical' method based on the active set search strategy. Therefore, the gain in conceptual simplicity by using the Fischer-Burmeister approach may be paid by a loss in computational efficiency which increases with the number of given constraints.

Remark 4. The Fischer-Burmeister complementarity function ϕ is non-differentiable at $(0, 0)$. As proposed by Kanzow [1996], it is reasonable from a numerical viewpoint to work with a

slightly modified functional $\phi_\epsilon(a, b) := a + b - \sqrt{a^2 + b^2 + 2\epsilon^2}$ which possess the property

$$\phi_\epsilon(a, b) = 0 \iff a \geq 0, b \geq 0, ab = \epsilon^2 \quad (4.71)$$

where ϵ plays the role of a numerical regularization parameter. Clearly, using ϕ_ϵ the original damage-plasticity problem is only solved approximately and becomes sensitive to the choice of the parameter ϵ . However, in the authors’ experience the parameter can be chosen quite small, e. g., $\epsilon = 10^{-8}$, such that the overall effect on the solution is negligible and is close to the usual precision of the numerical integration procedure itself.

Another issue is related to the rate of convergence and convergence radius using the Fischer-Burmeister approach. As reported by Auricchio et al. [2014] for the case of shape memory alloys and realized by the present authors as well for the discussed damage-plasticity model, the Newton iteration for solving equation system (4.70) depends more heavily on the quality of the initial guess for the solution than its active-set search counterpart solving the ‘classical’ equation system (4.64). Choosing an inappropriate initial guess may result in slow convergence or even divergence of the Newton iteration at the local Gauss-point level. In the present study, a quite noticeable improvement in this regard could be achieved by employing additionally a line-search technique to find a better starting point for the iteration. The authors made good experience with the same back-tracking method as used also by Auricchio et al. [2014] for their model. Details about the implementation and the applied parameters are omitted here for brevity but can be found in the latter reference and the cited references therein.

4.4.5 Consistent tangent operators

The calculation of the tangential stiffness matrix in a finite element program necessitates the computation of the algorithmic tangent moduli of the model (see, e. g., Simo and Taylor [1985]). The relationship between the increments $\Delta\sigma$, ΔD and $\Delta\epsilon$, $\Delta\bar{D}$ can be expressed as:

$$\Delta\sigma = \mathcal{C}_\epsilon [\Delta\epsilon] + \mathbf{C}_{\bar{D}} \Delta\bar{D} \quad (4.72)$$

$$\Delta D = \mathbf{E}_\epsilon \cdot \Delta\epsilon + E_{\bar{D}} \Delta\bar{D} \quad (4.73)$$

where $\mathcal{C}_\epsilon$ (fourth-order tensor), $\mathbf{C}_{\bar{D}}$, $\mathbf{E}_\epsilon$ (second-order tensors) and $E_{\bar{D}}$ (scalar) denote the consistent (algorithmic) tangent operators of the model. In the following, it will be shown how these quantities can be computed.

Since the stress σ is a function of ε , ε_p and D , the increment $\Delta\sigma$ can be expressed as

$$\begin{aligned}\Delta\sigma &= \frac{\partial\sigma}{\partial\varepsilon} [\Delta\varepsilon] + \frac{\partial\sigma}{\partial\varepsilon_p} [\Delta\varepsilon_p] + \frac{\partial\sigma}{\partial D} \Delta D = \\ &= \left(\frac{\partial\sigma}{\partial\varepsilon} + \frac{\partial\sigma}{\partial\varepsilon_p} : \frac{\partial\varepsilon_p}{\partial\varepsilon} + \frac{\partial\sigma}{\partial D} \otimes \frac{\partial D}{\partial\varepsilon} \right) [\Delta\varepsilon] + \left(\frac{\partial\sigma}{\partial\varepsilon_p} \left[\frac{\partial\varepsilon_p}{\partial\bar{D}} \right] + \frac{\partial\sigma}{\partial D} \frac{\partial D}{\partial\bar{D}} \right) \Delta\bar{D} \quad (4.74)\end{aligned}$$

By comparing the latter equation with (4.72), the expressions in the round brackets are identified as the moduli $\mathcal{C}_\varepsilon$ and $\mathcal{C}_{\bar{D}}$, respectively. The partial derivatives of σ can easily be computed from the stress-strain relationship (4.17)₁. The other partial derivatives can be computed by considering the relationships between the increments $\Delta\varepsilon_p$, ΔD and $\Delta\varepsilon$, $\Delta\bar{D}$ which are obtained after the local Gauss-point iteration for the equations in (4.64) (or the equations in (4.70) if the Fischer-Burmeister approach is used) has converged

$$\Delta\varepsilon_p = \frac{\partial\varepsilon_p}{\partial\varepsilon} [\Delta\varepsilon] + \frac{\partial\varepsilon_p}{\partial\bar{D}} \Delta\bar{D} = (-\mathcal{A}_p^{-1} : \mathcal{A}_\varepsilon) [\Delta\varepsilon] + (-\mathcal{A}_p^{-1} [\mathbf{A}_{\bar{D}}]) \Delta\bar{D} \quad (4.75)$$

$$\Delta D = \frac{\partial D}{\partial\varepsilon} \cdot \Delta\varepsilon + \frac{\partial D}{\partial\bar{D}} \Delta\bar{D} = (-B_{\Delta\lambda_d}^{-1} \mathbf{B}_\varepsilon) \cdot \Delta\varepsilon + (-B_{\Delta\lambda_d}^{-1} B_{\bar{D}}) \Delta\bar{D} \quad (4.76)$$

Again, by comparing (4.76) with (4.73), $\mathbf{E}_\varepsilon$ and $E_{\bar{D}}$ are identified as the corresponding expressions in the round brackets, respectively. The interested reader may find the specific expressions for $\mathcal{A}_p$, $\mathcal{A}_\varepsilon$ (fourth-order tensors), $\mathbf{A}_{\bar{D}}$, $\mathbf{B}_\varepsilon$ (second-order tensors) and $B_{\Delta\lambda_d}$, $B_{\bar{D}}$ (scalars) in Appendix 4.7.4.

Summarizing, the consistent tangent operators can be computed as

$$\mathcal{C}_\varepsilon = \frac{\partial\sigma}{\partial\varepsilon} - \frac{\partial\sigma}{\partial\varepsilon_p} : \mathcal{A}_p^{-1} : \mathcal{A}_\varepsilon - \frac{\partial\sigma}{\partial D} \otimes B_{\Delta\lambda_d}^{-1} \mathbf{B}_\varepsilon \quad (4.77)$$

$$\mathcal{C}_{\bar{D}} = -\frac{\partial\sigma}{\partial\varepsilon_p} [\mathcal{A}_p^{-1} [\mathbf{A}_{\bar{D}}]] - \frac{\partial\sigma}{\partial D} B_{\Delta\lambda_d}^{-1} B_{\bar{D}} \quad (4.78)$$

$$\mathbf{E}_\varepsilon = -B_{\Delta\lambda_d}^{-1} \mathbf{B}_\varepsilon \quad (4.79)$$

$$E_{\bar{D}} = -B_{\Delta\lambda_d}^{-1} B_{\bar{D}} \quad (4.80)$$

4.5 Numerical examples

4.5.1 Influence of the damage parameters in the model

Prior to the assessment of the model's ability to regularize the mesh size dependence in structural finite element simulations involving damage, the influences of the respective damage pa-

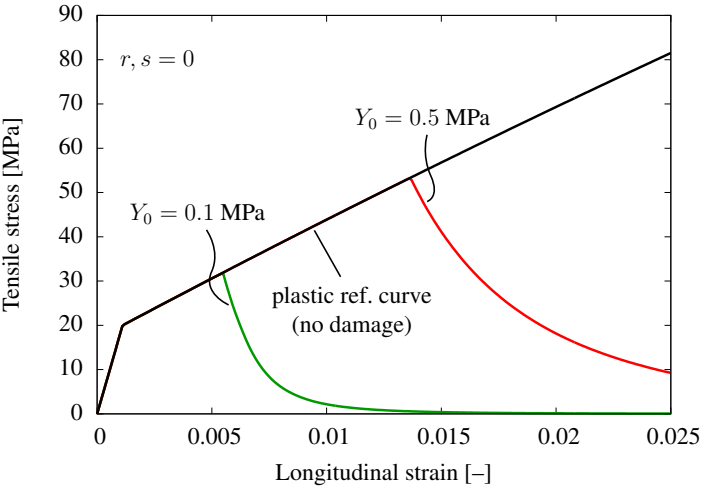
rameters Y_0 , r , s in the formulation are studied and illustrated in a simple and direct way. For this purpose, a single 3D finite element of unit length is subjected to a state of uniaxial tension and the model’s stress-strain response at a typical Gauss-point is examined. The remaining parameters of the model are prescribed as: $\lambda = 5000$ MPa, $\mu = 7500$ MPa, $a = 1900$ MPa, $b = 8.5$, $e = 400$ MPa, $f = 2.5$, $\sigma_0 = 20$ MPa, $H = 10^5$ MPa and $A = 10$ MPa mm².¹⁵ The function in Eqs. (4.7) - (4.9) is chosen as $f_{\text{dam}}(D) = 1 - D$.

The results of this investigation are shown in Figs. 4.1 - 4.3. Fig. 4.1 demonstrates the influence of the damage threshold Y_0 by neglecting any damage hardening, i. e., by setting $r = s = 0$. As expected, a higher value $Y_0 = 0.5$ MPa leads to a later onset of damage (red curve) in the simulation than in case of a lower value $Y_0 = 0.1$ MPa (green curve). Sudden increases of D and ξ_d along with a pronounced decrease in the tensile stress are noticeable in both cases as soon as the respective damage threshold is reached in the simulation. Apparently, the stress softening due to damage exceeds the plastic hardening effect for the particular material parameters chosen. As indicated in Fig. 4.1b, D and ξ_d are in fact equivalent in the present case which can readily be understood by inspecting Eq. (4.54) and considering $s = 0$. Owing to the specific choice of $f_{\text{dam}}(D)$ which leads to $\sigma = (1 - D)^2 \mathcal{C}[\epsilon_e]$ in Eq. (4.17), the tensile stress very smoothly approaches zero for increasing longitudinal strain and damage. A similar observation can be made for D and ξ_d which approach unity, respectively. For better illustration and as a reference, the stress-strain response of a purely elastoplastic material without damage is visualized in addition (black curve in Fig. 4.1a), a case which can be recovered by considering $Y_0 \rightarrow \infty$ in the model.

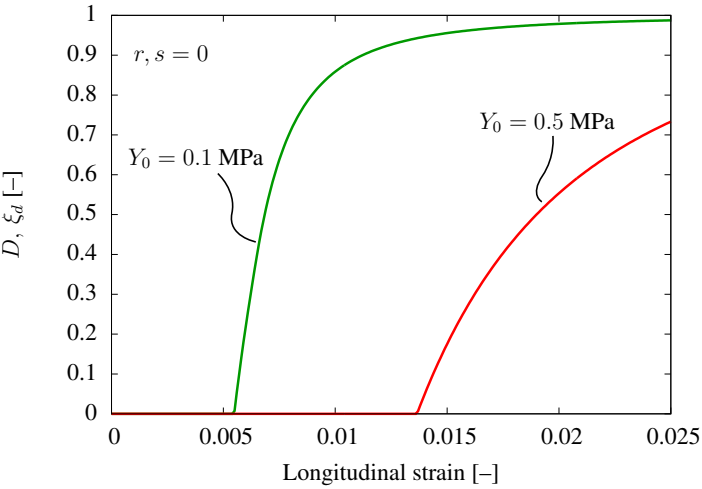
In Fig. 4.2, the influence of parameter r is studied by assuming further that $Y_0 = 0.1$ MPa and $s = 0$, effectively leading to the case of linear damage hardening in the model. From Eq. (4.54) it can again be inferred that D and ξ_d are equivalent in this case. By gradually increasing r , several different results for the stress-strain response as well as D and ξ_d are obtained (blue curves). The arrows in Figs. 4.2a and 4.2b indicate the change of the results for an increasing value of r , respectively. Apparently, damage hardening can be used for ‘slowing down’ the evolution of the damage variable D . For $r = 0$ and $r \rightarrow \infty$, one recovers the cases of no damage hardening (green dashed curve) and pure elastoplasticity without damage (black curve in Fig. 4.2a), respectively.

Finally, Fig. 4.3 demonstrates the meaning of nonlinear damage hardening in the model, visualized by gradually increasing parameter s in the simulation. For an insightful illustration, the damage threshold is again set to $Y_0 = 0.1$ MPa and the same values of r are used as in

¹⁵Since uniaxial tension leads to a completely homogeneous state within the element, the micromorphic parameters A , H do actually have no influence in the present case. This can be understood by inspecting Eq. (4.38) and considering that $\nabla \bar{D}$ vanishes identically, leading to $D = \bar{D}$ everywhere within the element, as desired.

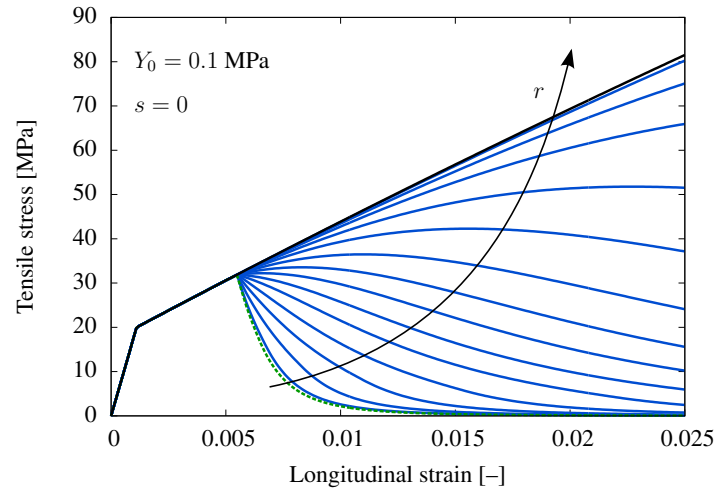


(a) Stress-strain response

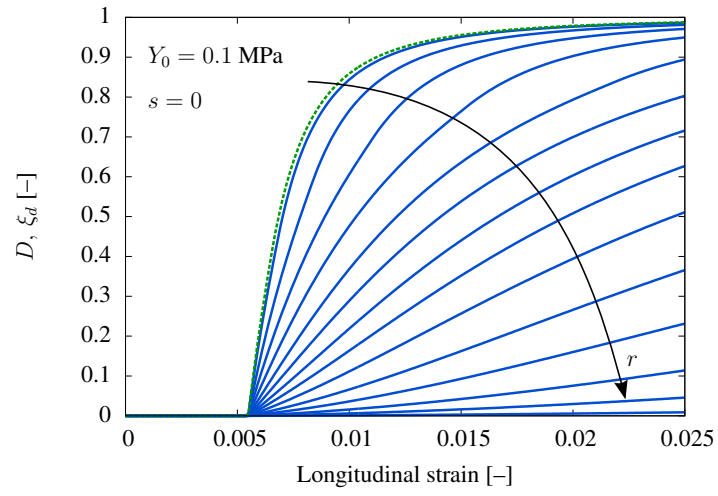


(b) Evolution of D and ξ_d

Figure 4.1: Influence of parameter Y_0 (assuming $r, s = 0$)



(a) Stress-strain response



(b) Evolution of D and ξ_d

Figure 4.2: Influence of parameter r (assuming $s = 0$)

Fig. 4.2. Moreover, s is adjusted such that the ratio r/s is always kept constant at 0.4 MPa (leading to the displayed blue curves). Arrows indicate the change of the results for increasing values of r and s , respectively. From Eq. (4.54) it can be inferred that ξ_d and D now truly differ from each other which is practically confirmed by inspecting Figs. 4.3b and 4.3c, respectively. For any $s > 0$, a certain saturation of ξ_d (and thus damage hardening) can be modeled. For instance, for $s = 0$ and $s \rightarrow \infty$ one recovers the same material behaviors as would be obtained for no damage hardening with damage thresholds $Y_0 = 0.1$ MPa and $Y_0 = 0.5$ MPa, respectively (green and red dashed curves). As such, nonlinear damage hardening allows for an additional flexibility of the model such that the latter can be adapted to even more possible softening behaviors of a material.

It should be recalled that yet another possibility exists to control the damage behavior of the model by choosing a different expression for $f_{\text{dam}}(D)$ in Eqs. (4.7) - (4.9). For brevity, this shall not be further discussed here.

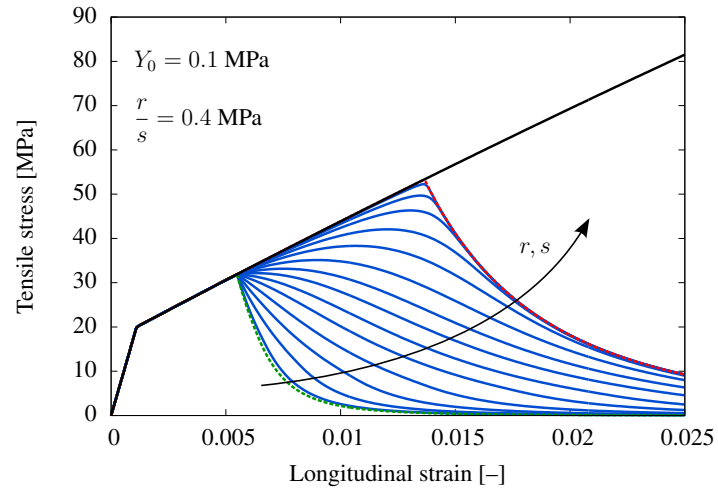
4.5.2 One-dimensional bar with imperfection under tension

4.5.2.1 Problem description and assumed material properties

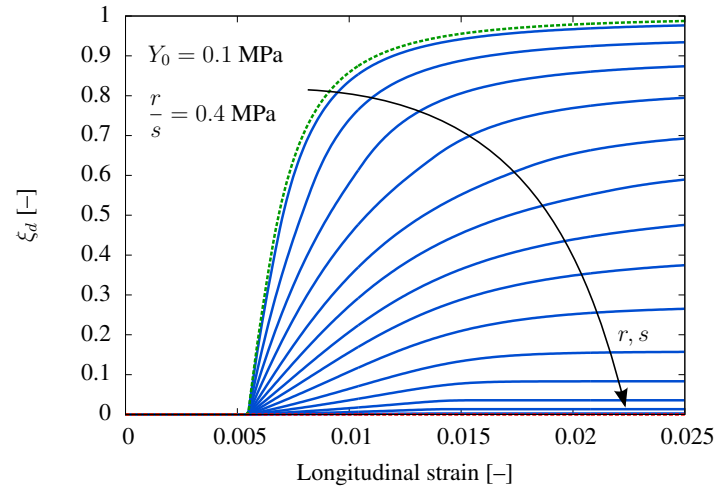
It is worthwhile to study the basic properties of the proposed micromorphic damage model in a simple context first. As a benchmark problem, a one-dimensional bar of length ℓ and cross section A_b is considered which is subjected to a state of uniaxial tension by applying two equal but opposite forces F at its both ends. The bar possesses a geometrical imperfection of length ℓ_w in its middle which is characterized by a cross section reduction α in order to control and trigger a localization process in this area. The elongation of the bar is measured by means of the displacement u at both ends. A schematic illustration of the problem is given in Fig. 4.4.

Due to a current lack of experimental data, the following arbitrary material properties are assumed throughout the analysis: $E = 210000$ MPa, $a = 1900$ MPa, $b = 8.5$, $e = 400$ MPa, $f = 2.5$, $r = 0.5$ MPa, $s = 0.1$, $\sigma_0 = 20$ MPa, $Y_0 = 0.1$ MPa and $H = 10^5$ MPa.¹⁶ Here, E denotes the Young's modulus of the material. The function in Eqs. (4.7) - (4.9) is defined as $f_{\text{dam}}(D) = 1 - D$. Furthermore, the length and cross section of the bar are set to $\ell = 100$ mm and $A_b = 1$ mm², respectively. Symmetry is exploited, only one-half of the specimen needs to be taken into account in the meshing process and during the simulation. Linear finite element approximations of the displacement field and the micromorphic damage field are considered (see Eqs. (4.44) - (4.45)).

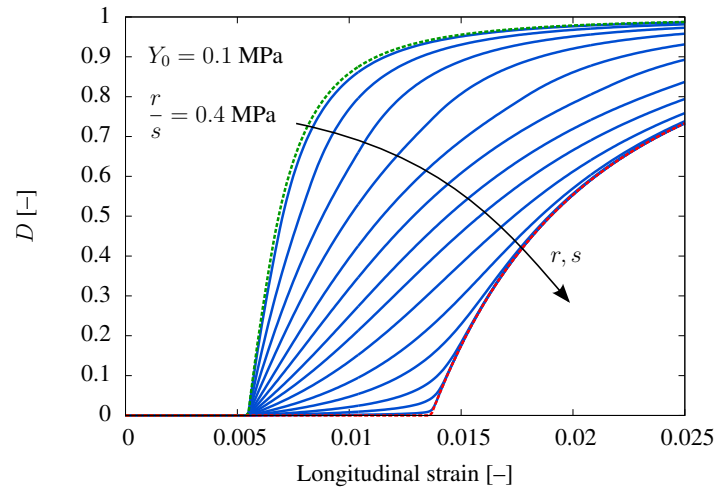
¹⁶The influence of the gradient parameter A is studied in detail and therefore varied during the example.



(a) Stress-strain response



(b) Evolution of ξ_d



(c) Evolution of D

Figure 4.3: Influence of parameter s (assuming $r/s = \text{const.} = 0.4 \text{ MPa}$)

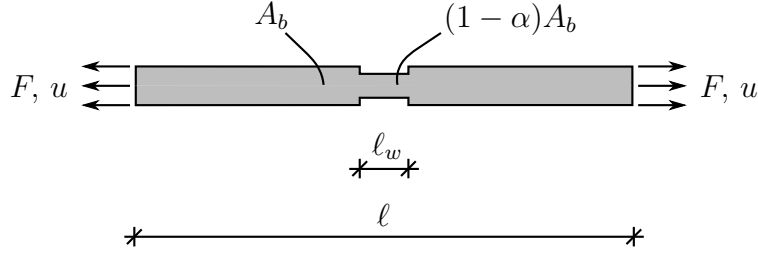


Figure 4.4: One-dimensional bar with imperfection under tension (schematic illustration)

4.5.2.2 General considerations

Before the numerical results of the example are to be discussed, two features shall briefly be mentioned which continuum damage models should desirably possess in order to serve as suitable tools in simulating damage processes. The first (here named F1) is related to the phase of crack initiation whereas the second (F2) belongs to the phase of crack opening:

F1: *Crack initiation phase.* During a localization process (which usually precedes the development of a crack), the model should be able to describe a progressive intensification of strains and damage within an ever-narrowing region of the considered structure. This process should ultimately end up in a fully developed failure zone (or initiation of a macro-crack) which is characterized by complete damage, i. e., in the present context by $D \approx D_{\text{cr}} = 1$. Ideally, this fully developed failure zone should preferably be a ‘sharp’ interface, i. e., nearly a point in a one-dimensional framework, whereas it should be close to a line or surface in a two- or three-dimensional setting, respectively.

F2: *Crack opening phase.* When damage has fully developed somewhere in the structure, the latter may essentially be regarded as ‘broken’ in this zone. From this point on, no (or only very little) loading can be transferred over this interface to neighboring elements. On the one hand, this means that damage should neither further increase in value in the failure zone nor should the damage zone itself further widen in a direction perpendicular to the crack where the material should unload elastically (Geers et al. [1998]). On the other hand, since almost no structural resistance is present anymore in this region, a strain increase should still be possible and the strain should with ongoing tension approach infinity in the fully developed failure zone (the crack ‘opens’).

Especially the modeling of crack opening (F2) in a continuous finite element framework has proven to be a difficult task even for gradient-extended damage models. For example, the popular implicit-gradient enhanced damage model based on nonlocal equivalent strain (see, e. g., Peerlings et al. [1995, 1996, 1998]) shows a tendency to predict a physically implausible

widening of the damage zone at highly damaged states within the material. Sophisticated modifications of the original formulation were proposed in order to partially overcome this problem (see, e. g., Geers et al. [1998], Saroukhani et al. [2013]).

The proposed micromorphic damage model shall be tested against the just mentioned requirements. In order to better illustrate its merits, a comparison is also conducted to a local version of the very same model which does not benefit from the micromorphic enhancement.

4.5.2.3 Results obtained by using the local version of the model

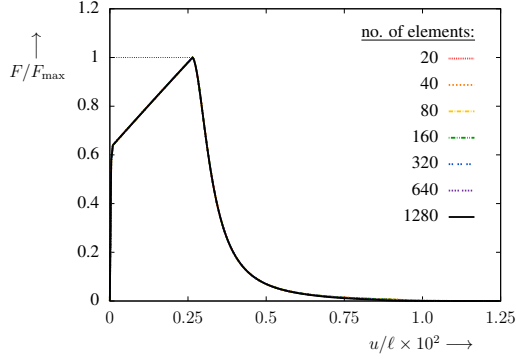
A local version of the model can be fully recovered from its micromorphic counterpart by setting the micromorphic parameters A and H and the additional degree of freedom $\bar{D}$ to zero everywhere in the considered structure. By utilizing this local model, the simulation is then repeatedly performed using an increasing number of elements. Equally-spaced meshes are used with 20 up to 1280 elements and a study of convergence is carried out. In the simulations, the imperfection zone is characterized by $\ell_w = 10$ mm and $\alpha = 0.1$, meaning a cross section reduction of 10% compared to the rest of the bar. The results are shown in Fig. 4.5a in terms of the (normalized) load-displacement curves. A nearly perfect mesh convergence is achieved, no more than 20 elements would actually be necessary for the computation. Initially, load F increases rapidly in the elastic range and then less pronounced when plasticity with both kinematic and isotropic hardening comes into play. At a certain load maximum (here denoted as $F_{\max}$), damage sets in and a severe drop in the curve becomes apparent after which the load subsequently approaches zero.¹⁷

The reason for the good convergence behavior becomes clear by inspecting the (pseudo-)time evolution of the stress and damage distributions in Figs. 4.5b and 4.5c for the case of 1280 elements, respectively.¹⁸ Due to balance of linear momentum, the stress in the imperfection zone is given by $F/A_b(1 - \alpha)^{-1}$ whereas it is F/A_b in the remaining part of the bar, i. e., in every (pseudo-)time step the stress is a piecewise constant function along the bar (for a better visualization, only the difference between the stress σ along the bar and the stress F/A_b outside of the imperfection zone is plotted in Fig. 4.5b). The stress plays a decisive role for the evolution of the internal variables and – in case of the local model – material points are not directly influenced by other surrounding points. It seems therefore reasonable that the internal variables at each material point within either the imperfection zone or outside of it develop equally, respectively, i. e., they all become piecewise constant functions along the bar

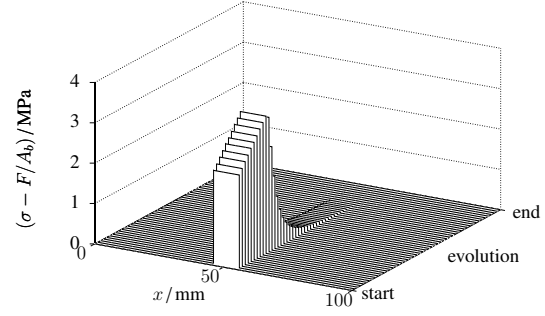
¹⁷The immediate load drop after the initiation of damage happens since the softening effect due to damage is, apparently, directly stronger than the effect of plastic hardening in the present case.

¹⁸‘Snapshots’ of the respective distributions are taken at 50 equally-spaced (pseudo-)time steps. This holds also true for all the evolution plots following later on.

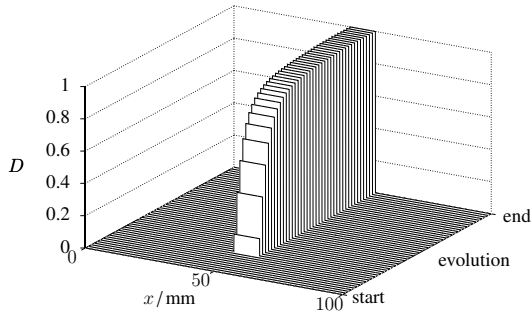
(see, e. g., Fig. 4.5c for the evolution of the damage variable D). In consequence, the strain becomes a piecewise constant function as well, as can be seen in Fig. 4.5d. The finite element method based on linear shape functions is capable of representing this solution exactly which is the reason for the good convergence behavior.



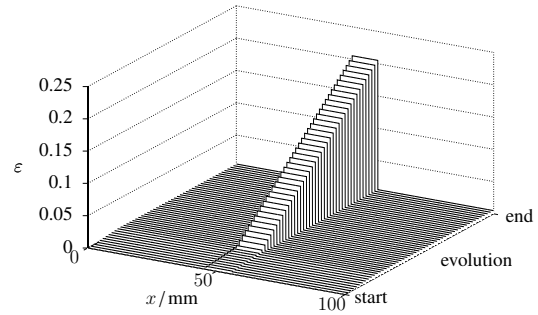
(a) Force-displacement curve



(b) Stress evolution (1280 elements)



(c) Damage evolution (1280 elements)



(d) Strain evolution (1280 elements)

Figure 4.5: Results obtained by using the local version of the model

Nevertheless, the results obtained for the local model are questionable since they violate the requirements of feature F1 stated above. More precisely, even though damage grows in this area up to $D \approx 1$ and remains bounded both in value and width from that point on (essentially fulfilling the requirements of feature F2), the process itself does, by its very nature, not resemble a localization process: no narrowing of the localization zone occurs and thus no ‘sharp’ failure zone develops. In fact, the damage zone is from the outset entirely determined by and restricted to the size of the imperfection zone itself which seems physically unjustifiable.

The geometrical imperfection was originally introduced in order to induce a stress inhomogeneity that triggers a localization process at a predefined location in the specimen. From a numerical point of view, this allows for a certain ‘manual’ control of the process which is

otherwise destined accidentally: more precisely, in a perfect bar under simple tension, localization can either be initiated at possibly multiple locations simultaneously by numerical round-off errors or not occur at all which leads to a completely uniform behavior within all elements.¹⁹ At the price of a slightly modified problem (i. e., by introducing the imperfection), it is therefore possible to study a single localization process at a well-defined location within the structure which is the actual goal of the example.²⁰ Furthermore, by gradually decreasing the size of the imperfection (here characterized by ℓ_w and α), it seems rational to expect that the obtained solution converges towards the actually desired single localization solution of the original perfect bar problem.

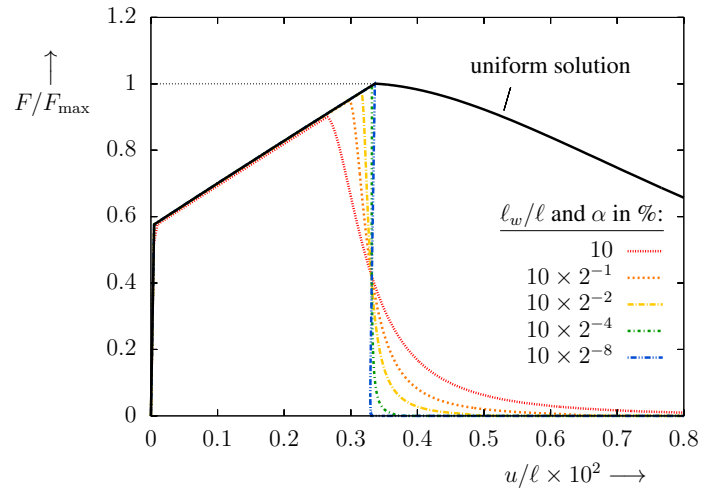
The results of such an imperfection sensitivity analysis are shown in Fig. 4.6 in terms of the obtained force-displacement curves and corresponding damage zones at the end of the simulations. An equally-spaced mesh of 10240 elements was used in all simulations. It can be observed that, the smaller the imperfection size becomes, the more the maximum load increases and shifts to the right in the diagram whereas the load drop following afterwards becomes heavier. In the limit, i. e., $\ell_w \rightarrow 0$ and $\alpha \rightarrow 0$, the force-displacement curve closely resembles that of a pure elastoplastic bar without damage which is merely unloaded at a certain stage of the process. More specifically, it is the same stage where damage would set in in case of a perfect bar without geometrical imperfection.²¹ The energy necessary to build the ‘crack’ becomes smaller and smaller and in the limit, perfectly brittle failure in a vanishing damage zone occurs (Fig. 4.6b) which requires no energy supply. This is not only a problem of the specific constitutive model considered here but indicates that a physically reasonable modeling of localization processes is usually beyond the capabilities of local damage models.

For completeness, it should be mentioned that an arclength method was utilized in all the aforementioned simulations. This was necessary in the cases of the two smallest imperfection sizes due to the occurrence of snapback in the force-displacement curves after the load maximum (see Fig. 4.6a). For better consistency and comparison purposes, the arclength method was then applied also in the remaining cases.

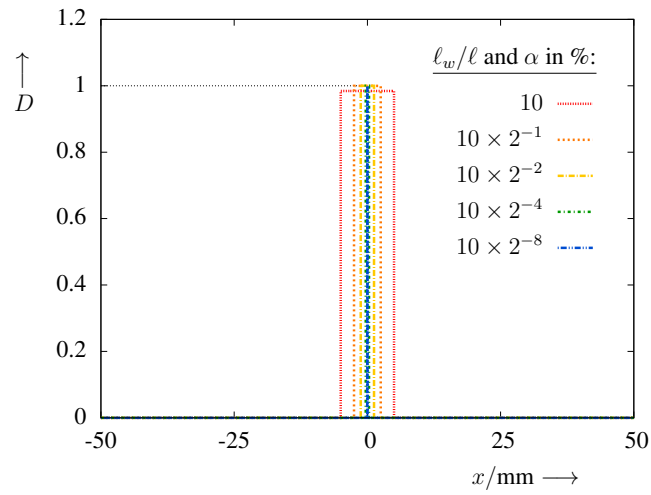
¹⁹It is worth mentioning that this sentence holds true for both the local and the micromorphic version of the model because their results are identical for an initially completely homogeneous problem as the perfect bar under simple tension.

²⁰Unfortunately, even the introduction of the imperfection zone does not preclude the existence of multiple solutions and the possibility of spontaneous strain localization in material points *within* the weakend zone of the bar during the simulation is still possible. However, in the authors’ experience the degree of numerical control of the process to reach the desired solution is largely increased by introducing the imperfection.

²¹For convenience, also the uniform solution (damage takes place equally in all elements) is illustrated in Fig. 4.6a which is obtained for the perfect bar under simple tension (black solid curve).



(a) Force-displacement curve



(b) Damage distribution at end of simulation

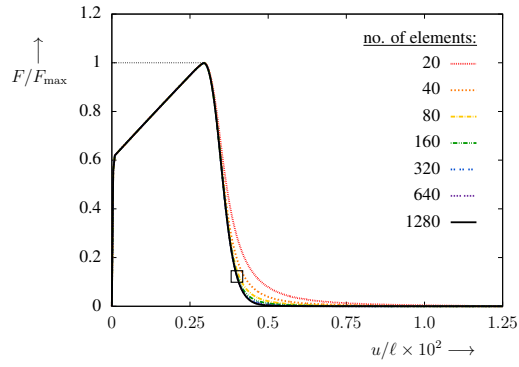
Figure 4.6: Influence of the imperfection size (local model, 10240 elements)

4.5.2.4 Results obtained by using the micromorphic model

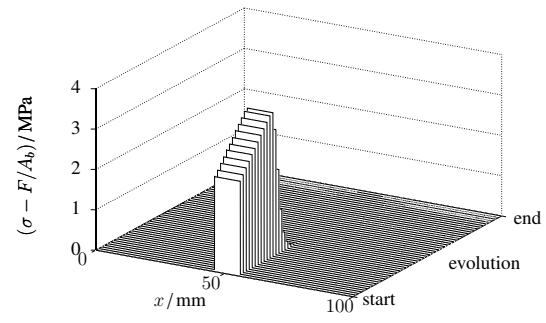
Fig. 4.7a shows the results of the convergence study obtained by using the regularized micromorphic damage model ($\ell_w = 10$ mm, $\alpha = 0.1$, $A = 10$ MPa mm²). Again, an arclength method was utilized in all computations in order to properly account for any possible occurrence of snapback in the simulations. This time, the force-displacement curves for the different meshes vary from each other. However, convergence towards a well-defined result is clearly visible. As desired, the stress distribution is still dictated by the linear momentum balance and remains a piecewise constant function in every step but the shapes of the damage and strain distributions are way more complex (see Figs. 4.7b - 4.7d). This is due to the gradient influence: material points within the imperfection zone are also influenced by neighboring points in the remaining part of the bar by means of the micromorphic damage variable $\bar{D}$. The non-linearity in the strain distribution explains the necessity of using sufficient elements to obtain a good and representative solution. The damage zone is not restricted to the imperfection size and a physically reasonable narrowing of the localization zone towards the middle of the bar is observable during the process which stands in contrast to the results obtained by using the local version of the model. In correspondence with the desired feature F1 mentioned above, this process leads ultimately to a ‘sharp’ failure interface when damage approaches $D \approx 1$. From this point on, further straining of the specimen does not alter the damage zone anymore. The strain in this region, however, can grow without bounds and approaches infinity with on-going tension, as desired by feature F2. The gradual transition of the strain from an initially piecewise constant distribution to a highly localized one is for better visibility also shown in Fig. 4.8, where a close-up of the process up to the indicated point in Fig. 4.7a is displayed. In summary, features F1 and F2 are both fulfilled by the proposed micromorphic damage model.

In Fig. 4.9, the dependence of the results on the imperfection size is studied (the same mesh as above with 10240 elements is used for the sensitivity analysis). As can be seen, if ℓ_w is taken smaller and smaller, the load maximum increases and shifts to the right in the diagram. In the limit $\ell_w \rightarrow 0$ and $\alpha \rightarrow 0$, the force-displacement curves tend towards a unique solution: load decreasing begins at the same stage where damage would start in case of a perfect bar with no geometrical imperfection (the uniform solution is again plotted in addition for convenience); however, this time, the damage zone remains finite (Fig. 4.9b) and the solution is therefore characterized by a finite amount of energy which is necessary to build the ‘crack’ which is physically reasonable.

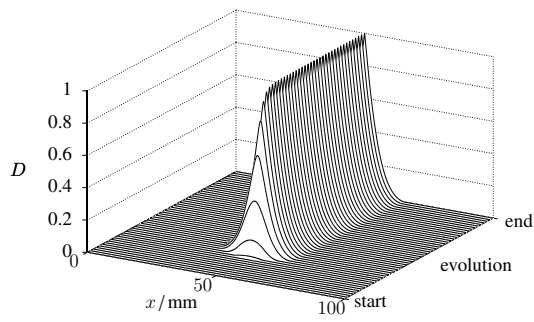
Finally, the influence of the gradient parameter A of the micromorphic model on the results is studied in Fig. 4.10 ($\ell_w = 10$ mm, $\alpha = 0.1$). The smaller the parameter becomes, the more



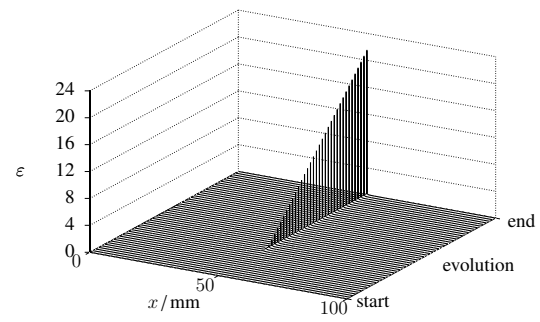
(a) Force-displacement curve



(b) Stress evolution (1280 elements)



(c) Damage evolution (1280 elements)



(d) Strain evolution (1280 elements)

Figure 4.7: Results obtained by using the micromorphic model

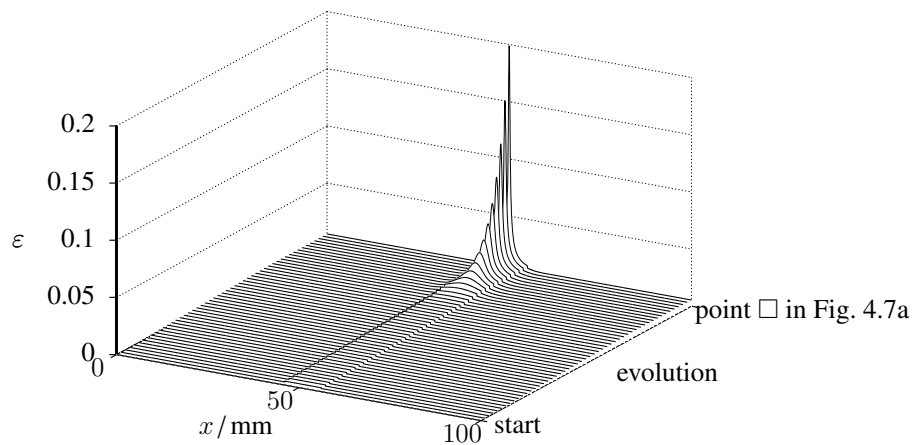
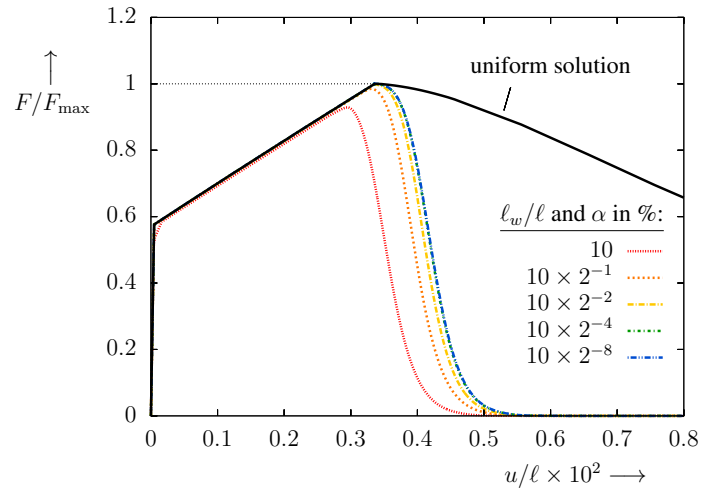
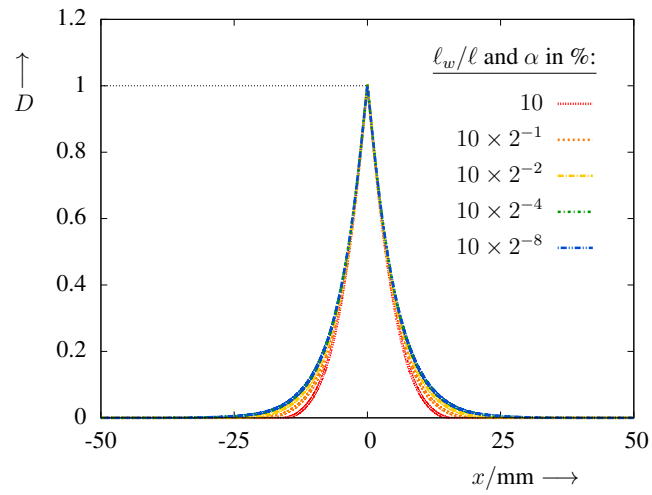


Figure 4.8: Strain evolution up to the indicated point in Fig. 4.7a (1280 elements)



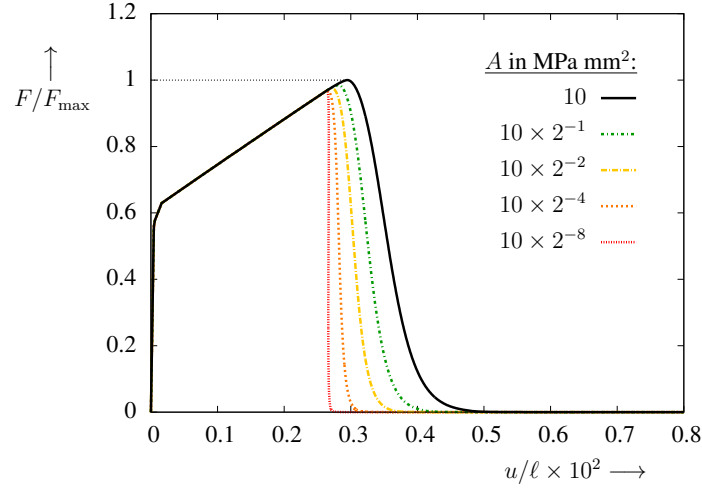
(a) Force-displacement curve



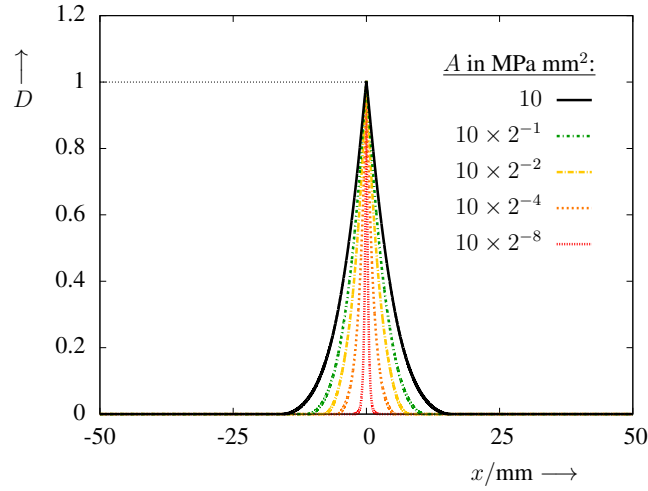
(b) Damage distribution at end of simulation

Figure 4.9: Influence of the imperfection size (micromorphic model, 10240 elements)

the point of maximum load decreases and shifts to the left in the diagram, tending towards the same point as in case of the local version of the model (compare the points of maximum load of the red curves in Figs. 4.6a and 4.10a, respectively). Moreover, the load drop becomes more severe which is reasonable since the damage zone shrinks (Fig. 4.10b) and localization occurs in a comparatively smaller zone. This leads in consequence to a more brittle-like failure behavior of the overall structure.



(a) Force-displacement curve



(b) Damage distribution at end of simulation

Figure 4.10: Influence of gradient parameter A (micromorphic model, 1280 elements)

4.5.3 Square specimen with circular hole

Next, a finite element problem is considered in which a 2D square specimen with a circular hole in its middle is subjected to a state of uniaxial tension by applying two equal but opposite horizontal forces $F(t)$ on the left and right edges of the specimen, respectively. The side length ℓ of the sample is 200 mm, the diameter of the circular cavity 100 mm. A plane strain deformation state is assumed. The dimensions of the specimen are illustrated in Fig. 4.11a.

Symmetry allows that only a quarter of the original sample needs to be considered during the simulation (highlighted in gray color). The actual boundary value problem is for convenience shown in Fig. 4.11b. Note that the applied force $F(t)$ is (pseudo-)time-dependent: a complete tensile test shall be simulated in which the specimen is first loaded gradually up to the point of maximum load and further deformed afterwards at a decreasing load level until the structure may essentially be regarded as ‘broken’. The loaded edge on the right is constrained such that it remains straight and perpendicular to the loading direction throughout the analysis.

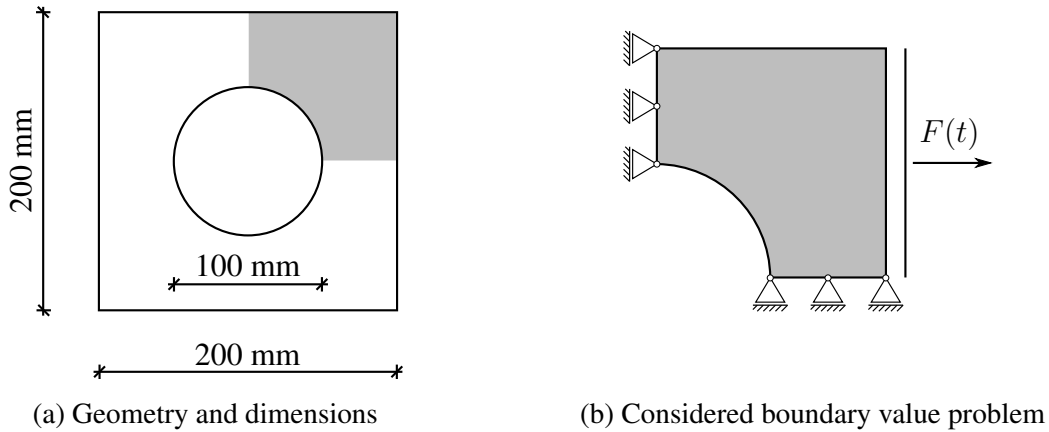


Figure 4.11: Square specimen with circular hole

Due to lack of experimental data, the parameters of the model are chosen as: $\lambda = 5000$ MPa, $\mu = 7500$ MPa, $a = 1900$ MPa, $b = 8.5$, $e = 400$ MPa, $f = 2.5$, $r = 0.5$ MPa, $s = 0.1$, $\sigma_0 = 20$ MPa, $Y_0 = 0.1$ MPa, $H = 10^5$ MPa and $A = 10$ MPa mm². Furthermore, the function in Eqs. (4.7) - (4.9) is defined as $f_{\text{dam}}(D) = 1 - D$. Linear finite element approximations of the displacement field and the micromorphic damage field are considered (see Eqs. (4.44) - (4.45)). The simulation is repeatedly performed using different mesh sizes and a study of convergence is carried out to practically judge the model’s regularization properties. Finite element meshes with 697, 2393, 6288 and 9077 elements are used in the simulations, respectively. In order to save computation time, the meshes are only refined in the area where damage is expected to occur. As can be seen exemplarily in Fig. 4.12 for the cases of 697

and 9077 elements, respectively, the mesh refinement is quite heavy in this region in order to properly account for the occurring high gradients of damage.²²

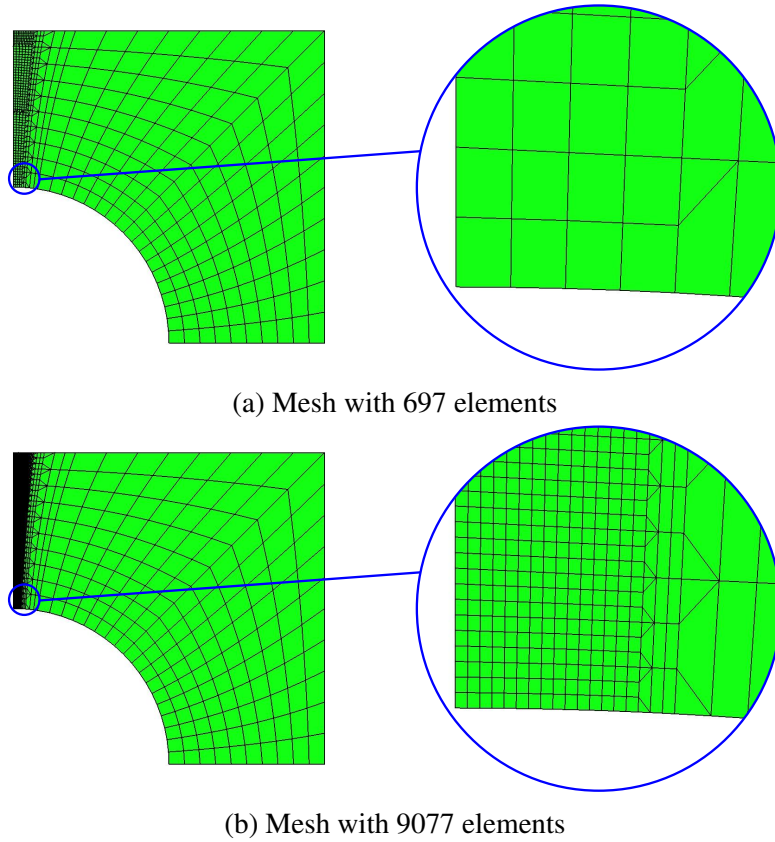


Figure 4.12: Mesh refinement

Fig. 4.13 is utilized to provide the reader with a general understanding of the process. Plotted are the damage contours D and the contours of the accumulated plastic strain κ during three different stages of the process, beginning with the initiation of damage at the cavity, an intermediate stage in which damage progresses vertically to the outer traction-free edges of the specimen and a final stage in which the specimen can essentially be considered as fully ‘broken’, respectively.²³

Fig. 4.14 illustrates the global response of the structure in terms of the normalized load-displacement curves for the different mesh sizes. Here, u denotes the horizontal displacement of the loaded ends of the specimen and $F_{\max}$ is the maximum load attained during the simulation. Mesh convergence is clearly visible, the differences between the individual curves can be

²²Quadrilateral elements are always preferred in the meshing process, triangular ones are only used rarely as transitional elements. This holds also for all examples which follow later on.

²³Here and henceforth, the top and bottom values in the legends of the figures indicate the actually attained minimum and maximum values within the contour plots.

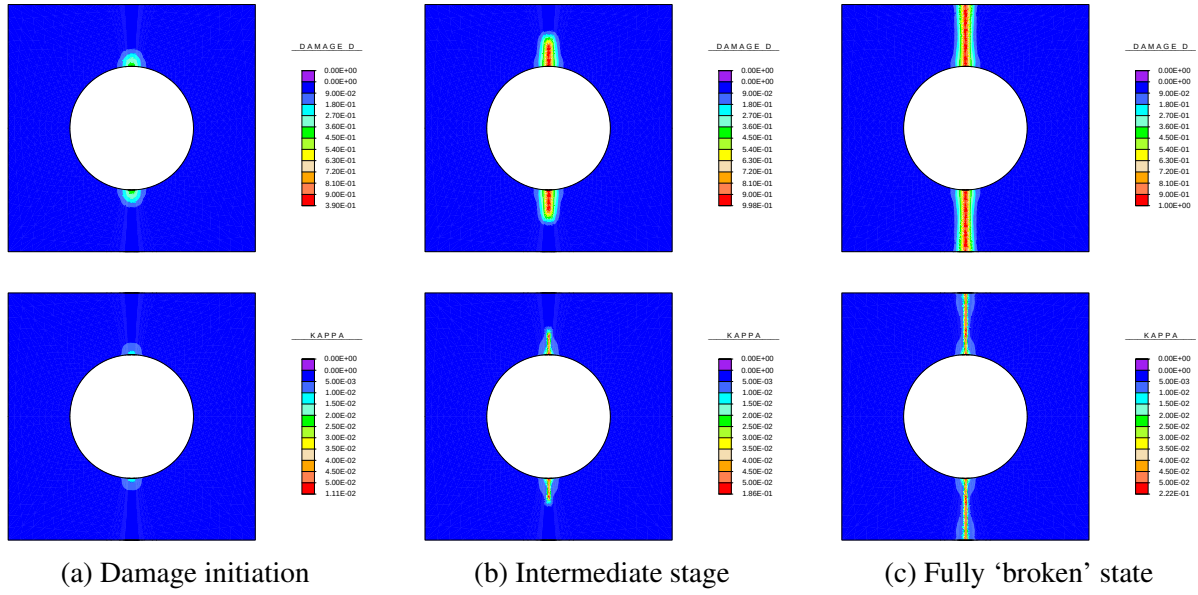


Figure 4.13: Damage contours D (top) and accumulated plastic strain κ (bottom) during three different stages of the process (9077 elements)

considered negligibly small. The points at which the damage contour ‘snapshots’ of Fig. 4.13 were taken are indicated by small rectangular boxes in the figure.

The occurrence of snapback after the point of maximum load is something which might deserve further clarification. Naturally, such an effect would hardly be observable in practical experiments. Its origin lies in the fact that any inertia (or dynamic) effects which usually accompany severe strain-localization processes are completely neglected in the quasi-static simulations performed in this study. If these dynamic effects were taken into account, rather a ‘sudden’ vertical drop of the load-displacement curve would be observable at the point where the tangent to the curve becomes infinite. Such points usually characterize the initiation of dynamic crack propagation, an effect which cannot be modeled using the present quasi-static framework (see, e. g., Heinrich et al. [2013], Hütter et al. [2013, 2014] for further explanations). Instead, the intention here is to track the equilibrium solution of the process by means of an arclength method. By doing so, one essentially assumes that the ‘crack’²⁴ grows in a quasi-static manner which is clearly an idealization. During the snapback phase, further loading happens only locally in a very narrow region within the structure whereas its major part unloads elastically. This results globally in a decrease of both the load and displacement simultaneously which necessitates the usage of an arclength method to further proceed the computation.

²⁴This terminology is here understood in a loose way, meaning a state of very high damage within the material which represents a crack in a continuous sense.

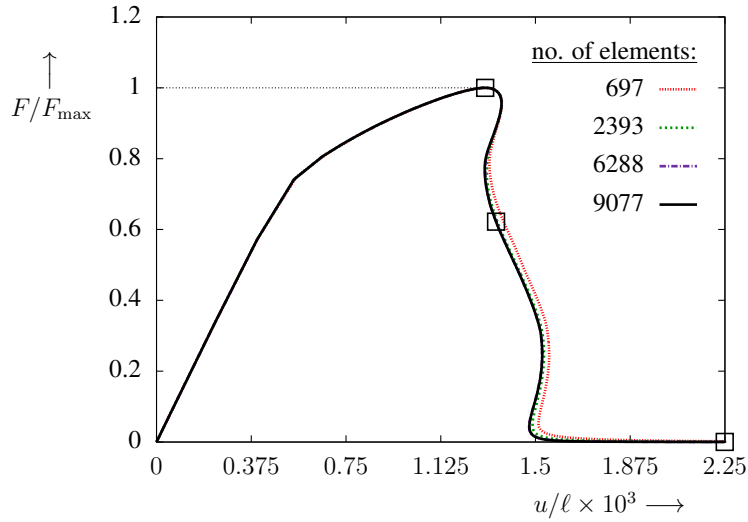
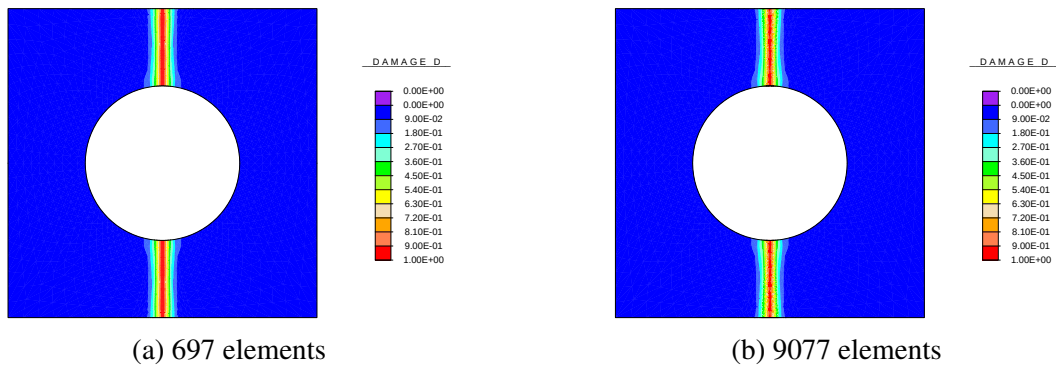


Figure 4.14: Convergence study: load-displacement curves

Convergence of the local fields is exemplarily demonstrated in Fig. 4.15 for the case of the damage variable D at the end of the process. For brevity, only the results for the coarsest and finest meshes are directly compared which show already a striking similarity to each other. In both cases, the totally damaged zone is confined to a relatively thin area in the middle part of the specimen which may be interpreted as a crack in a continuous sense. It is important to point out that the damaged zone remains nearly unchanged even if the structure is further strained at the end of the process at which deformation occurs at almost no structural resistance. This stands in contrast to some other formulations proposed in the literature which have shown the tendency to predict an artificial widening of the damaged zone at a nearly broken state of the structure.

Figure 4.15: Convergence study: damage contours D at the end of the simulation

Exemplarily, also the results shall be discussed briefly which are obtained if the local ver-

sion of the model is used in the simulations. Fig. 4.16 illustrates firstly the load-displacement curves for the same meshes as used before. At first sight, it almost seems as if the structure unloads elastically after the point of maximum load, however, this is not the case: in fact, severe snapback behavior of the structure occurs as damage initiates and grows in a small region at the cavity. When damage finally starts to propagate through the specimen from element to element, an oscillating behavior of the curves becomes visible. No clear convergence of the curves can be observed either, the response becomes more and more brittle for finer mesh discretizations which is in accordance with observations made in the one-dimensional example in Sect. 4.5.2. The energy dissipated during the damage process becomes increasingly smaller which can also visually be understood by examining Fig. 4.17. The smaller the mesh size becomes, the more the width of the damage zone shrinks and therefore also the energy which is dissipated during the failure process.

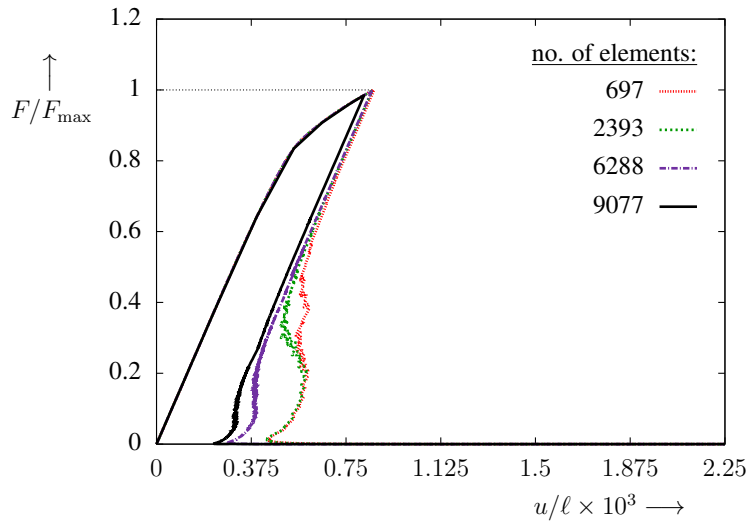


Figure 4.16: Local version of the model: load-displacement curves

The point of maximum load in Fig. 4.16 is also noticeably earlier reached for the finest mesh than in case of the other meshes for which $F_{\max}$ is approximately constant. The reason for this is that, in the former case, the damage process takes place slightly differently in the early stage of the process. Loosely speaking, damage develops along ‘a different path’ in the structure than in case of the other three meshes. This is due to the fact that the damage initiation and subsequent development seem to be largely dependent on the particular structure of the mesh itself. More precisely, damage does not start to develop at the cavity in the middle of the specimen and does not progress vertically through the specimen – which would seem physically reasonable and which was indeed observed in case of the micromorphic model – but

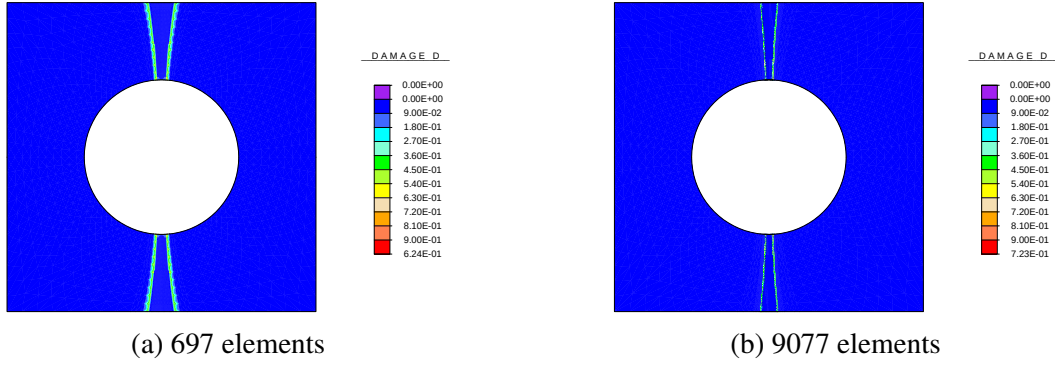


Figure 4.17: Local version of the model: damage contours D at the end of the simulation

along the transition area of the coarse to the fine mesh as indicated in Fig. 4.12. Apparently, the triangular elements in this region (which are commonly known to behave more stiffly than their quadrilateral counterparts) seem to trigger a spurious localization process in the nearby area. This problem is visualized in Fig. 4.18 where the results are illustrated which were obtained using four different meshes in which the coarse/fine mesh transition area was progressively shifted to the right. It can nicely be seen that damage develops in each case along a noticeably different path such that no convergence of the load-displacement curve can be expected. The observation that local damage models do not only suffer from a mesh size dependence but also from a mesh orientation and element-type dependence is well-known in the literature (see, e. g., Cervera and Chiumenti [2006], Grassl and Jirásek [2004], Jirásek and Grassl [2008]). No such spurious behavior as described above can be observed for the micromorphic model at hand (even though a corresponding counterpart to Fig. 4.18 confirming this claim is intentionally skipped here for brevity).

For completeness, it should be mentioned that the physically implausible influence of the coarse / fine mesh transition area can be significantly reduced, if the latter is positioned in a distance far enough from the middle of the specimen (not shown here for brevity). Nevertheless, the fundamental problems of the local version of the damage model remain.

4.5.4 Single-edge notched specimen

A 2D plane strain finite element problem is considered in which a square specimen with a side length $\ell = 100$ mm and a 50 mm sharp horizontal notch (zero width) located on the left side is subjected to a vertical force $F(t)$ on both the top and bottom edges of the specimen, respectively. Exploiting symmetry, only one-half of the specimen needs to be considered in the simulation (highlighted in gray color). The geometry and actual boundary value problem are illustrated in Figs. 4.19a and 4.19b, respectively. The loaded edge on the top is constrained

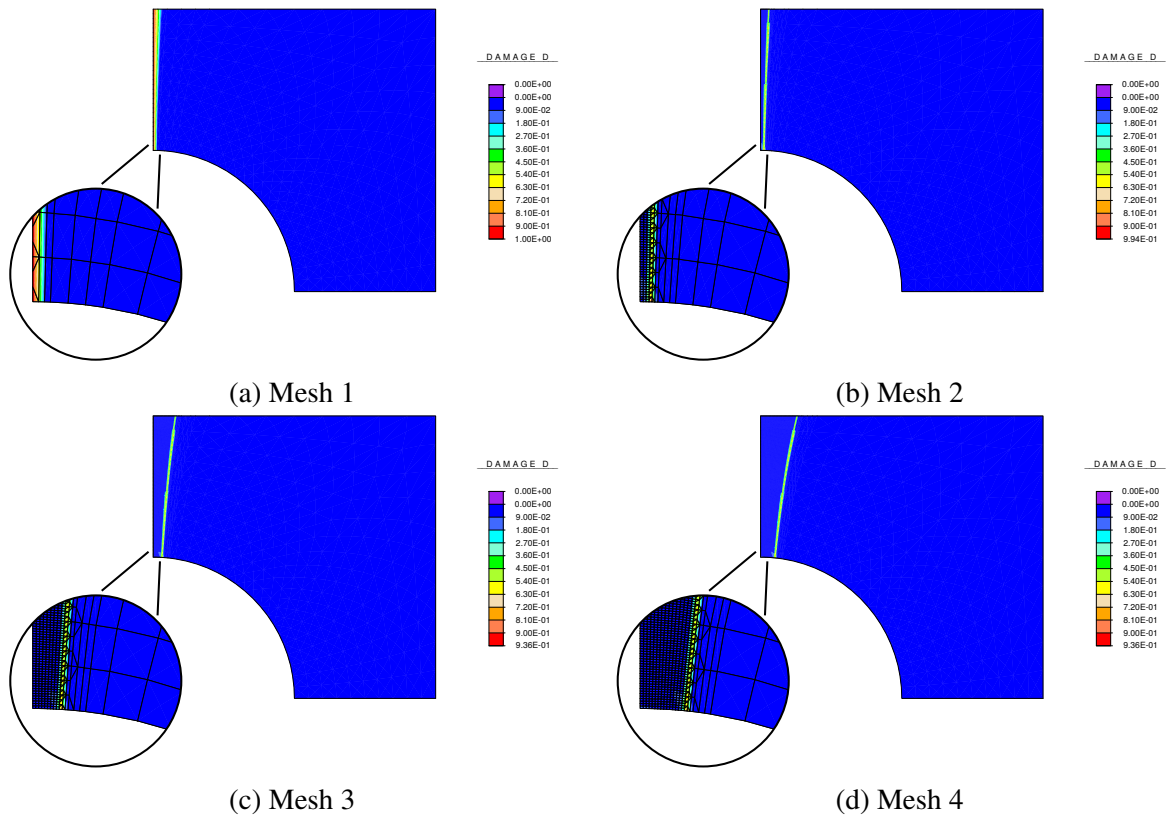


Figure 4.18: Local version of the model: influence of coarse/fine mesh transition area

such that it remains straight and perpendicular to the loading direction throughout the analysis.

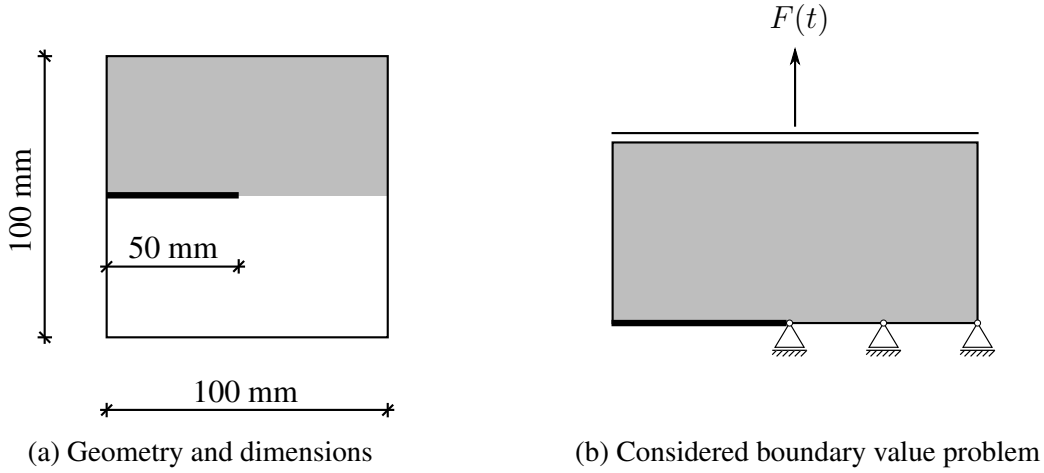


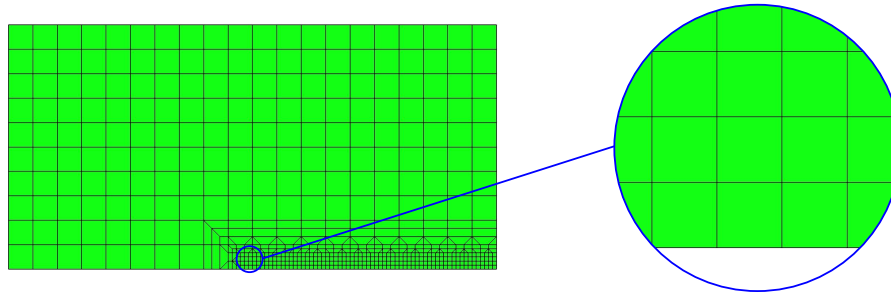
Figure 4.19: Single-edge notched specimen

The same set of material parameters is used as in Example 4.5.3 and the function in Eqs. (4.7) - (4.9) is again defined as $f_{\text{dam}}(D) = 1 - D$. Linear finite element approximations of the displacement field and the micromorphic damage field are considered (see Eqs. (4.44) - (4.45)). The simulation is repeatedly performed using different mesh sizes (602, 1303, 3440 and 10681 elements) in order to carry out a study of convergence. As exemplified in Fig. 4.20 for both the coarsest and finest discretizations, the refinement of the individual meshes is mainly limited to the area where damage is expected to occur during the process.

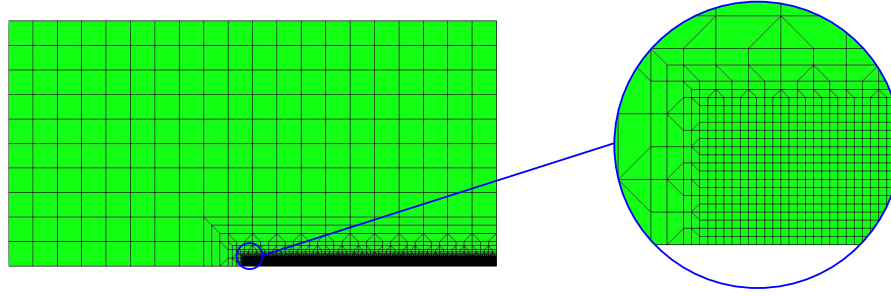
As illustrated in Fig. 4.21 for three distinct stages of the process (using the finest mesh discretization), the damage starts to develop at the notch tip and from there subsequently progresses towards the outer right edge until the specimen can be considered fully ‘broken’. The accumulated plastic strain κ in this region develops accordingly.

The normalized load-displacement curves obtained by using the different meshes are shown in Fig. 4.22 and illustrate the global response of the structure (v denotes the vertical displacements of the loaded ends). A clear mesh convergence is visible, the curves are almost congruent. Again, the small rectangular boxes in the figure indicate the points at which the damage contour ‘snapshots’ of Fig. 4.21 were taken.

A comparison between the respective meshes with regard to the local fields during the simulations reveals a very good agreement as well. Fig. 4.23 exemplarily demonstrates the damage contours at the end of the process for both the coarsest and finest mesh, respectively. Even though the totally damaged zone (area in red color) is a bit wider in case of the coarser mesh, the deviations from the converged result using the finest mesh discretization are quite small,

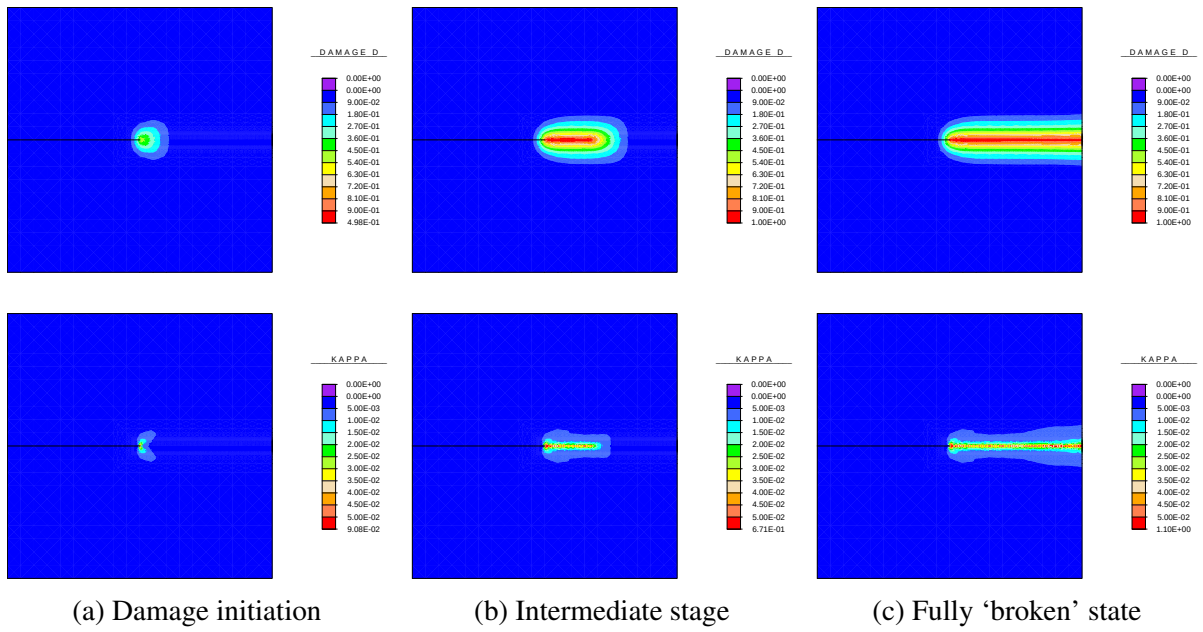


(a) Mesh with 602 elements



(b) Mesh with 10681 elements

Figure 4.20: Mesh refinement



(a) Damage initiation

(b) Intermediate stage

(c) Fully ‘broken’ state

Figure 4.21: Damage contours D (top) and accumulated plastic strain κ (bottom) during three different stages of the process (10681 elements)

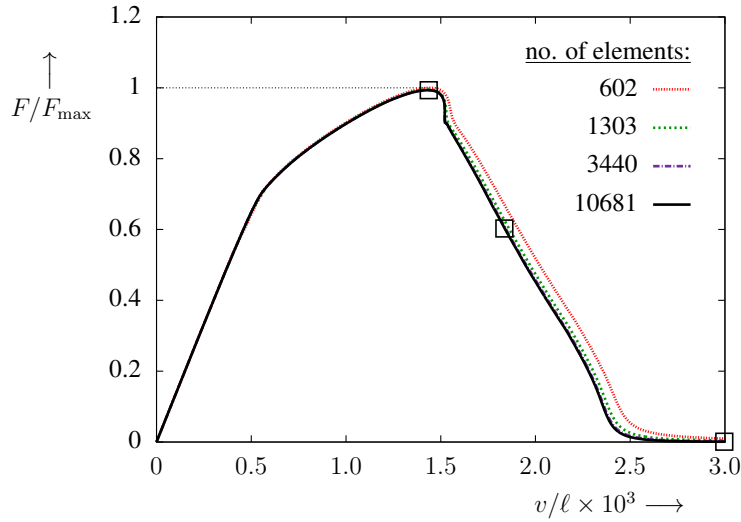
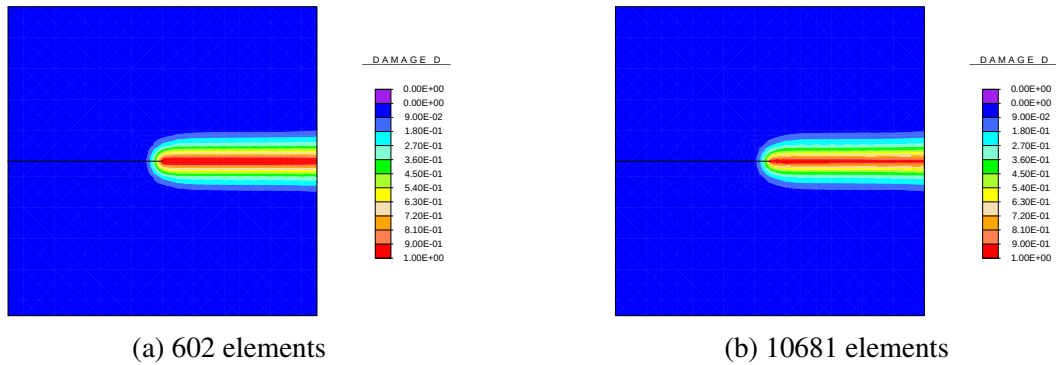


Figure 4.22: Convergence study: load-displacement curves

especially if one takes into account the large discrepancy in the number of elements between the two. For the finer meshes, the differences become negligible (not shown here for brevity). As in Example 4.5.3, the totally damaged zone is confined to a thin area in the middle of the specimen which may be interpreted as a crack in a continuous sense.

Figure 4.23: Convergence study: damage contours D at the end of the simulation

4.5.5 Moderately notched specimen

The following example is concerned with a tensile specimen of length $\ell = 200$ mm which is only moderately notched in its center on both sides as shown in Fig. 4.24a. The sample is subjected to a state of uniaxial tension via two horizontal forces $F(t)$ acting at its left and right ends, respectively. A 2D plane strain situation is considered and a corresponding finite element model is set up by exploiting symmetry conditions. Therefore, the boundary value

problem can be reduced to a quarter of its original size, see Fig. 4.24b. The loaded edge on the right is constrained such that it remains straight and perpendicular to the loading direction throughout the analysis.

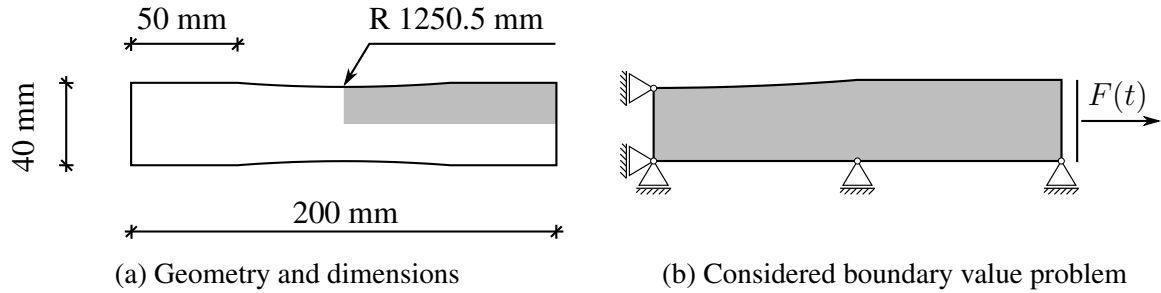


Figure 4.24: Moderately notched specimen

The regularization properties of the model shall be investigated by conducting a convergence study using different mesh sizes (540, 1800, 6450 and 9510 elements) and the same set of material parameters as in the examples of Sects. 4.5.3 and 4.5.4. The function in Eqs. (4.7) - (4.9) is taken as $f_{\text{dam}}(D) = 1 - D$. Linear finite element approximations of the displacement field and the micromorphic damage field are considered (see Eqs. (4.44) - (4.45)). The meshes are strongly refined in the middle area of the specimen where damage is expected to develop during the process. Fig. 4.25 illustrates both the coarsest and finest meshes with 540 and 9510 elements, respectively.

In the very early stages of the damage process, the area of maximum damage is located near the root of the notch. From there, it moves gradually towards the center of the specimen where it later starts to localize. Finally, when damage has reached a very high value in this region (i. e., D is near to 1), it progresses vertically towards the outer traction-free edges of the specimen, essentially resembling the formation of a ‘crack’ in a continuous sense. Damage contours during three different stages of the process are exemplarily illustrated in Fig. 4.26, along with the corresponding contours of the accumulated plastic strain.²⁵

The prediction of fracture onset in the center of the specimen is reasonable and in agreement with experimental observations made for ductile materials and certain notched configurations (see, e. g., Ambati et al. [2016]). The reason for this is the stress triaxiality ratio which is highest in the center of the sample (Bai et al. [2009]), a fact which is accounted for by the model via the first term in the damage driving force Y given in Eq. (4.19) (for further information, the reader is kindly referred to Lemaitre [1996]). The present example also underlines the importance of taking into account the softening effect of damage on the material’s properties: if a

²⁵It should be mentioned that the figures illustrate stages where the maximum damage has already reached the center of the specimen.

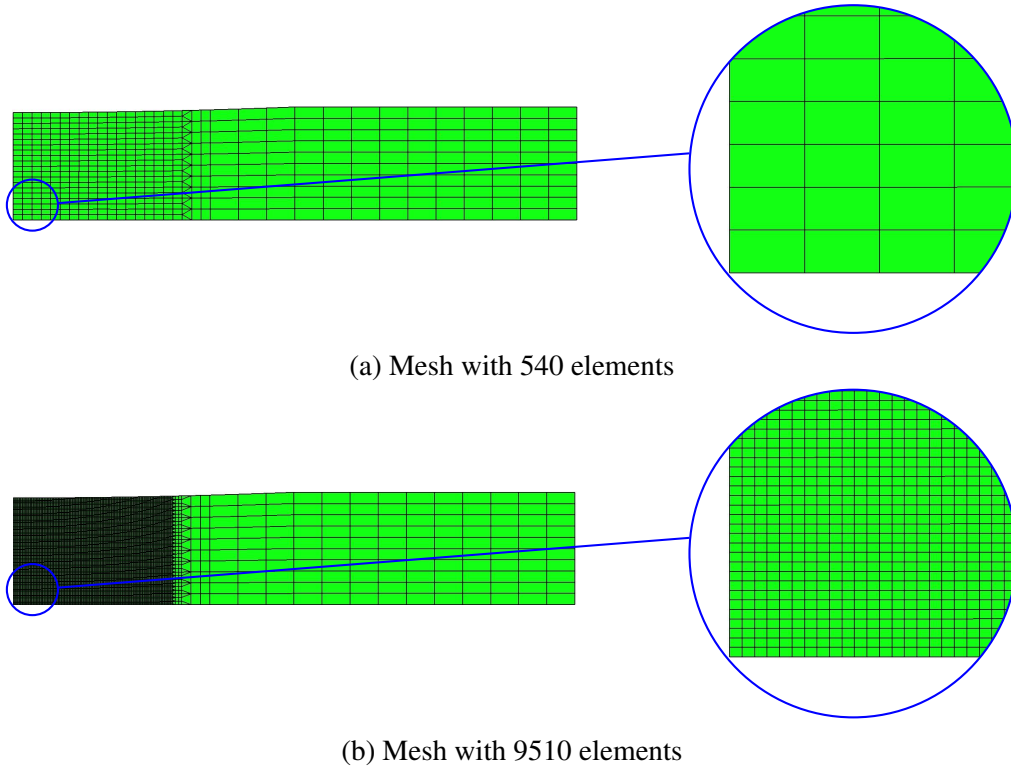


Figure 4.25: Mesh refinement

purely elastoplastic von Mises material model would be used in the simulations together with a critical value of accumulated plastic strain κ as failure criterion, failure were erroneously predicted at the root of the notch.

Fig. 4.27 shows the global response of the structure, i. e., the normalized load-displacement curves obtained by using the different meshes. Here, u denotes the horizontal displacements of the loaded ends at the left and right side, respectively, $F_{\max}$ is the maximum load occurring during the simulation. Mesh convergence is achieved, the curves lie very closely together. As before, the small rectangular boxes are used to indicate the different stages illustrated in Fig. 4.26.

Again, snapback behavior is observable shortly after the point of maximum load is exceeded. Reasons for this were already thoroughly explained in case of the example in Sect. 4.5.3: if dynamic effects were taken into account, a sudden vertical drop of the load-displacement curve would rather be visible.

A direct comparison between the damage contours at the end of the process of the coarsest and finest meshes is given in Fig. 4.28. The totally damaged zone is confined to a relatively thin area and slightly wider in case of the coarse mesh; however, the differences between the figures are quite small and, in the authors' opinion, acceptable results can already been obtained using

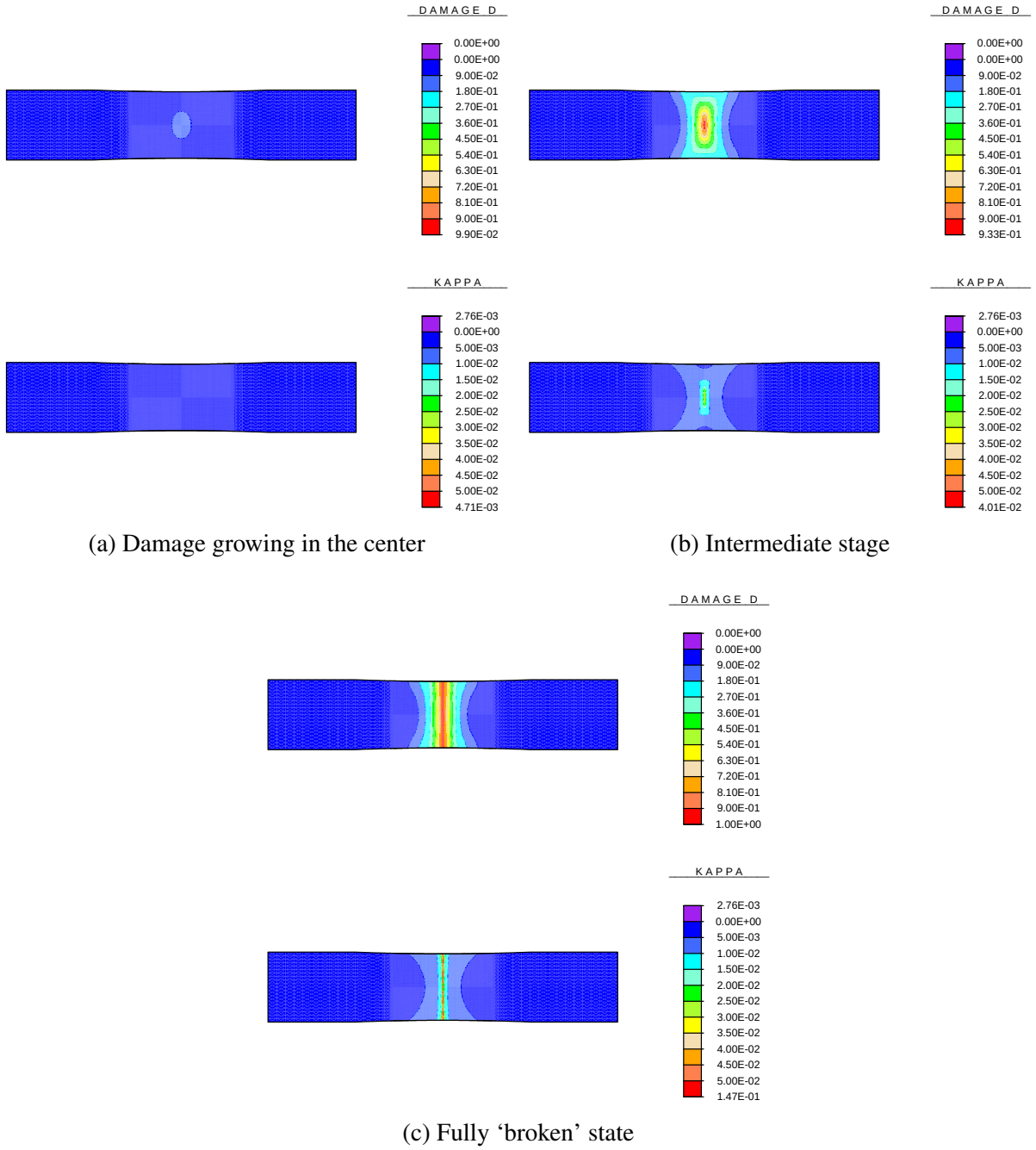


Figure 4.26: Damage contours D (top) and accumulated plastic strain κ (bottom) during three different stages of the process (9510 elements)

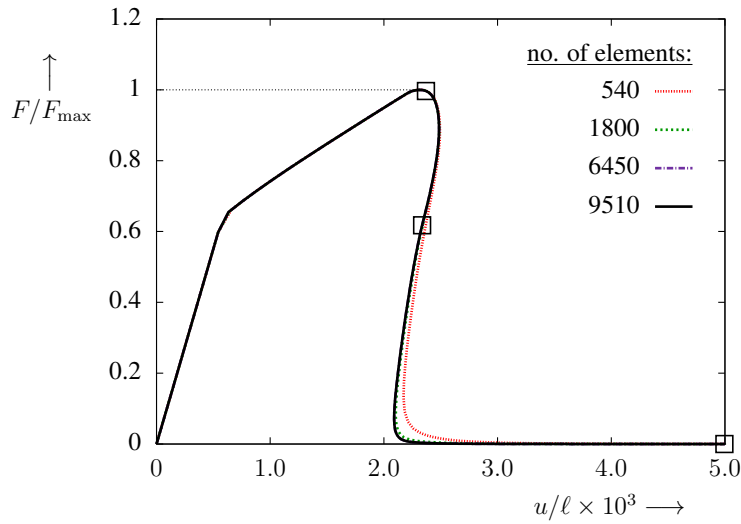
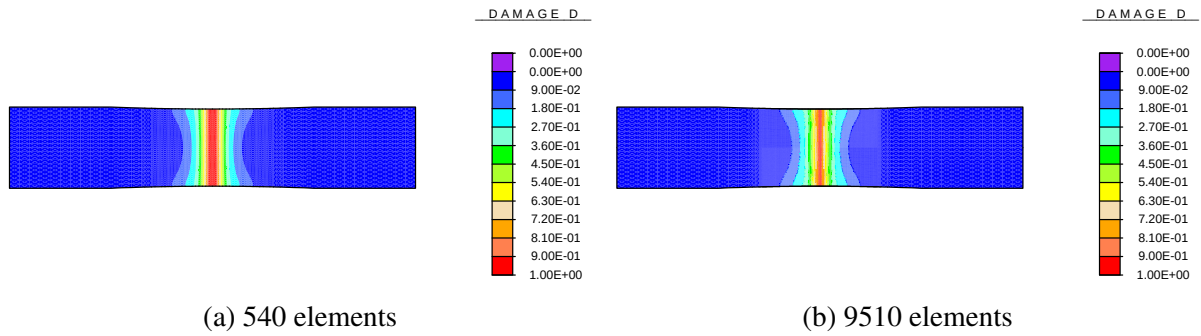


Figure 4.27: Convergence study: load-displacement curves

the coarse mesh. It bears also emphasis that no artificial widening of the damage zone under further straining takes place once the latter has fully developed in the middle of the structure.

Figure 4.28: Convergence study: damage contours D at the end of the simulation

4.5.6 Asymmetrically notched specimen

The last example deals with an asymmetrically notched 2D plane strain specimen of length $\ell = 100$ mm as shown in Fig. 4.29a. The sample is completely fixed at its left edge and subjected to a state of uniaxial tension via a horizontal force $F(t)$ acting at its right edge. The corresponding boundary value problem which is considered in the finite element simulation is illustrated in Fig. 4.29b. Note again that the loaded edge on the right is only allowed to deform in such a way that it remains straight and perpendicular to the loading direction throughout the analysis.

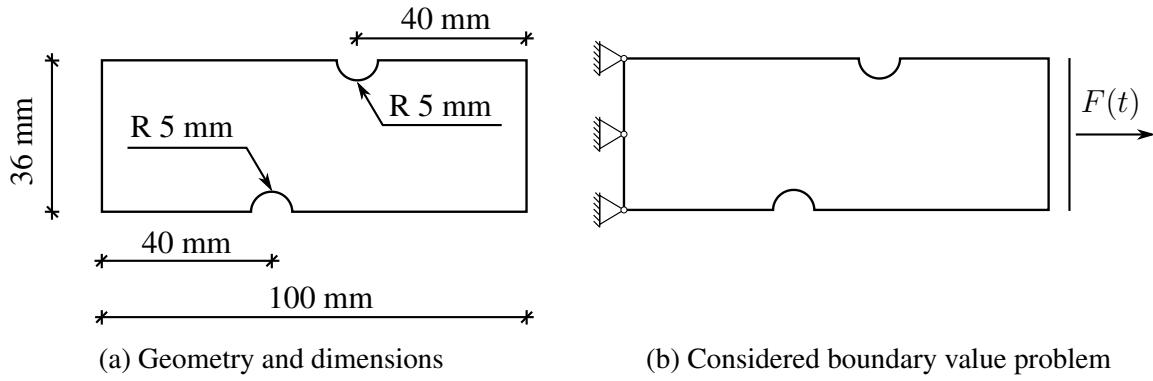
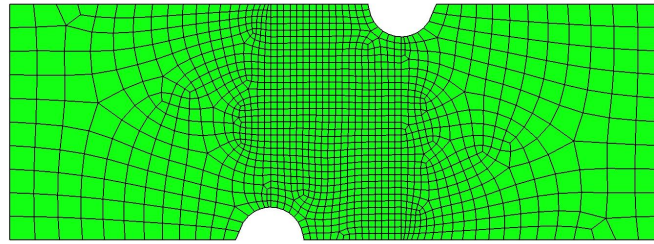
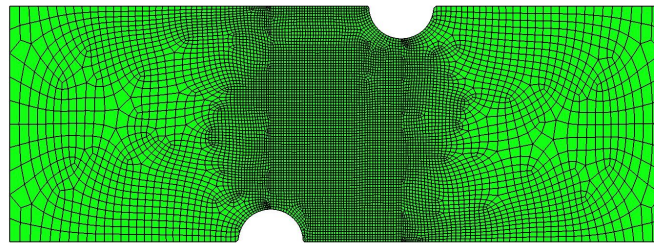


Figure 4.29: Asymmetrically notched specimen

A convergence study is conducted using meshes with 1374, 2190, 4075 and 8690 elements in the simulation, respectively. The material parameters are chosen as in the other examples of the study and the function in Eqs. (4.7) - (4.9) is defined as $f_{\text{dam}}(D) = 1 - D$. Linear finite element approximations are used for both the displacement and micromorphic damage field (see Eqs. (4.44) - (4.45)). The meshes are refined in the central part of the specimen where damage is expected to predominately occur. In Fig. 4.30, illustrations of the coarsest and finest meshes are given.



(a) Mesh with 1374 elements



(b) Mesh with 8690 elements

Figure 4.30: Mesh refinement

Fig. 4.31 is used to illustrate the different stages during the process by means of damage contours D and contours of the accumulated plastic strain κ . In the initial phase, damage

begins to evolve at the roots of both notches, at first more or less independently from each other, and from there distributes radially into the interior of the specimen, respectively. Quite soon, a relatively ‘thick’ damage zone forms between the notches which lies diagonally within the specimen. In the major part of this zone, damage stops to further increase after the latter has developed its full size. From this stage on, the actual process zone in which the level of damage reaches its critical value ($D \approx D_{\text{cr}} = 1$) is confined to a comparatively ‘thin’ area in the middle of this broader damage zone and it can be observed that ‘cracks’ (in a continuous sense) start to propagate from both notches towards the interior of the specimen, finally bridging the two notches. At the end of the process, this behavior leads to a fully developed failure zone (i. e., a zone in which D is near to 1) which has a slight ‘S’-like shape.

In Fig. 4.32, the global response of the structure in terms of the normalized load-displacement curves for the different meshes is shown. As above, u denotes the horizontal displacement of the right edge of the specimen and F_{max} the maximum load attained during the simulation. The convergence towards a unique solution is visible. In this example, no snapback of the load-displacement curves is observable which is, admittedly, strongly dependent on the particular choice of the geometry dimensions and material properties. The rectangular boxes in the figure are used to indicate the different stages shown in Fig. 4.31.

Finally, Fig. 4.33 provides a comparison between the damage contours using the coarsest and finest meshes. Illustrated are only the end states of the process, respectively. As in the other examples discussed above, differences in the plots (both in value and structure of the respective contour plots) are visible but seem to be rather small. No artificial widening of the damage zone under further straining becomes apparent after the latter has fully developed within the specimen.

4.6 Conclusions

In the present study, a regularized damage-plasticity model was discussed which is based on a two-surface formulation, i. e., damage and plasticity are treated as independent but possibly strongly coupled physical mechanisms. The model belongs to the class of micromorphic media as proposed by Forest [2009] and therefore a priori fulfills thermodynamic consistency. Regularization is achieved by means of an additional Helmholtz-type partial differential equation for the micromorphic (or ‘nonlocal’) damage variable which is solved next to the usual balance of linear momentum.

The numerical implementation of the model was discussed in detail in the present study.

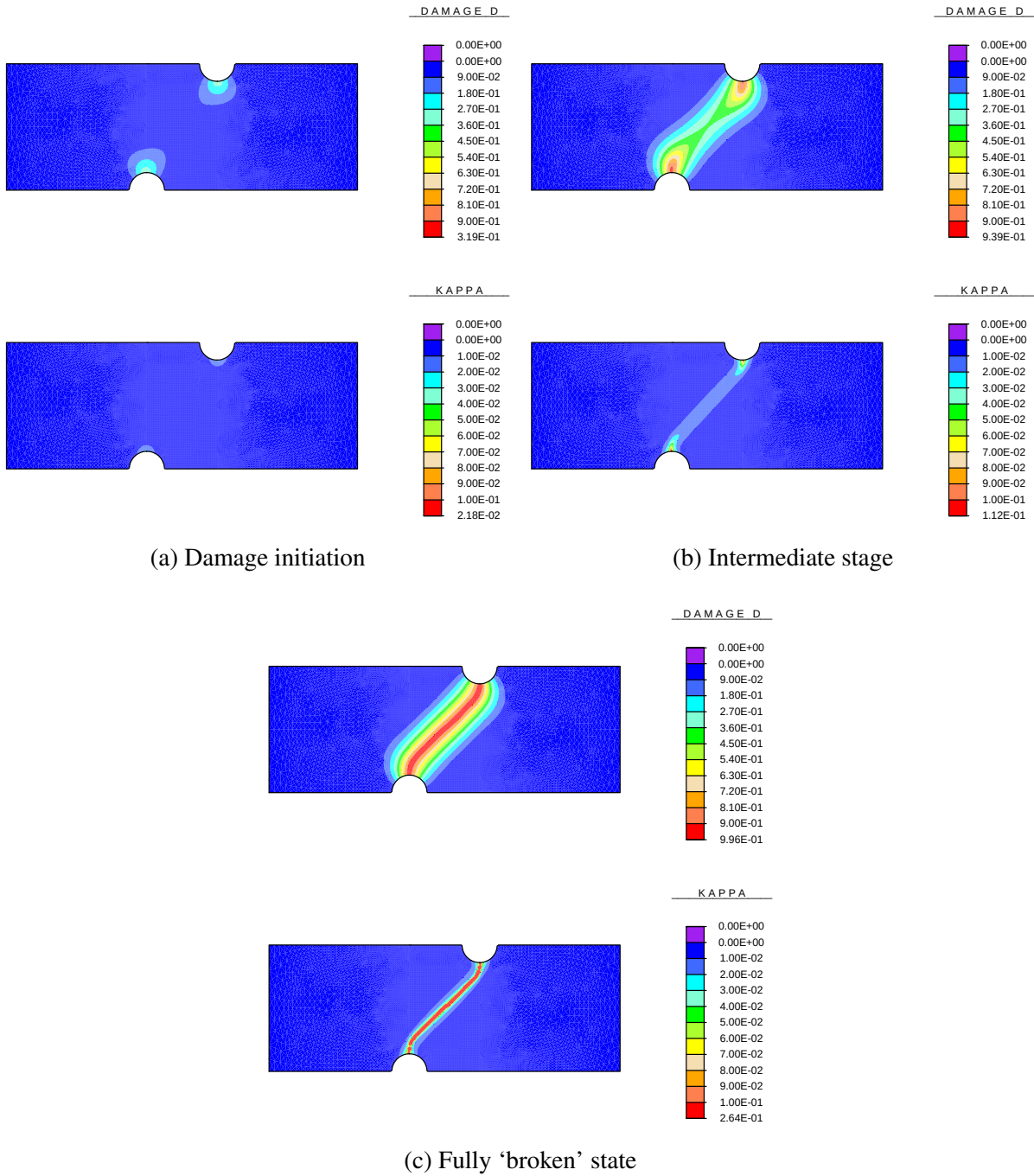


Figure 4.31: Damage contours D (top) and accumulated plastic strain κ (bottom) during three different stages of the process (8690 elements)

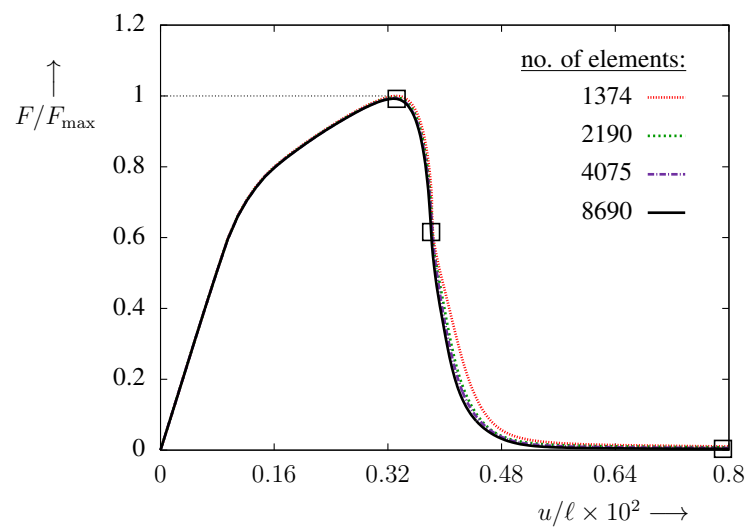


Figure 4.32: Convergence study: load-displacement curves

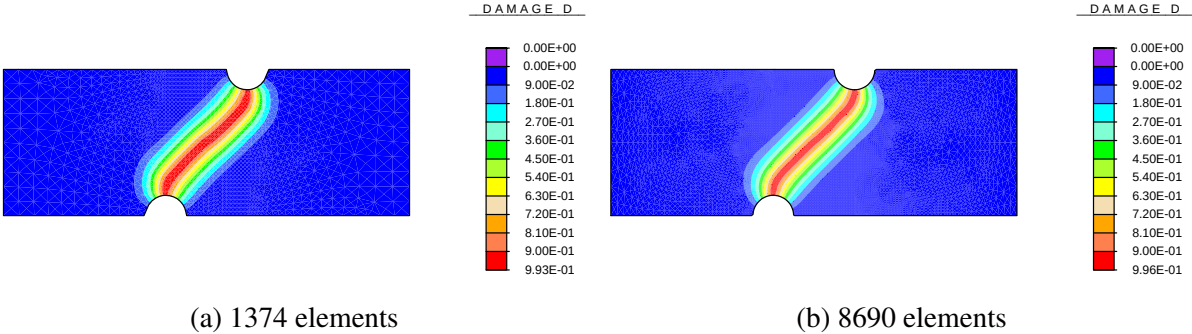


Figure 4.33: Convergence study: damage contours D at the end of the simulation

Particular emphasis was placed on two possible algorithms to integrate the model at the local Gauss-point level: the first is a (local) active-set search strategy borrowed from multisurface plasticity, the second a more recent and elegant strategy based on a reformulation of the existing inequality constraints by means of the Fischer-Burmeister complementarity function. Moreover, it was shown how the model can be implemented into nonlinear finite element codes by deriving the necessary (linearized) finite element equations. Naturally, one additional degree of freedom (namely the micromorphic damage variable) appears at the nodes of the mesh which needs to be solved for in addition to the usual nodal displacements. Due to the linearization of the finite element equations, four tangent operators need to be calculated in total. It was demonstrated how these quantities can be computed in a consistent manner such that a quadratic convergence of the global Newton iteration can still be preserved.

Several numerical simulations were carried out and discussed in the present study to examine the practical relevance of the model. Starting with a one-dimensional benchmark problem, its main regularization properties and features were illustrated in a relatively simple yet interesting and instructive context. By comparing the results with ones obtained by using a corresponding local version of the model, the benefits of the present micromorphic damage-plasticity approach could especially be emphasized. Next, the model was tested in several more complex 2D benchmark simulations. Also here, the model delivered reasonable mesh-independent results and the simulations could be performed up to very high values of damage. In particular, it was argued that the model is suitable for both the phases of crack initiation and crack propagation in a material, serving essentially as a tool to predict ‘cracks’ in a simple continuous sense.

In summary, the model appears – apart from its current restriction to plastic and damage isotropy which were both assumed here for conceptual simplicity – to be quite flexible in the sense that it can be adjusted to various possible situations: either elastic or elastoplastic material behavior with combined nonlinear hardening, in combination with or without regularized damage (if desired, a relapse into ‘local’ damage behavior is equally possible or damage can be neglected at all). Later studies could focus on several different enhancements of the model: e. g., incorporating suitable finite element technology into the formulation in order to avoid artificial locking effects and concurrently reducing the computational effort (see, e. g., Reese [2002, 2003, 2005]), extending the model to the large deformation regime (see, e. g., Vladimirov et al. [2008, 2009]) or taking into account anisotropic plasticity and/or damage (see, e. g., Pietryga et al. [2012], Vladimirov et al. [2010, 2014]).

4.7 Appendix

4.7.1

The general procedure for obtaining a micromorphic model is shortly presented for the geometrically linear and purely mechanical quasi-static case with a single micromorphic variable. For this, consider first that a certain conventional ‘local’ material model is given which depends on the displacement field $\mathbf{u}$ and state variables composed, e. g., of the strain ε and a set of internal variables α related to the various dissipative mechanisms of the material. Following an analogous presentation as given by Forest [2009], an ‘algorithm’ for constructing a micromorphic model can be formulated as follows:

Micromorphic approach:

Starting point: $\text{DOF}_0 := \{\mathbf{u}\}$, $\text{STATE}_0 := \{\varepsilon, \alpha\}$

- (1) from the basic set of state variables STATE_0 , select a variable ϕ which should exhibit gradient effects

$$\phi \in \{\varepsilon, \alpha\}, \quad \alpha: \text{set of internal variables}$$

- (2) introduce a so-called micromorphic variable $\bar{\phi}$ and extend the basic set of degrees of freedom DOF_0 for it, i. e.,

$$\text{DOF}_0 \rightarrow \text{DOF} := \{\mathbf{u}, \bar{\phi}\}$$

- (3) formulate the expression for the virtual work and extend it for work done by $\bar{\phi}$ and its gradient $\nabla \bar{\phi}$
- (4) apply the principle of virtual work to derive generalized balance equations and corresponding boundary conditions
- (5) extend the set of state variables for $\bar{\phi}$ and $\nabla \bar{\phi}$

$$\text{STATE}_0 \rightarrow \text{STATE} := \{\varepsilon, \alpha, \bar{\phi}, \nabla \bar{\phi}\}$$

- (6) exploit the extended Clausius-Duhem inequality to derive
 - generalized state relations from the state potential
 - generalized evolution equations from the analysis of dissipations

4.7.2

Requiring that the internal and external virtual work are the same leads to

$$\begin{aligned} \int_{\Omega} \boldsymbol{\sigma} \cdot \nabla^s \delta \mathbf{u} \, d\Omega - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} \, d\Omega - \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma + \\ + \int_{\Omega} (a_i \delta \bar{\Phi} + \mathbf{b}_i \cdot \nabla \delta \bar{\Phi}) \, d\Omega - \int_{\Omega} (a_e \delta \bar{\Phi} + \mathbf{b}_e \cdot \nabla \delta \bar{\Phi}) \, d\Omega - \int_{\Gamma_c} a_c \delta \bar{\Phi} \, d\Gamma = 0 \end{aligned}$$

By using the chain rule of differentiation

$$\begin{aligned} \operatorname{div}(\boldsymbol{\sigma}[\delta \mathbf{u}]) &= \operatorname{div}(\boldsymbol{\sigma}) \cdot \delta \mathbf{u} + \boldsymbol{\sigma} \cdot \nabla^s \delta \mathbf{u}, & \operatorname{div}(\mathbf{b}_i \delta \bar{\Phi}) &= \operatorname{div}(\mathbf{b}_i) \delta \bar{\Phi} + \mathbf{b}_i \cdot \nabla \delta \bar{\Phi} \\ \operatorname{div}(\mathbf{b}_e \delta \bar{\Phi}) &= \operatorname{div}(\mathbf{b}_e) \delta \bar{\Phi} + \mathbf{b}_e \cdot \nabla \delta \bar{\Phi} \end{aligned}$$

along with the divergence theorem

$$\begin{aligned} \int_{\Omega} \operatorname{div}(\boldsymbol{\sigma}[\delta \mathbf{u}]) \, d\Omega &= \int_{\Gamma} \boldsymbol{\sigma}[\delta \mathbf{u}] \cdot \mathbf{n} \, d\Gamma, & \int_{\Omega} \operatorname{div}(\mathbf{b}_i \delta \bar{\Phi}) \, d\Omega &= \int_{\Gamma} (\mathbf{b}_i \delta \bar{\Phi}) \cdot \mathbf{n} \, d\Gamma \\ \int_{\Omega} \operatorname{div}(\mathbf{b}_e \delta \bar{\Phi}) \, d\Omega &= \int_{\Gamma} (\mathbf{b}_e \delta \bar{\Phi}) \cdot \mathbf{n} \, d\Gamma \end{aligned}$$

and the fact that $\boldsymbol{\sigma}[\delta \mathbf{u}] \cdot \mathbf{n} = \boldsymbol{\sigma}[\mathbf{n}] \cdot \delta \mathbf{u}$, the expression can be reformulated as

$$\begin{aligned} - \int_{\Omega} (\operatorname{div}(\boldsymbol{\sigma}) + \mathbf{f}) \cdot \delta \mathbf{u} \, d\Omega + \int_{\Gamma} \boldsymbol{\sigma}[\mathbf{n}] \cdot \delta \mathbf{u} \, d\Gamma - \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma - \\ - \int_{\Omega} (\operatorname{div}(\mathbf{b}_i - \mathbf{b}_e) - a_i + a_e) \delta \bar{\Phi} \, d\Omega + \int_{\Gamma} (\mathbf{b}_i - \mathbf{b}_e) \cdot \mathbf{n} \delta \bar{\Phi} \, d\Gamma - \int_{\Gamma_c} a_c \delta \bar{\Phi} \, d\Gamma = 0 \end{aligned}$$

Finally, considering that $\boldsymbol{\sigma}[\mathbf{n}] = \mathbf{t}$ on Γ_t , $(\mathbf{b}_i - \mathbf{b}_e) \cdot \mathbf{n} = a_c$ on Γ_c , $\mathbf{u} = \hat{\mathbf{u}}$ on Γ_u , $\bar{\Phi} = \hat{\bar{\Phi}}$ on $\Gamma_{\bar{\Phi}}$ as well as the fact that the test functions $\delta \mathbf{u}$ and $\delta \bar{\Phi}$ vanish on Γ_u and $\Gamma_{\bar{\Phi}}$, respectively, but are otherwise arbitrary and independent from each other, results in the statements

$$\begin{aligned} \operatorname{div}(\boldsymbol{\sigma}) + \mathbf{f} &= \mathbf{0} & \text{in } \Omega & & \operatorname{div}(\mathbf{b}_i - \mathbf{b}_e) - a_i + a_e &= 0 & \text{in } \Omega \\ \mathbf{t} &= \boldsymbol{\sigma}[\mathbf{n}] & \text{on } \Gamma_t & & a_c &= (\mathbf{b}_i - \mathbf{b}_e) \cdot \mathbf{n} & \text{on } \Gamma_c \\ \mathbf{u} &= \hat{\mathbf{u}} & \text{on } \Gamma_u & & \bar{\Phi} &= \hat{\bar{\Phi}} & \text{on } \Gamma_{\bar{\Phi}} \end{aligned}$$

which are valid in a point-wise sense.

4.7.3

The linearization of g in (4.39) about a known state $(\mathbf{u}^*, \bar{D}^*)$ can be written as

$$\begin{aligned} L_g(\Delta \mathbf{u}, \Delta \bar{D}, \delta \mathbf{u}) &\equiv g(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u}) \\ &\quad + \mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] + \mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \bar{D}] \stackrel{!}{=} 0 \quad \forall \delta \mathbf{u} \end{aligned}$$

where the Gâteaux derivatives $\mathcal{D}g_u[\Delta \mathbf{u}]$ and $\mathcal{D}g_{\bar{D}}[\Delta \bar{D}]$ are defined as

$$\begin{aligned} \mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} g(\mathbf{u}^* + \epsilon \Delta \mathbf{u}, \bar{D}^*, \delta \mathbf{u}) \\ \mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \bar{D}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} g(\mathbf{u}^*, \bar{D}^* + \epsilon \Delta \bar{D}, \delta \mathbf{u}) \end{aligned}$$

More precisely, the calculation of $\mathcal{D}g_u[\Delta \mathbf{u}]$ is carried out as

$$\begin{aligned} \mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \left(\int_{\Omega} (\boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\epsilon), \bar{D}^*) \cdot \nabla^s \delta \mathbf{u} - \mathbf{f} \cdot \delta \mathbf{u}) \, d\Omega - \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma \right) \\ &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}(\epsilon), \bar{D}^*) \cdot \nabla^s \delta \mathbf{u} \, d\Omega \\ &= \int_{\Omega} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} \left[\frac{\partial \boldsymbol{\varepsilon}}{\partial \epsilon} \right] \right) \bigg|_{\epsilon=0} \cdot \nabla^s \delta \mathbf{u} \, d\Omega \\ &= \int_{\Omega} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} [\nabla^s(\Delta \mathbf{u})] \right) \cdot \nabla^s \delta \mathbf{u} \, d\Omega \end{aligned}$$

with

$$\boldsymbol{\varepsilon}(\epsilon) := \nabla^s(\mathbf{u}^* + \epsilon \Delta \mathbf{u})$$

Analogously, $\mathcal{D}g_{\bar{D}}[\Delta \bar{D}]$ is calculated as

$$\begin{aligned} \mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \bar{D}] &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \left(\int_{\Omega} (\boldsymbol{\sigma}(\boldsymbol{\varepsilon}^*, \bar{D}(\epsilon)) \cdot \nabla^s \delta \mathbf{u} - \mathbf{f} \cdot \delta \mathbf{u}) \, d\Omega - \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{u} \, d\Gamma \right) \\ &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}^*, \bar{D}(\epsilon)) \cdot \nabla^s \delta \mathbf{u} \, d\Omega \\ &= \int_{\Omega} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \bar{D}} \frac{\partial \bar{D}}{\partial \epsilon} \right) \bigg|_{\epsilon=0} \cdot \nabla^s \delta \mathbf{u} \, d\Omega \\ &= \int_{\Omega} \left(\frac{\partial \boldsymbol{\sigma}}{\partial \bar{D}} \Delta \bar{D} \right) \cdot \nabla^s \delta \mathbf{u} \, d\Omega \end{aligned}$$

where

$$\bar{D}(\epsilon) := \bar{D}^* + \epsilon \Delta \bar{D}$$

In the same manner, the linearization of h in (4.40) about a known state $(\mathbf{u}^*, \bar{D}^*)$ is carried out as

$$\begin{aligned} L_h(\Delta \mathbf{u}, \Delta \bar{D}, \delta \bar{D}) &\equiv h(\mathbf{u}^*, \bar{D}^*, \delta \bar{D}) \\ &+ \mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \mathbf{u}] + \mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \bar{D}] \stackrel{!}{=} 0 \quad \forall \delta \bar{D} \end{aligned}$$

with $\mathcal{D}h_u[\Delta \mathbf{u}]$ and $\mathcal{D}h_{\bar{D}}[\Delta \bar{D}]$ denoting the Gâteaux derivatives

$$\begin{aligned} \mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \mathbf{u}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} h(\mathbf{u}^* + \epsilon \Delta \mathbf{u}, \bar{D}^*, \delta \bar{D}) \\ \mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \bar{D}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} h(\mathbf{u}^*, \bar{D}^* + \epsilon \Delta \bar{D}, \delta \bar{D}) \end{aligned}$$

In more detail, $\mathcal{D}h_u[\Delta \mathbf{u}]$ is computed as

$$\begin{aligned} \mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \mathbf{u}] &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \left(\int_{\Omega} (H(D(\boldsymbol{\varepsilon}(\epsilon), \bar{D}^*) - \bar{D}^*) \delta \bar{D} - A \nabla \bar{D}^* \cdot \nabla \delta \bar{D}) d\Omega \right) \\ &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \int_{\Omega} H D(\boldsymbol{\varepsilon}(\epsilon), \bar{D}^*) \delta \bar{D} d\Omega \\ &= \int_{\Omega} H \left(\frac{\partial D}{\partial \boldsymbol{\varepsilon}} \cdot \frac{\partial \boldsymbol{\varepsilon}}{\partial \epsilon} \right) \bigg|_{\epsilon=0} \delta \bar{D} d\Omega \\ &= \int_{\Omega} H \left(\frac{\partial D}{\partial \boldsymbol{\varepsilon}} \cdot \nabla^s(\Delta \mathbf{u}) \right) \delta \bar{D} d\Omega \end{aligned}$$

and $\mathcal{D}h_{\bar{D}}[\Delta \bar{D}]$ as

$$\begin{aligned} \mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \bar{D}] &= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \left(\int_{\Omega} (H(D(\boldsymbol{\varepsilon}^*, \bar{D}(\epsilon)) - \bar{D}(\epsilon)) \delta \bar{D} - A \nabla \bar{D}(\epsilon) \cdot \nabla \delta \bar{D}) d\Omega \right) \\ &= \int_{\Omega} \left(H \left(\frac{\partial D}{\partial \bar{D}} \frac{\partial \bar{D}}{\partial \epsilon} - \frac{\partial \bar{D}}{\partial \epsilon} \right) \bigg|_{\epsilon=0} \delta \bar{D} - A \frac{\partial \nabla \bar{D}}{\partial \epsilon} \bigg|_{\epsilon=0} \cdot \nabla \delta \bar{D} \right) d\Omega \\ &= \int_{\Omega} \left(H \left(\frac{\partial D}{\partial \bar{D}} \Delta \bar{D} - \Delta \bar{D} \right) \delta \bar{D} - A \nabla(\Delta \bar{D}) \cdot \nabla \delta \bar{D} \right) d\Omega \\ &= \int_{\Omega} \left(H \Delta \bar{D} \left(\frac{\partial D}{\partial \bar{D}} - 1 \right) \delta \bar{D} - A \nabla(\Delta \bar{D}) \cdot \nabla \delta \bar{D} \right) d\Omega \end{aligned}$$

4.7.4

After a somewhat lengthy calculation, the corresponding expressions in (4.75) - (4.76) are obtained as

$$\begin{aligned}
 \mathcal{A}_p &= \mathcal{T}_{1p} - \mathbf{T}_{1\Delta\lambda_d} \otimes (T_{3\Delta\lambda_d})^{-1} \mathbf{T}_{3p} \\
 \mathcal{A}_\varepsilon &= \mathcal{T}_{1\varepsilon} - \mathbf{T}_{1\Delta\lambda_d} \otimes (T_{3\Delta\lambda_d})^{-1} \mathbf{T}_{3\varepsilon} \\
 \mathbf{A}_{\bar{D}} &= \mathbf{T}_{1\bar{D}} - \mathbf{T}_{1\Delta\lambda_d} (T_{3\Delta\lambda_d})^{-1} \mathbf{T}_{3\bar{D}} \\
 \mathbf{B}_\varepsilon &= \mathbf{T}_{3\varepsilon} - (\mathcal{T}_{1p}^{-1} : \mathcal{T}_{1\varepsilon})^T [\mathbf{T}_{3p}] \\
 B_{\Delta\lambda_d} &= T_{3\Delta\lambda_d} - \mathbf{T}_{3p} \cdot \mathcal{T}_{1p}^{-1} [\mathbf{T}_{1\Delta\lambda_d}] \\
 B_{\bar{D}} &= T_{3\bar{D}} - \mathbf{T}_{3p} \cdot \mathcal{T}_{1p}^{-1} [\mathbf{T}_{1\bar{D}}]
 \end{aligned}$$

in which the fourth-order tensors $\mathcal{T}_{1p}$, $\mathcal{T}_{1\varepsilon}$, second-order tensors $\mathbf{T}_{1\Delta\lambda_d}$, $\mathbf{T}_{3p}$, $\mathbf{T}_{3\varepsilon}$, $\mathbf{T}_{1\bar{D}}$ and scalars $T_{3\Delta\lambda_d}$, $T_{3\bar{D}}$ are used to represent

$$\begin{aligned}
 \mathcal{T}_{1p} &= \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}_p} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \boldsymbol{\varepsilon}_p} \\
 \mathcal{T}_{1\varepsilon} &= \frac{\partial \mathbf{r}_1}{\partial \boldsymbol{\varepsilon}} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \boldsymbol{\varepsilon}} \\
 \mathbf{T}_{1\Delta\lambda_d} &= \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_d} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \Delta\lambda_d} \\
 \mathbf{T}_{1\bar{D}} &= \frac{\partial \mathbf{r}_1}{\partial \bar{D}} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \bar{D}} \\
 \mathbf{T}_{3p} &= \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}_p} - \frac{\partial r_3}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \boldsymbol{\varepsilon}_p} \\
 \mathbf{T}_{3\varepsilon} &= \frac{\partial r_3}{\partial \boldsymbol{\varepsilon}} - \frac{\partial r_3}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \boldsymbol{\varepsilon}} \\
 T_{3\Delta\lambda_d} &= \frac{\partial r_3}{\partial \Delta\lambda_d} - \frac{\partial r_3}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \Delta\lambda_d} \\
 T_{3\bar{D}} &= \frac{\partial r_3}{\partial \bar{D}} - \frac{\partial r_3}{\partial \Delta\lambda_p} \left(\frac{\partial r_2}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_2}{\partial \bar{D}}
 \end{aligned}$$

The residuals $\mathbf{r}_1$, r_2 and r_3 are defined as shown in (4.64) (or (4.70) if the Fischer-Burmeister approach is used).

Clearly, certain derivatives in the above vanish because not all residuals depend on each variable. However, the expressions are here stated in their most general form such that they are also applicable to other specific forms of the residuals in (4.64) or (4.70), respectively.

5 | Article 4:

A micromorphic damage-plasticity model to counteract mesh dependence in finite element simulations involving material softening

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Disclosure of the individual authors’ contributions to the article:

T. Brepols reviewed the relevant existing literature, developed the ‘two-surface’ gradient-extended damage-plasticity model and implemented it into the academic finite element software FEAP (as an own element subroutine using a corresponding interface in the software). It was his idea to apply the Fischer-Burmeister approach in the context of the algorithmic implementation of the model and he presented a procedure to locally enforce stress constraints for 3D gradient-extended material models. He set up and performed all simulations, interpreted the results and wrote the article. It was S. Wulfinghoff’s original idea to use the micromorphic approach for the gradient-extension of the model. He and S. Reese gave conceptual advice, contributed to the discussion of the results, read the article and gave valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

5.1 Abstract

A gradient-extended damage-plasticity material model is presented which belongs to the class of micromorphic media as proposed by Forest [2009]. A ‘two-surface’ formulation is utilized in which damage and plasticity are treated as independent but strongly coupled dissipative phenomena. To this end, separate yield and damage criteria as well as loading / unloading conditions are introduced. The model is thermodynamically consistent and accounts for both nonlinear kinematic and isotropic hardening as well as damage hardening. Various theoretical and numerical aspects of the formulation are discussed. Emphasis is also put on a procedure to enforce stress constraints at the local integration point level which provides, for instance, the basis for a straightforward integration of 3D gradient-extended material models into beam or shell elements or for their usage in 2D plane stress computations. A structural example problem is used to illustrate the merits of the model and its ability to deliver mesh-independent results in coupled damage-plasticity finite element simulations.

5.2 Introduction

Studying damage and fracture processes within materials and structures is a subject of major interest in the mechanics community. The availability of today’s computing power, the ongoing improvement of sophisticated simulation software as well as the increasing knowledge of the physical backgrounds of the aforementioned phenomena due to better experimental insights have provided the basis for a steadily growing number of interesting numerical studies on this topic in more recent times (among many others, see, e. g., Dimitrijevic and Hackl [2008, 2011], Duda et al. [2015], Junker et al. [2016], Kiefer et al. [2018], Miehe, Aldakheel and Raina [2016], Mozaffari and Voyiadjis [2016], Naderi et al. [2016], Seabra et al. [2013]). Naturally, along with these developments has come also a considerable progress in and application of advanced and ‘non-standard’ material modeling techniques.

A common example is the consideration of ‘nonlocal’ gradient effects in damage and fracture computations. For long, it has been recognized that finite element simulations involving conventional ‘local’ continuum damage models may suffer from strongly mesh-dependent results which are caused by an oversimplified approach to model material softening (see, e. g., Bažant et al. [1984], Cervera and Chiumenti [2006], de Borst et al. [1993], Grassl and Jirásek [2004], Jirásek and Grassl [2008]). Gradient-enhanced damage models can provide a way out of this dilemma by incorporating internal material length scales acting as ‘localization limiters’ in the underlying formulation and thus restoring its physical and mathematical soundness. For

this reason and due to the above mentioned technical achievements, gradient-extended material models find an increasing application in more and more practically relevant computational investigations nowadays (e. g., Miehe [2014], Miehe et al. [2014], Saanouni and Hamed [2013], Waffenschmidt et al. [2014], to name only a few).

However, especially with regard to gradient-enhanced models coupling damage and plasticity, a lot of open questions remain and a need for further clarification and research is noticeable within the scientific community. In this regard, the present study aims at making a valuable contribution by presenting and discussing a gradient-extended damage-plasticity model which fits into the rather general framework of micromorphic media as proposed by Forest [2009, 2016]. The latter may be considered an approach for unifying concepts among the various existing types of gradient-enhancements in the literature that is applied by an increasing number of authors, see, e. g., also Bayerschen et al. [2015] or Wulfinghoff et al. [2013]. A ‘two-surface’ formulation is utilized in which damage and plasticity are modeled as separate dissipative mechanisms using independent damage and yield criteria and corresponding sets of loading / unloading conditions. The latter fact makes the model flexibly adaptable to various cases in which the material’s behavior is either only (quasi-)brittle-like, ductile-like or possibly anything in between. Nonlinear kinematic and isotropic hardening as well as damage hardening are considered and thermodynamical consistency of the model is ensured via suitable choices for the evolution equations.

An additional point is the discussion of a procedure to enforce stress constraints for 3D gradient-extended material models at the local integration point level. The method makes it possible to use these models without modifications in 2D plane stress computations or to integrate the latter, e. g., in beam or shell element formulations. In a variety of different ways, many authors have worked in the past on the subject of incorporating stress constraints into conventional ‘local’ material models at the integration point level (among many others, see, e. g., Aravas [1987], de Borst [1991], Dodds [1987], Dvorkin et al. [1995], Jetteur [1986], Kirchner et al. [1997], Klinkel and Govindjee [2002], Simo and Taylor [1986]). The present study, however, is concerned with gradient-extended materials and explains, e. g., how to appropriately condense the additional material tangent operators showing up due to a gradient-extension. This makes it possible to retain the quadratic rate of convergence in a Newton-Raphson iteration scheme at the global finite element level. To the best knowledge of the authors, this issue has not been presented or discussed for gradient-extended material models in the literature, yet.

Finally, the application of the just-mentioned procedure and the mesh regularization properties of the presented model are carefully examined by means of a structural 2D plane stress

benchmark simulation.

5.3 Constitutive theory

This section discusses the theoretical details and constitutive theory of the gradient-extended damage-plasticity model. Starting with a brief explanation of the origin of the considered type of gradient-extension and a presentation of the model's strong and weak form in Sect. 5.3.1, the fundamental kinematic assumptions and general thermodynamic considerations are dealt with in Sect. 5.3.2. In Sect. 5.3.3, the individual parts of the underlying Helmholtz free energy are defined, whereas Sect. 5.3.4 describes the derivation of the state relations and thermodynamic conjugate forces of the model based on the second-law of thermodynamics. Finally, Sects. 5.3.5 and 5.3.6 are concerned with a thermodynamically consistent modeling of plasticity and damage, respectively.

5.3.1 Micromorphic extension, strong and weak form of the problem

The gradient-extended model under consideration is derived from the micromorphic theory proposed by Forest [2009, 2016] which may be regarded as a systematic approach for constructing higher-order gradient material models from already existing 'local' counterparts. In the case of the present study, a scalar 'micromorphic' damage variable is introduced as an additional degree of freedom of the model and a further generalized micromorphic balance equation needs to be solved next to the classical balance of linear momentum. As will be described in Sect. 5.3.3, a coupling between the micromorphic damage variable and its local counterpart is enforced by introducing a direct dependence of the underlying free energy on the difference between the just-mentioned quantities. Omitting any details of the derivation process for brevity (the interested reader is kindly referred to the above mentioned references), the 'strong form' of the problem consists of the following partial differential equations and boundary conditions which are valid in a pointwise sense:

$$\begin{array}{ll}
 \text{linear momentum balance:} & \text{micromorphic balance:} \\
 \text{div}(\boldsymbol{\sigma}) + \mathbf{f} = \mathbf{0} & \text{in } \Omega \quad H(D - \bar{D}) + A \text{div}(\nabla \bar{D}) = 0 \quad \text{in } \Omega \\
 \boldsymbol{\sigma}[\mathbf{n}] = \hat{\mathbf{t}} & \text{on } \Gamma_t \quad \nabla \bar{D} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma \\
 \mathbf{u} = \hat{\mathbf{u}} & \text{on } \Gamma_u
 \end{array} \tag{5.1}$$

In the above, $\boldsymbol{\sigma}$ denotes the stress tensor, $\mathbf{u}$ is the displacement vector, D is the local damage variable and $\bar{D}$ its corresponding micromorphic counterpart. Conventional body forces acting

in the domain of body Ω are represented by $\mathbf{f}$, whereas $\hat{\mathbf{t}}$ and $\hat{\mathbf{u}}$ are prescribed tractions and displacements at the Dirichlet (Γ_t) and Neumann (Γ_u) parts of the boundary, i. e., $\Gamma = \Gamma_u \cup \Gamma_t$, $\Gamma_u \cap \Gamma_t = \emptyset$. Moreover, by $\mathbf{n}$ appropriate unit outward normals at the boundary are denoted and A , H are micromorphic material parameters to be described in more detail in Sect. 5.3.3. It is noted that the very same set of Eqs. (5.1) may also be used to model size effects in, for example, gradient crystal plasticity, if D is replaced by an equivalent plastic strain measure, see Wulfinghoff and Böhlke [2012] and Ziemann et al. [2015].

With (5.1) at hand, the ‘weak form’ of the problem is obtained in the usual way by multiplying the partial differential equations (linear momentum balance and micromorphic balance) by appropriate vectorial and scalar test functions $\delta \mathbf{u}$ and $\delta \bar{D}$, respectively, and integrating over the domain Ω . By further considering Gauss’ theorem and taking into account the boundary conditions, the weak form of the problem follows as:¹

$$g(\mathbf{u}, \bar{D}, \delta \mathbf{u}) := \int_{\Omega} (\boldsymbol{\sigma} \cdot \nabla^s \delta \mathbf{u} - \mathbf{f} \cdot \delta \mathbf{u}) \, d\Omega - \int_{\Gamma_t} \hat{\mathbf{t}} \cdot \delta \mathbf{u} \, d\Gamma = 0 \quad \forall \delta \mathbf{u} \quad (5.2)$$

$$h(\mathbf{u}, \bar{D}, \delta \bar{D}) := \int_{\Omega} (H (D - \bar{D}) \delta \bar{D} - A \nabla \bar{D} \cdot \nabla \delta \bar{D}) \, d\Omega = 0 \quad \forall \delta \bar{D} \quad (5.3)$$

Since g and h are generally nonlinear, a linearization is carried out with respect to the unknowns $\mathbf{u}$ and $\bar{D}$ which leads to a coupled system of linear algebraic equations in the increments $\Delta \mathbf{u}$ and $\Delta \bar{D}$. The latter equation system is then ready for being solved, e. g., by means of an iterative finite element analysis (details are omitted here).

5.3.2 Kinematic assumptions and thermodynamic considerations

A geometrically linear theory is assumed. As such, the total strain $\boldsymbol{\varepsilon} := \nabla^s \mathbf{u}$ is separable into elastic ($\boldsymbol{\varepsilon}_e$) and plastic ($\boldsymbol{\varepsilon}_p$) parts in an additive manner. Furthermore, in order to model nonlinear kinematic hardening, an additional additive split of the plastic part into recoverable ($\boldsymbol{\varepsilon}_{pe}$) and irrecoverable ($\boldsymbol{\varepsilon}_{pi}$) parts is considered, leading to the following relationship:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_{pe} + \boldsymbol{\varepsilon}_{pi} \quad (5.4)$$

The additional split of the plastic strain is physically motivated. According to Lion [2000], $\boldsymbol{\varepsilon}_{pe}$ accounts for dislocation-induced lattice rotations and stretches on the microscale, whereas $\boldsymbol{\varepsilon}_{pi}$ results from local plastic deformations coming from inelastic slip on crystallographic slip

¹ $\nabla^s (\bullet) := \frac{1}{2} [(\bullet) + (\bullet)^T]$ denotes the symmetric part of a quantity $(\bullet)$.

systems.

With regard to the isotropic continuum damage framework considered in this study, the scalar internal damage variable D measures the degree of material degradation at a certain point in an averaged sense. Furthermore, the model makes use of the concept of effective stress, originally introduced by Kachanov [1958] and Rabotnov [1963], and the hypothesis of strain equivalence, proposed by Lemaitre [1971]. The effective stress is denoted and defined as

$$\tilde{\sigma} := \frac{\sigma}{f_{\text{dam}}(D)} \quad (5.5)$$

where $f_{\text{dam}}(D)$ is a scalar-valued positive and decreasing function which is unity for a virgin material ($D = 0$) and progressively approaches zero for increasing damage, until a predefined critical value is reached ($D = D_{\text{cr}}$) that represents complete material failure.

The model is based on the framework of irreversible thermodynamics (see, e. g., Chaboche [2003], Germain et al. [1983], Lemaitre and Chaboche [1990], Truesdell and Noll [1965]). All thermomechanical processes within the material are characterized by means of state couples $(\mathbf{a}_i, \mathbf{A}_i)$ where index i is used to distinguish the various processes available. Quantity $\mathbf{a}_i$ is a strain-like state variable and $\mathbf{A}_i$ a thermodynamically conjugated stress-like state variable, both can be tensors of arbitrary order according to the physical phenomena they represent.

In more detail, the present damage-plasticity model is characterized in every material point by a set of couples $\{(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma}), (\boldsymbol{\varepsilon}_{pe}, \mathbf{X}_p), (\xi_p, q_p), (D, Y), (\xi_d, q_d), (\bar{D}, a_i), (\nabla \bar{D}, \mathbf{b}_i)\}$. The pairs $(\boldsymbol{\varepsilon}_e, \boldsymbol{\sigma})$, $(\boldsymbol{\varepsilon}_{pe}, \mathbf{X}_p)$ and (ξ_p, q_p) describe the state of plastic flow, kinematic and isotropic plastic hardening, whereas (D, Y) and (ξ_d, q_d) characterize the state of damage and damage hardening, respectively. The two couples $(\bar{D}, a_i)$ and $(\nabla \bar{D}, \mathbf{b}_i)$ are related to the micromorphic damage and its first gradient, respectively.

5.3.3 State potential in terms of the Helmholtz free energy

The reversible processes taking place within the material are described by means of a state potential which is expressed in terms of the Helmholtz free energy ψ . The latter energy functional depends on the strain-like variables of the model and is assumed to be additively separable into individual parts. More precisely, there exist energetic contributions related to elasticity (ψ_e), plasticity (ψ_p), damage hardening (ψ_d) and micromorphic damage ($\psi_{\bar{d}}$), leading in total to the following expression and dependencies:

$$\psi = \psi_e(\boldsymbol{\varepsilon}_e, D) + \psi_p(\boldsymbol{\varepsilon}_{pe}, \xi_p, D) + \psi_d(\xi_d) + \psi_{\bar{d}}(D - \bar{D}, \nabla \bar{D}) \quad (5.6)$$

The elastic part of the energy is defined as

$$\psi_e(\boldsymbol{\varepsilon}_e, D) := f_{\text{dam}}(D) \frac{1}{2} \boldsymbol{\varepsilon}_e \cdot \boldsymbol{\mathcal{C}}[\boldsymbol{\varepsilon}_e] \quad (5.7)$$

The quantity $\boldsymbol{\mathcal{C}} := \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \boldsymbol{\mathcal{I}}$ denotes the isotropic fourth-order elasticity tensor in which λ, μ are the Lamé parameters, $\mathbf{I}$ is the second-order identity tensor and $\boldsymbol{\mathcal{I}}$ is the fourth-order symmetric identity tensor. The plastic part of the energy is also affected by damage through function $f_{\text{dam}}(D)$ and reads

$$\psi_p(\boldsymbol{\varepsilon}_{pe}, \xi_p, D) := f_{\text{dam}}(D) \left(\frac{1}{2} a \boldsymbol{\varepsilon}_{pe} \cdot \boldsymbol{\varepsilon}_{pe} + e \left(\xi_p + \frac{\exp(-f \xi_p) - 1}{f} \right) \right) \quad (5.8)$$

The first term inside the outer parentheses accounts for kinematic hardening, the second term is related to nonlinear isotropic hardening. The constants a, e and f are corresponding plastic material parameters. In simple analogy, the energetic part related to nonlinear damage hardening is defined as

$$\psi_d(\xi_d) := r \left(\xi_d + \frac{\exp(-s \xi_d) - 1}{s} \right) \quad (5.9)$$

with r and s being damage material parameters. Finally, the part of the energy belonging to micromorphic damage is expressed as

$$\psi_{\bar{d}}(D - \bar{D}, \nabla \bar{D}) := \frac{1}{2} H (D - \bar{D})^2 + \frac{1}{2} A \nabla \bar{D} \cdot \nabla \bar{D} \quad (5.10)$$

and consists of two terms. The first term penalizes the difference between the local and the micromorphic damage variable with H being a penalty parameter, thus enforcing a certain degree of coupling between the two quantities. The second term accounts for the influence of the gradient of $\bar{D}$ in the free energy. Parameter A introduces implicitly an ‘internal material length’ into the formulation.

5.3.4 State relations and thermodynamic conjugate forces

The second-law of thermodynamics in terms of the Clausius-Duhem inequality is used to derive consistent state relations of the model. The latter reads in its isothermal local form (see Forest [2009] for further information):

$$-\dot{\psi} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} + \underbrace{a_i \dot{\bar{D}} + \mathbf{b}_i \cdot \nabla \dot{\bar{D}}}_{\text{micromorphic extension}} \stackrel{!}{\geq} 0 \quad (5.11)$$

Naturally, two additional terms appear in the Clausius-Duhem inequality due to the micromorphic extension which account for the contributions of the micromorphic damage and its first gradient to the second-law.

With the chain rule of differentiation and expressions (5.4) and (5.6) in mind, inequality (5.11) can be rewritten as:

$$\begin{aligned} & \left(\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(a_i - \frac{\partial \psi}{\partial \bar{D}} \right) \dot{\bar{D}} + \left(\mathbf{b}_i - \frac{\partial \psi}{\partial \nabla \bar{D}} \right) \cdot \nabla \dot{\bar{D}} + \\ & + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \cdot \dot{\boldsymbol{\varepsilon}}_p - \frac{\partial \psi}{\partial D} \dot{D} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_{p_e}} \cdot \dot{\boldsymbol{\varepsilon}}_{p_e} - \frac{\partial \psi}{\partial \xi_p} \dot{\xi}_p - \frac{\partial \psi}{\partial \xi_d} \dot{\xi}_d \geq 0 \end{aligned} \quad (5.12)$$

The latter expression must hold for arbitrary thermomechanical processes. One possibility is now to set the expressions in the parentheses intentionally to zero, such that the state relations of the model follow as:

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} = f_{\text{dam}}(D) \mathbf{C}[\boldsymbol{\varepsilon}_e], \quad a_i = \frac{\partial \psi}{\partial \bar{D}} = -H(D - \bar{D}), \quad \mathbf{b}_i = \frac{\partial \psi}{\partial \nabla \bar{D}} = A \nabla \bar{D} \quad (5.13)$$

As shown, using the micromorphic approach one obtains in addition to the stress-strain relation further state relations for the thermodynamic conjugate forces a_i and $\mathbf{b}_i$ to $\bar{D}$ and $\nabla \bar{D}$, respectively.

What remains left to be fulfilled is the remaining dissipation inequality which reads

$$(\boldsymbol{\sigma} - \mathbf{X}_p) \cdot \dot{\boldsymbol{\varepsilon}}_p + Y \dot{D} + \mathbf{X}_p \cdot \dot{\boldsymbol{\varepsilon}}_{p_i} - q_p \dot{\xi}_p - q_d \dot{\xi}_d \geq 0 \quad (5.14)$$

The abbreviations of the thermodynamic conjugate forces have been introduced for notational convenience and are defined as:

$$\begin{aligned} Y = -\frac{\partial \psi}{\partial D} = & -\frac{df_{\text{dam}}(D)}{dD} \left(\frac{1}{2} \boldsymbol{\varepsilon}_e \cdot \mathbf{C}[\boldsymbol{\varepsilon}_e] + \frac{1}{2} a \boldsymbol{\varepsilon}_{p_e} \cdot \boldsymbol{\varepsilon}_{p_e} + \right. \\ & \left. + e \left(\xi_p + \frac{\exp(-f \xi_p) - 1}{f} \right) \right) - H(D - \bar{D}) \end{aligned} \quad (5.15)$$

$$\mathbf{X}_p = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_{p_e}} = f_{\text{dam}}(D) a \boldsymbol{\varepsilon}_{p_e} \quad (5.16)$$

$$q_p = \frac{\partial \psi}{\partial \xi_p} = f_{\text{dam}}(D) e (1 - \exp(-f \xi_p)) \quad (5.17)$$

$$q_d = \frac{\partial \psi}{\partial \xi_d} = r (1 - \exp(-s \xi_d)) \quad (5.18)$$

As can be seen from Eq. (5.15), Y (sometimes loosely referred to as the ‘energy release rate’) is directly influenced by the micromorphic damage variable $\bar{D}$ and will in Sect. 5.3.6 be used in the definition of the damage loading function. According to this fact, a ‘nonlocal’ character is introduced into the constitutive equations at the local integration point level. Further, Y contains both elastic and plastic contributions which proves to be beneficial since a purely elastic ‘energy release rate’ would maybe be too restrictive from a physical point of view (for arguments supporting this hypothesis, see, e. g., Chaboche [2003], Chow and Wang [1987], Ju [1989], Kachanov [1993], Saanouni et al. [1994]).

5.3.5 Modeling of plasticity

Deviatoric plastic behavior of the material is assumed for simplicity which is modeled by means of a von Mises-type yield function:²

$$\Phi_p(\tilde{\boldsymbol{\sigma}}, \tilde{\mathbf{X}}_p, \tilde{q}_p) = \sqrt{\frac{3}{2}} \left\| \tilde{\boldsymbol{\sigma}}' - \tilde{\mathbf{X}}_p' \right\| - (\sigma_0 + \tilde{q}_p) \leq 0 \quad (5.19)$$

The initial yield stress is given by material parameter σ_0 and nonlinear kinematic and isotropic hardening are taken into account via $\tilde{\mathbf{X}}_p$ and $\tilde{q}_p$, respectively. As indicated, a further coupling between plasticity and damage is considered in the formulation since Φ_p is expressed in terms of effective quantities, i. e., in terms of $\tilde{\boldsymbol{\sigma}}$ as defined in (5.5) and

$$\tilde{\mathbf{X}}_p := \frac{\mathbf{X}_p}{f_{\text{dam}}(D)}, \quad \tilde{q}_d := \frac{q_d}{f_{\text{dam}}(D)} \quad (5.20)$$

Furthermore, the following thermodynamically consistent plastic evolution equations for the strain-like plastic internal variables are postulated:

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda}_p \frac{\partial \Phi_p}{\partial \boldsymbol{\sigma}} = \sqrt{\frac{3}{2}} \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} \frac{\boldsymbol{\sigma}' - \mathbf{X}_p'}{\|\boldsymbol{\sigma}' - \mathbf{X}_p'\|} \quad (5.21)$$

$$\dot{\boldsymbol{\varepsilon}}_{p_i} = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} \frac{b}{a} \tilde{\mathbf{X}}_p' = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} b \boldsymbol{\varepsilon}_{p_e} \quad (5.22)$$

$$\dot{\xi}_p = -\dot{\lambda}_p \frac{\partial \Phi_p}{\partial q_p} = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} \quad (5.23)$$

Constant b in expression (5.22) is an additional plastic material parameter necessary for modeling nonlinear kinematic hardening. By inspecting the remaining dissipation inequality (5.14),

² $(\bullet)' := (\bullet) - \frac{1}{3} \text{trace}(\bullet) \mathbf{I}$ denotes the deviatoric part of a second-order tensor $(\bullet)$.

it can be easily verified that evolution equations (5.21) – (5.23) lead to a thermodynamically consistent plastic behavior of the model.

As usual, the plastic loading / unloading conditions of the model have to be taken into account, i. e.,

$$\dot{\lambda}_p \geq 0, \quad \Phi_p \leq 0, \quad \dot{\lambda}_p \Phi_p = 0 \quad (5.24)$$

5.3.6 Modeling of damage

Damage is modeled by means of the damage loading function

$$\Phi_d(Y, q_d) = Y - (Y_0 + q_d) \leq 0 \quad (5.25)$$

The structural analogy to plasticity is apparent. The onset of damage is represented by material parameter Y_0 , whereas q_d accounts for nonlinear damage hardening.

Thermodynamically consistent evolution equations for the strain-like damage variables are postulated as

$$\dot{D} = \dot{\lambda}_d \frac{\partial \Phi_d}{\partial Y} = \dot{\lambda}_d \quad (5.26)$$

$$\dot{\xi}_d = -\dot{\lambda}_d \frac{\partial \Phi_d}{\partial q_d} = \dot{\lambda}_d \quad (5.27)$$

and, finally, the damage loading / unloading conditions need to be considered, i. e.,

$$\dot{\lambda}_d \geq 0, \quad \Phi_d \leq 0, \quad \dot{\lambda}_d \Phi_d = 0 \quad (5.28)$$

As was mentioned in Sect. 5.3.4, a ‘nonlocal’ character of the constitutive equations exists due to the dependence of Φ_d on Y which itself is directly influenced by the micromorphic damage variable $\bar{D}$.

To summarize, there exist 12 material parameters of the model: $\lambda, \mu, \sigma_0, a, b, e, f, r, s, Y_0, A$ and H . In the present study, constant H plays the role of a penalty constant controlling the degree of coupling between D and $\bar{D}$ which is typically desired to be strong. In other words, H is intentionally chosen as a large number. All other parameters should be determined via suitable experiments.

5.4 Numerical and algorithmic aspects

The present section discusses some fundamental numerical and algorithmic aspects which are practically relevant, if the model is to be implemented into, e. g., finite element codes. More concretely speaking, Sect. 5.4.1 is concerned with the time-discretization of the model's evolution equations and a solution strategy for the resulting algebraic equation system, whereas Sect. 5.4.2 explains a procedure to enforce stress constraints for 3D gradient-extended material models at the local integration point level in finite elements.

5.4.1 Discretization of the evolution equations and remarks on the incremental problem

The evolution equations (5.21) – (5.23) and (5.26) – (5.27) of the model are discretized in time by means of a fully implicit backward Euler scheme, leading to a coupled system of nonlinear algebraic equations. Considering a time interval $[t_n, t_{n+1}]$ during the Newton-Raphson iteration at the global finite element level, this equation system needs to be solved iteratively (for given values of ε and $\bar{D}$) in every integration point for the following unknowns at time t_{n+1} : ε_p , ε_{p_i} , ξ_p , D , ξ_d , $\Delta\lambda_p$, $\Delta\lambda_d$, where $\Delta\lambda_p = \Delta t \dot{\lambda}_p$ and $\Delta\lambda_d = \Delta t \dot{\lambda}_d$ denote the incremental plastic and damage multipliers, respectively.³ In the actual iteration process, the variables ε_{p_i} , ξ_p , D and ξ_d do not need to be treated as additional unknowns but can be expressed in terms of the quantities ε_p , $\Delta\lambda_p$, $\Delta\lambda_d$, thus reducing the computational effort. The stress-like quantities σ , $\mathbf{X}_p$, q_p , Y and q_d at time t_{n+1} can be computed according to the formulas given in Sect. 5.3.4.

The resulting equation system is additionally subject to the time-discrete version of the loading / unloading conditions (5.24) and (5.28) which leads to four mutually exclusive scenarios: the step can either be 1.) elastic, 2.) elastic with concurrently evolving damage, 3.) elastoplastic or 4.) elastoplastic with concurrently evolving damage. In order to determine the correct solution, a suitable algorithmic strategy needs to be adopted. With regard to monolithic approaches in which the plastic and damage variables are computed simultaneously, a classical approach would be, e. g., to apply a local active set search strategy similar as in multi-surface plasticity (see, e. g., Simo et al. [1988]). Another more recent alternative would be to reformulate the two sets of loading / unloading conditions by means of the so-called Fischer-Burmeister functional, thus rigorously eliminating the need for any kind of case differentiation within the algorithm (see, e. g., Auricchio et al. [2014], Bartel and Hackl [2009], Brepols et al.

³In the following, if not explicitly denoted otherwise, any quantity is referred to time $t_{n+1} = t_n + \Delta t$.

[2017], Kiefer et al. [2012], Kiefer et al. [2018]). Both algorithmic strategies possess advantages and disadvantages. Further details about this and other numerical issues (e. g., finite element discretization of the equations, computation of the consistent tangent operators etc.) are omitted here for brevity but are thoroughly discussed by Brepols et al. [2017].

The final equations which need to be solved in case of an elastoplastic step with concurrently evolving damage are given below in a residuum format:⁴

$$\begin{aligned} \mathbf{r}_1 &= \boldsymbol{\varepsilon}_p - \boldsymbol{\varepsilon}_{p_n} - \sqrt{\frac{3}{2}} \frac{\Delta\lambda_p}{f_{\text{dam}}(D_n + \Delta\lambda_d)} \frac{\boldsymbol{\sigma}' - \mathbf{X}'_p}{\|\boldsymbol{\sigma}' - \mathbf{X}'_p\|} = \mathbf{0} \\ r_2 &= \Phi_p = 0 \\ r_3 &= \Phi_d = 0 \end{aligned} \tag{5.29}$$

Taking symmetry into account, the resulting number of scalar equations and unknowns to be solved for in this particular case is eight (six components of $\boldsymbol{\varepsilon}_p$ plus two scalars $\Delta\lambda_p$ and $\Delta\lambda_d$).

5.4.2 Enforcing stress constraints for 3D gradient-extended material models in finite elements

In engineering applications, it is frequently desirable and convenient to work with beam or shell instead of classical solid finite elements. The validity of some of these element formulations fundamentally depends upon special zero-stress conditions prevailing within the respective elements, a fact which needs to be considered by the applied material formulation as well. However, sophisticated material models are often only available for three-dimensional problems and a consideration of such zero-stress conditions would necessitate a reformulation of these models which proves to be complicated. Similar problems can arise, if 2D plane stress computations are to be performed using a complex 3D material model, as is, e. g., the case in the present study.

In this section, it is shown how arbitrary nonlinear 3D gradient-extended material models (introducing one additional degree of freedom) can be consistently integrated into beam, shell or 2D plane stress elements of the above mentioned kind which rely upon additional zero-stress conditions. For this, an iterative algorithm will be described which enforces these constraints at the local integration point level. The style of presentation is very similar to that given by Klinkel and Govindjee [2002] who explained a corresponding strategy for conventional ‘local’ 3D material models. In the following, the method is extended to account also for

⁴The corresponding residuals in case of a purely elastoplastic step or elastic step with concurrently evolving damage are obtained by deleting either r_3 or $\mathbf{r}_1$ and r_2 in (5.29), respectively.

gradient-extended material models of the type presented in this study.

For the development of the procedure, consider the time-discretized version of the weak form constituted by (5.2) – (5.3). During a time interval $[t_n, t_{n+1}]$ in a global Newton-Raphson iteration, the stress $\boldsymbol{\sigma}$ and the damage variable D are considered as functions of the strain $\boldsymbol{\varepsilon}$ and the micromorphic damage variable $\bar{D}$ only, i. e.,⁵

$$\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, \bar{D}), \quad D \equiv D(\boldsymbol{\varepsilon}, \bar{D}) \quad (5.30)$$

A consistent linearization of the weak form requires to derive $\boldsymbol{\sigma}$ and D with respect to $\boldsymbol{\varepsilon}$ and $\bar{D}$, respectively, leading to

$$\Delta \boldsymbol{\sigma} = \mathcal{A}[\Delta \boldsymbol{\varepsilon}] + \mathbf{B} \Delta \bar{D}, \quad \Delta D = \mathbf{E} \cdot \Delta \boldsymbol{\varepsilon} + F \Delta \bar{D} \quad (5.31)$$

where $\mathcal{A} := \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}}|_{\bar{D}=\text{const}}$ (fourth-order tensor), $\mathbf{B} := \frac{\partial \boldsymbol{\sigma}}{\partial \bar{D}}|_{\boldsymbol{\varepsilon}=\text{const}}$, $\mathbf{E} := \frac{\partial D}{\partial \boldsymbol{\varepsilon}}|_{\bar{D}=\text{const}}$ (second-order tensors) and $F := \frac{\partial D}{\partial \bar{D}}|_{\boldsymbol{\varepsilon}=\text{const}}$ (scalar).

In all the element formulations considered in this section, certain components of the stress tensor vanish. Assuming a standard Cartesian frame, these are components $\{\sigma^{22}, \sigma^{33}, \sigma^{23}\}$ in case of beam formulations, whereas σ^{33} and $\{\sigma^{33}, \sigma^{13}, \sigma^{23}\}$ are assumed to be zero in case of shell and 2D plane stress elements, respectively. To describe a single algorithm which is applicable in all cases, a matrix-vector notation of all quantities is adopted⁶ and the expressions in (5.31) are rewritten in the following partitioned matrix format:

$$\begin{bmatrix} \Delta \boldsymbol{\sigma}_m \\ \Delta \boldsymbol{\sigma}_z \end{bmatrix} = \begin{bmatrix} \mathcal{A}_{mm} & \mathcal{A}_{mz} \\ \mathcal{A}_{zm} & \mathcal{A}_{zz} \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{\varepsilon}_m \\ \Delta \boldsymbol{\varepsilon}_z \end{bmatrix} + \begin{bmatrix} \mathbf{B}_m \\ \mathbf{B}_z \end{bmatrix} \Delta \bar{D} \quad (5.32)$$

$$\Delta D = \begin{bmatrix} \mathbf{E}_m & \mathbf{E}_z \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{\varepsilon}_m \\ \Delta \boldsymbol{\varepsilon}_z \end{bmatrix} + F \Delta \bar{D} \quad (5.33)$$

In the respective cases, $\boldsymbol{\sigma}_m$ and $\boldsymbol{\sigma}_z$ are defined as

$$\text{beam:} \quad \boldsymbol{\sigma}_m = [\sigma^{11}, \sigma^{12}, \sigma^{13}]^T, \quad \boldsymbol{\sigma}_z = [\sigma^{22}, \sigma^{33}, \sigma^{23}]^T = \mathbf{0} \quad (5.34)$$

$$\text{shell:} \quad \boldsymbol{\sigma}_m = [\sigma^{11}, \sigma^{22}, \sigma^{12}, \sigma^{13}, \sigma^{23}]^T, \quad \boldsymbol{\sigma}_z = [\sigma^{33}] = \mathbf{0} \quad (5.35)$$

$$\text{2D plane stress:} \quad \boldsymbol{\sigma}_m = [\sigma^{11}, \sigma^{22}, \sigma^{12}]^T, \quad \boldsymbol{\sigma}_z = [\sigma^{33}, \sigma^{13}, \sigma^{23}]^T = \mathbf{0} \quad (5.36)$$

⁵Remember that, during the considered time interval, $\boldsymbol{\sigma}$ and D do additionally depend on the history variables at time t_n which are, however, constant within $[t_n, t_{n+1}]$.

⁶No extra symbols are introduced to avoid an excessive proliferation of notation. The change in meaning of the quantities is implicitly understood.

The vectors σ_m and ε_m contain the components of the stress and strain which are actually included in the weak form of the underlying formulation.

An algorithm enforcing the stress constraint(s) at the local integration point level can be obtained by arguing that σ_z should vanish. Expanding this condition in a Taylor series in terms of the unknown strain ε_z delivers

$$\sigma_z^{(i+1)} = \sigma_z^{(i)} + \left. \frac{\partial \sigma_z}{\partial \varepsilon_z} \right|^{(i)} \Delta \varepsilon_z + \dots \stackrel{!}{=} 0 \quad (5.37)$$

where a superscript denotes the corresponding local iteration number. By neglecting higher-order terms and identifying $\mathcal{A}_{zz}^{(i)} = (\partial \sigma_z / \partial \varepsilon_z)|^{(i)}$, expression (5.37) can then be rewritten as

$$\Delta \varepsilon_z = -\mathcal{A}_{zz}^{(i)-1} \sigma_z^{(i)} \quad (5.38)$$

which suggests the following iterative procedure for the calculation of ε_z at time t_{n+1} :

$$\varepsilon_z^{(i+1)} \leftarrow \varepsilon_z^{(i)} + \Delta \varepsilon_z, \quad \varepsilon_z^{(0)} := \varepsilon_z \text{ at time } t_n \quad (5.39)$$

The iteration must be performed until $\|\sigma_z^{(i)}\| \approx 0$; the rate of convergence is quadratic. As indicated, the algorithm requires to additionally store the converged components of ε_z during the computation.

A new point discussed here is the computation of the appropriate material tangent moduli in case of gradient-extended material models. The latter are necessary to retain a quadratic rate of convergence in a Newton-Raphson iteration at the global finite element level. For this, one needs to compute the variations of σ_m and D with respect to ε_m and $\bar{D}$, respectively. Since these quantities do implicitly depend on the complete strain state ε , a proper condensation procedure is necessary as follows:

Remember that $\Delta \sigma_z = 0$ and plug this condition into the second equation of (5.32), leading to

$$\Delta \varepsilon_z = -\mathcal{A}_{zz}^{-1} \mathcal{A}_{zm} \Delta \varepsilon_m - \mathcal{A}_{zz}^{-1} \mathbf{B}_z \Delta \bar{D} \quad (5.40)$$

Inserting this result both into the first equation of (5.32) and Eq. (5.33) delivers, after simple rearranging, the expressions:

$$\Delta \sigma_m = \hat{\mathcal{A}} \Delta \varepsilon_m + \hat{\mathbf{B}} \Delta \bar{D}, \quad \Delta D = \hat{\mathbf{E}} \Delta \varepsilon_m + \hat{F} \Delta \bar{D} \quad (5.41)$$

where $\hat{\mathcal{A}}$, $\hat{\mathbf{B}}$, $\hat{\mathbf{E}}$ and $\hat{F}$ denote the appropriate material tangent moduli of the stress-constrained

problem in matrix format:

$$\hat{\mathcal{A}} := \left. \frac{\partial \sigma_m}{\partial \epsilon_m} \right|_{\bar{D}=\text{const}} = \mathcal{A}_{mm} - \mathcal{A}_{mz} \mathcal{A}_{zz}^{-1} \mathcal{A}_{zm} \quad (5.42)$$

$$\hat{\mathbf{B}} := \left. \frac{\partial \sigma_m}{\partial \bar{D}} \right|_{\epsilon=\text{const}} = \mathbf{B}_m - \mathcal{A}_{mz} \mathcal{A}_{zz}^{-1} \mathbf{B}_z \quad (5.43)$$

$$\hat{\mathbf{E}} := \left. \frac{\partial D}{\partial \epsilon_m} \right|_{\bar{D}=\text{const}} = \mathbf{E}_m - \mathbf{E}_z \mathcal{A}_{zz}^{-1} \mathcal{A}_{zm} \quad (5.44)$$

$$\hat{F} := \left. \frac{\partial D}{\partial \bar{D}} \right|_{\epsilon=\text{const}} = F - \mathbf{E}_z \mathcal{A}_{zz}^{-1} \mathbf{B}_z \quad (5.45)$$

The above procedure can equally be applied in case of a geometrically nonlinear theory. It could furthermore readily be extended to account for more general cases with multiple gradient variables.

5.5 Numerical example

In the following, in order to illustrate the merits of the gradient-extended material model and to test the functionality of the procedure presented in Sect. 5.4.2, a 2D plane stress finite element problem is considered. A tensile specimen with length $\ell = 200$ mm, width 80 mm and two sharp vertical notches of 16 mm length (zero width) located at the upper and lower edges is subjected to a state of uniaxial tension by applying a horizontal force $F(t)$ at the left and right ends of the sample, respectively. Note that the applied force $F(t)$ is (pseudo-)time-dependent: the tensile specimen is first loaded gradually up to the point of maximum load $F_{\max}$ and further deformed afterwards at a decreasing load level (due to evolving damage) until the structure may essentially be regarded as ‘broken’.

The geometry and its dimensions are shown in Fig. 5.1a. By exploiting symmetry conditions, the original boundary-value problem can be reduced to a quarter of its original size, see Fig. 5.1b. The loaded edge on the right is constrained such that it remains straight and perpendicular to the loading direction throughout the analysis. Moreover, note that, due to the assumed elastoplastic isotropy of the model, the plane stress condition implies that components σ_{13} , σ_{23} and ε_{13} , ε_{23} of the stress and strain tensor automatically vanish, meaning that σ_z in Eq. (5.36) as well as ε_z directly reduce to $\sigma_z = [\sigma_{33}] = 0$ and $\varepsilon_z = [\varepsilon_{33}]$, respectively.

The regularization properties of the model shall be investigated by conducting a convergence study using different mesh sizes (640, 1715, 4415 and 8330 elements) and the fol-

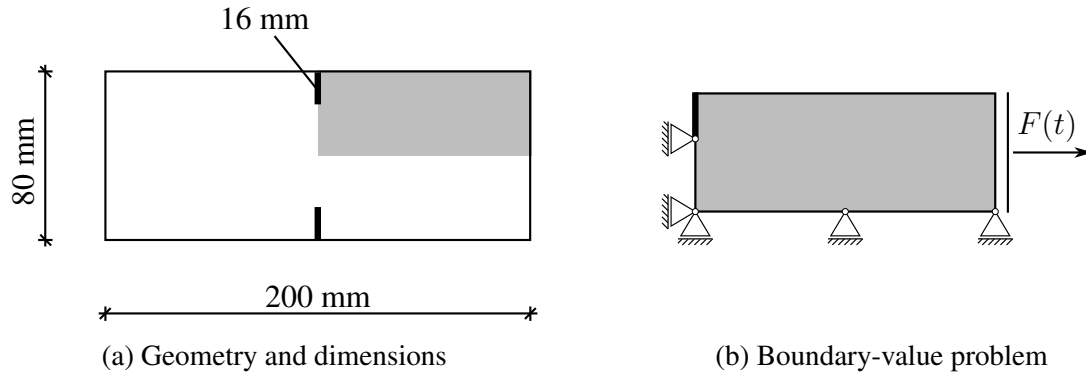


Figure 5.1: Double-edge notched specimen

lowing set of material parameters: $\lambda = 5000$ MPa, $\mu = 7500$ MPa, $a = 1900$ MPa, $b = 8.5$, $e = 400$ MPa, $f = 2.5$, $r = 0.5$ MPa, $s = 0.1$, $\sigma_0 = 20$ MPa, $Y_0 = 0.1$ MPa, $H = 10^5$ MPa and $A = 10$ MPa mm². The function in Eqs. (5.5) and (5.20) is defined as $f_{\text{dam}}(D) = (1 - D)^2$. As will be illustrated below, this choice allows for very stable computations up to values of $D = D_{\text{cr}} \approx 1$. Linear finite element approximations of the displacement field and the micromorphic damage field are considered. The meshes are strongly refined in the region of the notch tip(s) and the area(s) where damage is expected to develop during the process, see Fig. 5.2 illustrating exemplarily both the coarsest and finest meshes with 640 and 8330 elements, respectively.⁷

In the process, damage starts to develop at the notch tip(s) and from there on progresses into the interior of the specimen until the latter may be regarded as fully ‘broken’, meaning that, practically, no further load can be carried by the structure. Three different stages during the process are exemplarily illustrated in Fig. 5.3. The corresponding accumulated plastic strain is shown as well.⁸

Fig. 5.4 shows the global response of the structure, i. e., the normalized load-displacement curves obtained by using the different meshes. Here, u denotes again the horizontal displacements of the loaded ends at the left and right side, respectively. Mesh-convergence is recognized, the curves lie very close together. The points at which the damage contours of Fig. 5.3 were taken are indicated by small rectangular boxes.

A noticeable snapback of the load-displacement curve is visible shortly after exceeding the point of maximum load which deserves further clarification. It should be kept in mind that a quasi-static analysis is performed of a process which is accompanied by dynamic effects at the

⁷Quadrilateral elements are preferred in the meshing process, triangular ones are only used rarely as transitional elements.

⁸The top and bottom values in the legends of the contour plots always indicate the corresponding minimum and maximum values attained in the computations.

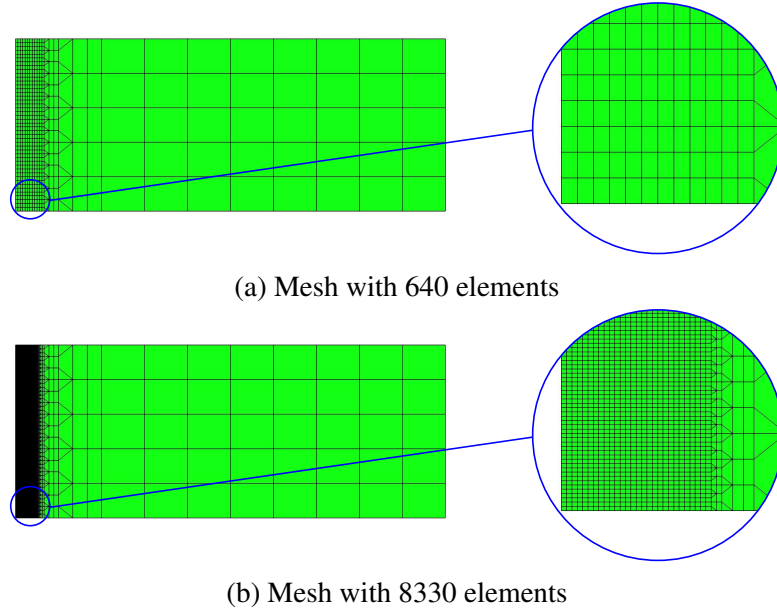


Figure 5.2: Mesh refinement

point when severe strain-localization sets in and the ‘crack’ starts to run through the specimen. If these effects were taken into account, the load-displacement curve would show a ‘sudden’ vertical drop when the tangent to the curve becomes infinite. This usually marks the beginning of dynamic crack propagation which cannot be modeled using a purely quasi-static framework (see, e. g., Heinrich et al. [2013], Hütter et al. [2013, 2014] for more detailed explanations). Instead, an arclength method is used in the present study to compute the equilibrium solution of the process, practically considering the ‘crack’ to grow quasi-statically.

Convergence of the local fields is exemplarily demonstrated in Fig. 5.5 for the case of the damage variable D . For brevity, only the end states of the process for the coarsest and finest meshes are shown, respectively. The highly damaged zone ($D \geq 0.9$, marked in red color) is confined to a relatively thin area (representing a crack in a continuous sense) and slightly wider in case of the coarser mesh; however, the differences between the plots can be considered negligibly small.

5.6 Conclusions

A gradient-enhanced damage-plasticity material model was presented and discussed in this study which can be considered as a particular instance of the general class of micromorphic media as proposed by Forest [2009, 2016]. The gradient-extension is characterized by a Helmholtz-type partial differential equation for a newly introduced ‘micromorphic’ (i. e., non-

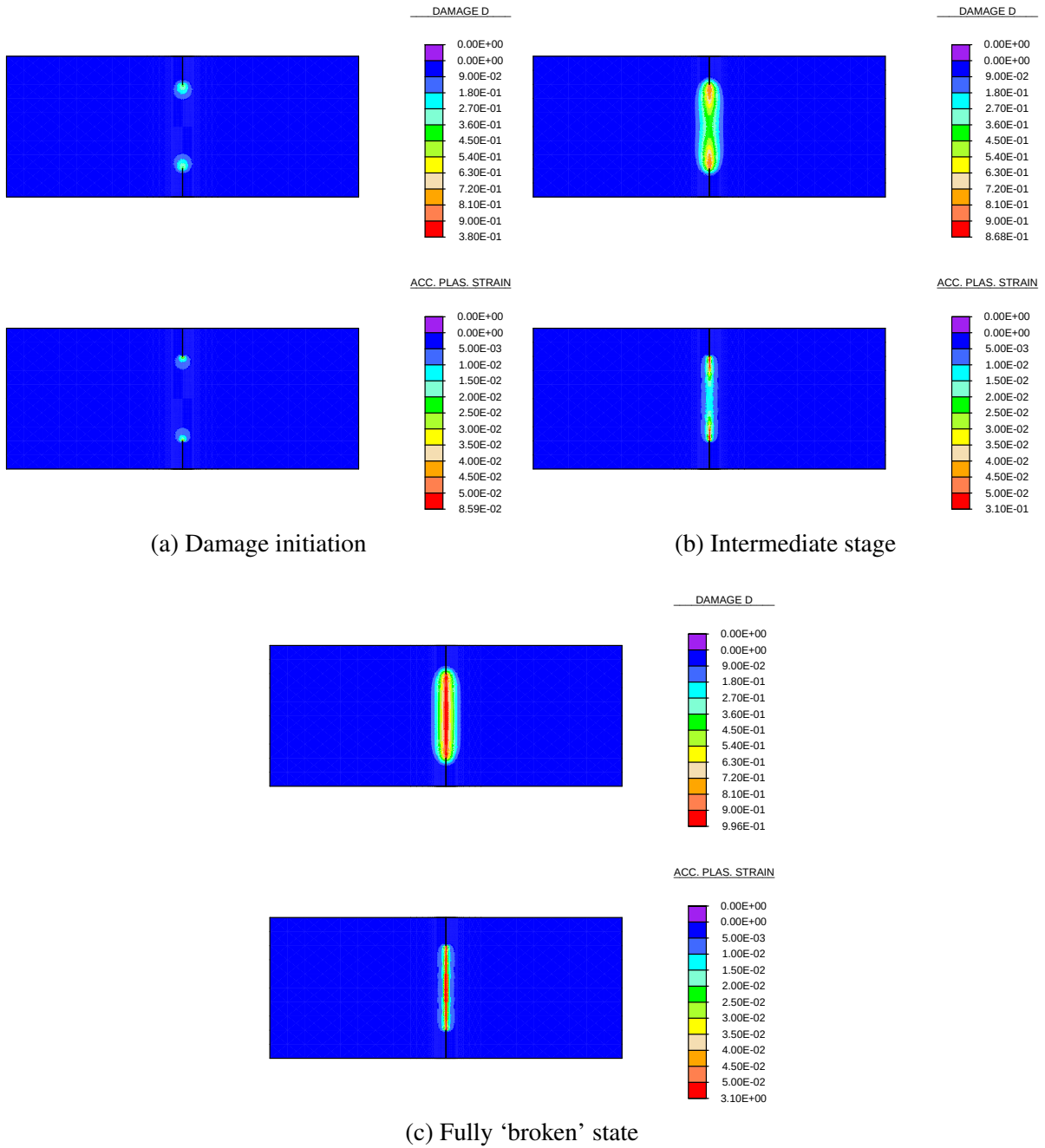


Figure 5.3: Damage contours D (top) and accumulated plastic strain (bottom) during three different stages of the process (8330 elements)

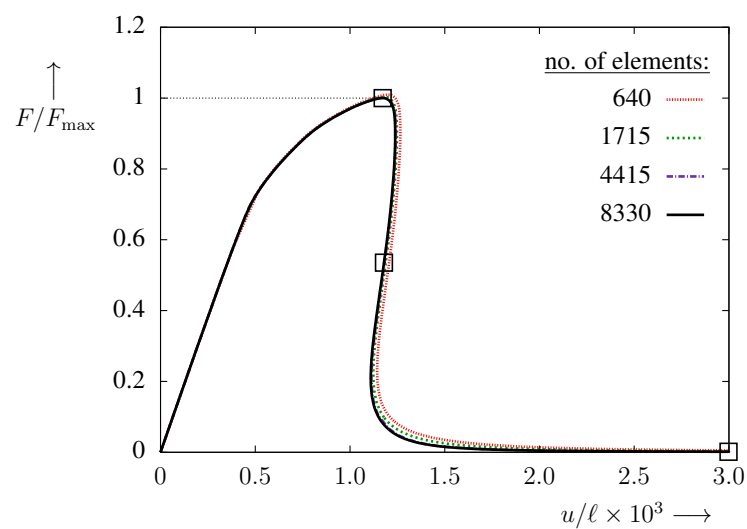


Figure 5.4: Convergence study: load-displacement curves

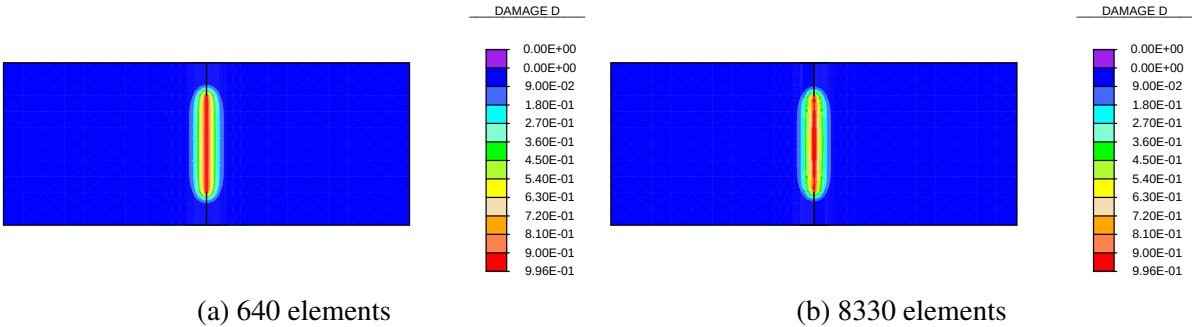


Figure 5.5: Convergence study: damage contours D at the end of the simulation

local) damage variable which needs to be solved in addition to the classical balance of linear momentum. In finite element computations, this micromorphic damage variable shows up as a further degree of freedom at the nodes (similar, e. g., to the temperature in thermomechanically coupled problems). Damage and plasticity are regarded as distinct physical mechanisms which was realized by postulating individual damage and yield criteria as well as corresponding sets of loading / unloading conditions. Nonlinear kinematic and isotropic hardening as well as damage hardening are considered in the formulation.

Besides a detailed description of the model's equations and some remarks about its numerical implementation into finite element codes, the present study focused also on a procedure to locally enforce stress constraints in computations involving 3D gradient-extended material models. Special emphasis was put here on a condensation procedure for the four consistent tangent operators which is necessary to retain the rate of quadratic convergence in a Newton-Raphson iteration scheme at the global finite element level. The procedure can, e. g., be utilized to easily carry out 2D plane stress computations using 3D gradient-extended material models or to incorporate the latter in a straightforward manner in beam or shell elements without the need of a (possibly) complicated reformulation of the model's constitutive equations.

Finally, a numerical benchmark test was conducted in which the evolution of damage within a 2D double-edge notched specimen was examined. To demonstrate the practical applicability of the above mentioned procedure, the underlying mechanical problem was assumed to be plane stress. The results showed that the micromorphic damage-plasticity model is able to suitably regularize the mesh-dependence which is otherwise present for finite element simulations involving conventional 'local' continuum damage models. Stable computations were performed up to very high values of the damage variable at which the structure could essentially be regarded as 'broken'.

The promising results of the study naturally pave the way for further possible enhancements of the model. Currently, the authors are working on a finite strain extension which relies upon a multiplicative description of plasticity and nonlinear kinematic hardening in the spirit of Vladimirov et al. [2008, 2009]. Furthermore, the incorporation of suitable finite element technology (see, e. g., Reese [2002, 2003, 2005]) into the formulation in order to avoid artificial locking effects and concurrently reducing the computational effort seems sensible, especially with regard to large plastic deformations. Another interesting point would be to take account of anisotropic plasticity and/or damage (for related works of the authors on the mentioned subject, see, e. g., Pietryga et al. [2012], Vladimirov et al. [2010, 2014]).

6 | Article 5:

A ‘two-surface’ gradient-extended damage-plasticity model for large deformations

This chapter represents a preliminary version of the following article:

Brepols, T., Wulfinghoff, S. and Reese, S., ‘Gradient-extended two-surface damage-plasticity for large deformations: Micromorphic formulation and numerical aspects’ (working title), *in preparation*.

Disclosure of the individual authors’ contributions to the article:

T. Brepols reviewed the relevant existing literature, developed the ‘two-surface’ gradient-extended damage-plasticity model for large deformations and implemented it into the academic finite element software FEAP (as an own element subroutine using a corresponding interface in the software). It was his idea to employ the finite strain elastoplasticity framework by Vladimirov et al. [2008] as the basis for the model development. He set up and performed all simulations, interpreted the results and wrote the preliminary version of the article. In previous works dealing with a small strain version of the model presented here (see Brepols et al. [2017, 2018]), it was S. Wulfinghoff’s original idea to apply the micromorphic approach in order to achieve the gradient-extension. T. Brepols then adopted the same approach also for the development of the large deformation model presented in this work. Moreover, S. Wulfinghoff and S. Reese gave conceptual advice, contributed to the discussion of the results, read the current version of the article and gave valuable suggestions for improvement. All authors approved the preliminary publication of the article in the present dissertation.

6.1 Abstract

This work is concerned with the theoretical development, algorithmic implementation and numerical investigation of a thermodynamically consistent ‘two-surface’ gradient-extended damage-plasticity material model for arbitrarily large deformations. It can be considered the geometrically nonlinear version of a corresponding model for small deformations which was presented recently (Brepols et al. [2017, 2018]). The terminology ‘two-surface’ stems from the fact that damage and plasticity are treated in the model as truly distinct dissipative mechanisms, meaning that individual damage loading and plastic yield criteria as well as appropriate loading / unloading conditions are used in the formulation, respectively. Such an approach makes the model flexibly adaptable to various situations in which the material under consideration shows either a (quasi-)brittle-type, ductile-type or possibly a mixed-type damaging behavior. Nonlinear Armstrong-Frederick kinematic hardening, nonlinear Voce isotropic hardening as well as nonlinear damage hardening are accounted for in the presented formulation that relies exclusively on symmetric internal variables, being beneficial, e. g., from the computational point of view. The model’s gradient-extension is derived on the basis of the micromorphic approach according to Forest [2009, 2016] and allows for the computation of mesh-insensitive results in finite element simulations involving material softening which is exemplarily confirmed through the discussion of a numerical benchmark problem. Furthermore, many other interesting and practically relevant aspects are highlighted, as, e. g., the model’s implementation into finite elements, the computation of the algorithmically consistent tangent operators necessary to retain a quadratic rate of convergence in a global Newton-Raphson scheme, or a suitable time-integration of the model’s evolution equations at the integration point level.

6.2 Introduction

The modeling of damage and fracture in solid materials has always been a major concern in mechanics. Through the further development of corresponding methods in this scientific discipline and the increase in computing power of modern computers, simulation tools on the basis of the finite element method for predicting failure in structures have found their way also into, e. g., the automotive or aerospace industries and often play an essential role in the design phase of new (large-scale) processes to reduce experimental costs. Typical examples of such processes are the machining and forming of ductile materials which usually undergo significant elastoplastic distortion before finally fracturing. It goes without saying that the

quality of corresponding simulations to a large extent depends also on the accuracy of the applied material models and the way the latter account for the complex inelastic phenomena plasticity and damage as well as the interplay between the two. This topic is intriguingly challenging from a scientific point of view and there is a pressing need for further research in this area.

The actual phenomena causing damage in ductile materials, i. e., nucleation, growth and coalescence of microvoids, are nowadays quite well understood and documented, see, e. g., Hancock and Mackenzie [1976], Hosokawa et al. [2013], Landron et al. [2013], McClintock [1968], Rice and Tracey [1969] and Tekoğlu et al. [2015]. If the main interest is to model the effective material response, continuum mechanical models are often appropriate which usually only consider the overall impact of damage on the material's behavior and are virtually predestined for the usage in finite element analyses. Many such models were proposed in the past and it is impossible to mention all of them here. For a more comprehensive literature review the reader is referred to Besson [2010].

Very roughly, such material formulations can be classified into 'uncoupled' and 'coupled' ones. Uncoupled models make use of phenomenological / empirical failure criteria or damage variables which estimate the degree of deterioration at a material point in a certain sense (e. g., by means of 'strain-to-failure' curves). If a failure criterion is met or damage reaches a predefined limit during the computation, the material element is considered to fail which usually means that the corresponding finite element is simply removed from the mesh or the equivalent stress is set to zero at the integration point. The terminology 'uncoupled' means that damage has no effect whatsoever on the model's constitutive response, i. e., it causes no material softening nor does it affect the plastic behavior. Some well-known representatives of this class of models were proposed by Bao and Wierzbicki [2004], Cockcroft and Latham [1968], Johnson and Cook [1985], Kamoulakos et al. [2003], Oh et al. [1979], Wierzbicki and Xue [2005], Wilkins et al. [1980], Xue [2007], to name only a few. Uncoupled formulations are used in a variety of different applications and there is still active research in this field (see, e. g., Bai and Wierzbicki [2008], Børvik et al. [2009], Buchkremer et al. [2016], Ghandehariun et al. [2016], Huang et al. [2017], Nguyen et al. [2012] or Tarigopula et al. [2008]). Nevertheless, the predictive capabilities of uncoupled models might be insufficient in cases in which pronounced damaged zones occur in the material, such that the influence of damage on the material behavior cannot actually be neglected anymore.

Coupled formulations can sometimes be a better alternative which themselves are further distinguishable into two major groups. The first group consists of micromechanically motivated models which use (one or more) internal variables that represent the volume fraction

of microvoids within the material. These variables are usually incorporated into the model's yield function(s) and affect the material's strength. Corresponding evolution equations for these variables are then derived based on a deeper knowledge of the true physical mechanisms causing ductile damage (i. e., void nucleation, growth and coalescence, as mentioned earlier). Essentially, a stress decrease is induced whenever the void volume fraction in the material increases. The probably best-known and most important representative in this field is the Gurson–Tvergaard–Needleman (GTN) model (Tvergaard and Needleman [1984]) whose development was based on earlier works by Gurson [1977] and Tvergaard [1981, 1982*a,b*], respectively. Since then, the original GTN model has been (and still is) continuously further developed and improved. For instance, Gologanu et al. [1993, 1994, 1997], Madou and Leblond [2012*a,b*] incorporated the effect of the void shape into the model, whereas Wen et al. [2005] and Xue [2008] took the void size and void shear effect into account, respectively. Some other features which were implemented and investigated are kinematic hardening (Arndt et al. [1997], Besson and Guillemer-Neel [2003], Klingbeil et al. [2016], Leblond et al. [1995], Mear and Hutchinson [1985], Mühlich and Brocks [2003], Ristinmaa [1997]), plastic anisotropy (Benzerga and Besson [2001], Keralavarma and Benzerga [2008, 2010], Monchiet et al. [2006, 2008], Morin et al. [2015]) and strain rate sensitivity (Needleman and Tvergaard [1984], Pan et al. [1983]).

Models belonging to the second group are based on the continuum damage mechanics (CDM) concept and are phenomenological in nature. Abstract scalar- or tensor-valued internal variables are utilized in a continuum mechanics framework which account for the effects of damage in an averaged sense only by causing softening, e. g., by weakening the stiffness and / or strength of the material. In contrast to the micromechanically motivated models described above, constitutive relationships (such as the evolution equations) are often quite formally derived on the basis of strict thermodynamic considerations. Furthermore, the notion of 'effective stress' (and maybe other 'effective variables') as well as an equivalence hypothesis between the damaged and a fictitious undamaged state of the material may play a role. The CDM concept goes back to works by Kachanov [1958] and Rabotnov [1963, 1969] in the context of creep modeling and was later established as a sound and general theory on its own by embedding it into the framework of irreversible thermodynamics (see, e. g., Chaboche [1978]). Later, Lemaitre [1984, 1985*a,b*] proposed a model for predicting isotropic ductile damage in metals which is still popular in the CDM community. Here, the evolution of damage is strongly dependent upon the stress triaxiality ratio and causes softening by reducing the material's stiffness. The model is based on a 'single-surface' formulation in which damage is not regarded as an own 'mechanism' but can only develop under concurrently evolving plastic

deformation of the material (i. e., formally, a yield criterion and loading / unloading conditions for plasticity are present in the model but no corresponding counterparts for damage). Lemaitre's original model was further modified to account for, e. g., ageing effects (Marquis and Lemaitre [1988]), damage anisotropy (Lemaitre et al. [2000]), the crack closure effect (Andrade Pires et al. [2003], Bouchard et al. [2011], Desmorat and Cantournet [2008]) and large deformations (de Souza Neto et al. [1998]). Other damage-plasticity models based on a 'two-surface' approach with separate yield and damage criteria as well as loading / unloading conditions, respectively, were developed by Hansen and Schreyer [1994], Ju [1989], Simo and Ju [1987] for the geometrically linear case and by Voyiadjis and Kattan [1992], Zhu and Cescotto [1995] for the geometrically nonlinear case.

A severe disadvantage of conventional (i. e., 'local') coupled models involving material softening behavior (as the micromechanically motivated and phenomenological CDM models discussed above) is that their usage in finite element simulations can lead to strongly mesh-dependent results. Whenever damage starts to concentrate in a narrow region of the structure during a simulation, it can usually be observed that both the predicted damage zone and corresponding energy dissipation during the damage process progressively decrease upon mesh refinement (among others, see Bažant et al. [1984], de Borst et al. [1993]). In final consequence, this means that, for a theoretically infinitely fine mesh, failure of the structure would occur in a zone of measure zero without any energy dissipation which is unrealistic. Moreover, also the initial location of the damage zone and its direction of propagation can be influenced by the mesh structure itself and the specific element types used (Cervera and Chiumenti [2006], Grassl and Jirásek [2004], Jirásek and Grassl [2008]). It seems clear that this complicates, if not even prevents, a meaningful interpretation of the results. Even worse, the issue cannot simply be cured by using a different numerical solution method, since it is an intrinsic problem of the material formulation itself that leads to a mathematically ill-posed boundary value problem (see, e. g., Bažant and Belytschko [1985], Benallal et al. [1993], de Borst et al. [2012], Jirásek and Bažant [2001], Lasry and Belytschko [1988], Pham and Marigo [2009]).

In order to restore the well-posedness of the problem, the model can be equipped with an internal material length scale which can be understood as a 'localization limiter' that prevents the damage zone from shrinking below a tolerable bound and that cures also the sensitivity issue with regard to the mesh structure and element types. This is achieved by making the damage variable at the integration point level dependent on quantities that contain information about the state at surrounding points, and the very size of the selected influence area exactly defines the internal length. More technically speaking, there are integral-type formulations in which damage is defined as a function of a spatial integral of a variable, and gradient-

type formulations in which damage is considered a function of a variable exhibiting gradient effects. In the literature, both approaches are referred to as 'nonlocal', even though only the former type truly abandons the principle of local action (for physical arguments supporting the assertion of the nonlocal character of damage, see Bažant [1991]). Gradient-type models are typically easier to implement and are the focus of this work, therefore the subsequent discussion is limited to these. For a survey of integral-type formulations, the interested reader is referred to Bažant and Jirásek [2002].

Gradient-type formulations may be distinguished into 'explicit' and 'implicit' ones. In explicit models, higher-order gradient terms of an existing local quantity are directly included in some of the model's constitutive relations. Examples of such models in the context of damage are Comi [1999] and Comi and Driemeier [1998]. In implicit models, a new 'nonlocal' variable is introduced into the formulation and a corresponding partial differential equation (PDE) is utilized that describes its development and spatial distribution within the body under consideration. Typically, an associated local quantity acts as a source term in the PDE, the latter of which often (but not necessarily) has a Helmholtz-type format, and the model's internal material length is characterized by the pre-factor of the gradient term in the equation. In consequence, a coupled problem is obtained which is constituted by the balance of linear momentum and the mentioned PDE (in the purely mechanical case). Both the displacement and nonlocal variable become global unknowns of the system that need to be solved for in a computation. In case of a finite element discretization of the problem, this means that additional degrees of freedom appear at every respective node of the mesh, the number of which depends on the specific order of the nonlocal variable.

Based on the particular implicit gradient approach by Peerlings et al. [1995, 1996, 1998], nonlocal versions of the micromechanically motivated GTN model were developed by, e. g., Hütter et al. [2013, 2014] and Linse et al. [2012]. Aldakheel et al. [2017] and Miehe, Kienle, Aldakheel and Teichtmeister [2016] presented a model, respectively, in which the phase field of fracture approach is coupled with a modified Gurson-type plasticity model that is valid for large deformations. With regard to models based on the CDM concept, Brepols et al. [2015a,b] proposed and investigated an implicit gradient Lemaitre-type damage-plasticity model which takes into account nonlinear Armstrong-Frederick kinematic hardening, nonlinear Voce isotropic hardening and in which damage is chosen as the nonlocal variable. A conceptually quite similar model was suggested by César de Sá et al. [2006] which accounts also for the crack closure effect. Other gradient-enhanced damage-plasticity models in which damage affects the elastic stiffness of the material but which are not based on the Lemaitre approach were presented by, e. g., de Borst et al. [1999] and Nedjar [2001]. In contrast to that,

Engelen et al. [2002] developed an implicit gradient damage-plasticity model in which damage weakens the yield stress and, thus, leads to material softening. Conceptually similar models for the geometrically nonlinear case were suggested and examined by Geers [2004] and Geers et al. [2001, 2003], respectively. Saanouni and Hamed [2013] established a damage-plasticity model for large deformations whose gradient-extension is based on the micromorphic approach by Forest [2009, 2016] and in which damage is modeled by means of a Lemaitre-type ansatz. They tested the model's practical behavior in several structural finite element simulations. Brepols et al. [2017, 2018] also applied the micromorphic approach to derive two slightly different versions of a two-surface gradient-extended damage-plasticity model which take both nonlinear plastic and damage hardening into account, respectively. Besides the theory, the authors discussed many numerical aspects of the model in great detail, as, for instance, the models' implementation into finite elements, the algorithmic treatment at the integration point level (either by means of a local active set search strategy or the Fischer-Burmeister approach) and the derivation of the four consistent tangent operators which are necessary to retain a quadratic rate of convergence in a Newton scheme at the global finite element level. Furthermore, in various structural simulations they illustrated that mesh-independent results can be obtained with the models up to very high values of damage. Kiefer et al. [2018] developed a conceptually quite similar two-surface damage-plasticity model, whose gradient-extension is based on an approach originally proposed by Dimitrijevic and Hackl [2008], and they confirmed the model's mesh regularization properties in monotonic and cyclic loading finite element simulations of a plate with hole. Micromorphic gradient-extended models in which damage is coupled with crystal plasticity were established by Aslan and Forest [2009], Aslan, Quilici and Forest [2011] for the geometrically linear case and by Aslan, Cordero, Gaubert and Forest [2011] for the geometrically nonlinear case. In more recent times, models were developed and investigated that make use of two internal material length scales, i. e., which couple gradient damage with gradient plasticity (see, e. g., Dimitrijevic and Hackl [2011] or the works by Miehe, Aldakheel and Raina [2016] and Miehe, Teichtmeister and Aldakheel [2016], the latter two of which utilized the phase field approach). In this way, one can, for instance, additionally account for the plastic size effect or ensure that a developing damage zone remains inside of a plastic zone (or even vice versa, theoretically).

Outline of the work. In the present study, a novel geometrically nonlinear two-surface gradient-extended damage-plasticity model is presented and numerically examined for its mesh regularization properties in finite element simulations involving both large plastic deformations and severe damage. Chapter 6.3 deals with the theory of the model. Multiplicative splits

of the deformation gradient and its plastic part are introduced, the latter of which proves useful for the modeling of nonlinear Armstrong-Frederick kinematic hardening. The micromorphic approach is utilized to achieve the model's gradient-extension and, for a quite general form of the Helmholtz free energy, the state relations of the model are derived in accordance with the second law of thermodynamics. A yield and damage loading function are postulated and plastic and damage evolution equations are chosen which fulfill thermodynamic consistency. It is then shown that a pull-back of all constitutive equations to the reference configuration leads to a convenient model formulation with a relatively low number of symmetric internal variables which is suitable for further numerical treatment. Both the strong and weak form of the problem are presented and a linearization of the weak form is carried out, laying the foundation for the subsequent finite element discretization in Chap. 6.4 which is concerned with various algorithmic aspects of the model. Through the introduction of independent finite element interpolations of the displacement and micromorphic damage field, an additional degree of freedom naturally appears at the nodes of the mesh (being the nodal value of the micromorphic damage variable in the present case). The coupled system of finite element equations, the element stiffness matrix and the element residual vector are derived. Furthermore, an implicit exponential map time integration scheme for the evolution equations at the integration point level is presented which preserves both the plastic incompressibility of the model and the symmetry of the tensorial internal variables. The solution of the incremental problem is discussed and analytical formulas for the four consistent tangent operators are given which are necessary to retain the quadratic rate of convergence in the Newton iteration at the global finite element level. Finally, numerical examples in Chap. 6.5 illustrate the practical meaning of the model's damage parameters and confirm its mesh regularizing properties in finite element simulations involving large plastic deformations and severe damage. A conclusion of the work is given in Chap. 6.6.

Notational conventions. A direct tensor notation is preferred throughout the text. Scalars and scalar-valued functions are represented by light-face italic characters of either case, e. g., A or a . Vectors and vector-valued functions are denoted by bold-face italic letters of either case, e. g., $\mathbf{B}$ or $\mathbf{b}$. Second-order tensors and tensor-valued functions are usually written as bold-face roman characters of either case, e. g., $\mathbf{C}$ or $\mathbf{c}$. However, if greek symbols are used to denote second-order tensors, the latter are written in italic style, as, e. g., $\boldsymbol{\sigma}$ or $\boldsymbol{\varepsilon}$. Upper-case calligraphic bold-face letters in italic style are used to represent fourth-order tensors and tensor-valued functions, e. g., $\mathcal{D}$.

The operators $\text{grad}(\bullet)$, $\text{Grad}(\bullet)$ and $\text{div}(\bullet)$, $\text{Div}(\bullet)$ describe the gradient of a scalar, vector

or tensor with respect to Eulerian and Lagrangian coordinates, respectively. The symmetric part of a second-order tensor $\mathbf{C}$ is designated by $\text{sym}(\mathbf{C}) := (\mathbf{C} + \mathbf{C}^T) / 2$ where $\mathbf{C}^T$ means its transpose. The deviatoric part of a second-order tensor is abbreviated as $\mathbf{C}' := \mathbf{C} - \frac{1}{3} \text{tr}(\mathbf{C}) \mathbf{I}$ in which $\mathbf{I}$ is the second-order identity tensor and $\text{tr}(\mathbf{C})$ the trace of $\mathbf{C}$. A single contraction of a second-order tensor $\mathbf{C}$ from the right with a first-order tensor $\mathbf{d}$ (which might also be considered as a linear mapping of $\mathbf{d}$ by $\mathbf{C}$) is written as $\mathbf{C}[\mathbf{d}]$. A double contraction of a fourth-order tensor $\mathcal{D}$ from the right with a second-order tensor $\mathbf{C}$ (which might also be considered as a linear mapping of $\mathbf{C}$ by $\mathcal{D}$) is denoted as $\mathcal{D}[\mathbf{C}]$. The scalar and dyadic products of two first-order tensors $\mathbf{a}$ and $\mathbf{b}$ are written as $\mathbf{a} \cdot \mathbf{b}$ and $\mathbf{a} \otimes \mathbf{b}$, respectively. Analogous conventions hold for second-order tensors. Finally, a double contraction between two fourth-order tensors $\mathcal{D}$ and $\mathcal{E}$ is denoted as $\mathcal{D} : \mathcal{E}$.

6.3 Constitutive modeling

6.3.1 Gradient-extended isotropic damage based on the micromorphic approach

The gradient-extended two-surface damage-plasticity model presented in the following belongs to the class of micromorphic media in the sense of Forest [2009]. Loosely speaking, the micromorphic approach is a systematic procedure for constructing higher-order gradient-extended materials in which additional internal (micromorphic) degrees of freedom are used in the formulation, also called ‘microvariables’. In contrast to internal variables, these microvariables show up as further degrees of freedom in generalized balance equations which need to be solved in addition to the classical ones, as, for example, the balance of linear momentum in the purely mechanical case. A coupling between the microvariables and selected strain-like variables of the model is realized by introducing a direct dependence of the Helmholtz free energy on the difference between the just mentioned quantities. It is interesting to note that many other well-known gradient-extended models in the literature can be understood as special instances of the general class of micromorphic media (e. g., see Forest [2009, 2016], Forest et al. [2011]).

The balance equations are derived using the principle of virtual work (PVW). In the present case, assuming a geometrically nonlinear, quasi-static, and purely mechanical theory with a single scalar micromorphic damage variable $\bar{D}$, the expressions for the internal (g_{int}) and external (g_{ext}) virtual work can, for instance, be formulated with respect to quantities defined

in the reference configuration B_0 of the body as follows:

$$g_{\text{int}} = \int_{B_0} \mathbf{S} \cdot \delta \mathbf{E} \, dV + \underbrace{\int_{B_0} (a_{0_i} \delta \bar{D} + \mathbf{b}_{0_i} \cdot \text{Grad}(\delta \bar{D})) \, dV}_{\text{micromorphic extension}} \quad (6.1)$$

$$g_{\text{ext}} = \int_{B_0} \mathbf{f}_0 \cdot \delta \mathbf{u} \, dV + \int_{\partial B_{0_t}} \mathbf{t}_0 \cdot \delta \mathbf{u} \, dA + \underbrace{\int_{B_0} (a_{0_e} \delta \bar{D} + \mathbf{b}_{0_e} \cdot \text{Grad}(\delta \bar{D})) \, dV + \int_{\partial B_{0_c}} a_{0_c} \delta \bar{D} \, dA}_{\text{micromorphic extension}} \quad (6.2)$$

In the above, $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor, $\mathbf{u}$ is the displacement vector, $\mathbf{E}$ is the Green-Lagrange strain tensor and a_{0_i} , $\mathbf{b}_{0_i}$ are internal forces related to the micromorphic damage variable $\bar{D}$ and its gradient $\text{Grad}(\bar{D})$, respectively. Conventional body forces are denoted by $\mathbf{f}_0$ whereas a_{0_e} , $\mathbf{b}_{0_e}$ are generalized body forces. Quantities $\mathbf{t}_0$ and a_{0_c} are conventional and generalized tractions defined on parts ∂B_{0_t} and ∂B_{0_c} of the outer surface of the body where tractions and generalized tractions are prescribed (Neumann boundary), respectively. Moreover, the abbreviation

$$\delta \mathbf{E} := \frac{1}{2} \left(\mathbf{F}^T \text{Grad}(\delta \mathbf{u}) + \text{Grad}(\delta \mathbf{u})^T \mathbf{F} \right) \quad (6.3)$$

is defined where $\mathbf{F} := \partial \mathbf{x} / \partial \mathbf{X}$ is the deformation gradient ($\mathbf{X}$ and $\mathbf{x}$ are position vectors of a material point in the reference and current configuration, respectively) and $\delta \mathbf{u}$ and $\delta \bar{D}$ denote test functions constructed such that $\delta \mathbf{u} = \mathbf{0}$ on ∂B_{0_u} and $\delta \bar{D} = 0$ on $\partial B_{0_{\bar{D}}}$, respectively (Dirichlet boundary).

By applying the PVW, one derives the classical balance of linear momentum as well as a generalized balance equation for the micromorphic damage variable with corresponding

boundary conditions (mathematical details of the derivation are given in Appendix 6.7.1):

$$\text{PVW : } g_{\text{int}} \stackrel{!}{=} g_{\text{ext}} \implies \left\{ \begin{array}{l} \text{linear momentum balance:} \\ \text{Div}(\mathbf{FS}) + \mathbf{f}_0 = \mathbf{0} \quad \text{in } B_0 \\ \mathbf{FS}[\mathbf{n}_0] = \mathbf{t}_0 \quad \text{on } \partial B_{0_t} \\ \mathbf{u} = \hat{\mathbf{u}} \quad \text{on } \partial B_{0_u} \\ \\ \text{micromorphic balance:} \\ \text{Div}(\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) - a_{0_i} + a_{0_e} = 0 \quad \text{in } B_0 \\ (\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) \cdot \mathbf{n}_0 = a_{0_c} \quad \text{on } \partial B_{0_c} \\ \bar{D} = \hat{\hat{D}} \quad \text{on } \partial B_{0_{\bar{D}}} \end{array} \right. \quad (6.4)$$

Here, $\mathbf{n}_0$ represents an outward unit normal vector at the Neumann boundaries ∂B_{0_t} and ∂B_{0_c} whereas $\hat{\mathbf{u}}$ and $\hat{\hat{D}}$ are prescribed values of the displacement and the micromorphic damage variable at the Dirichlet boundaries ∂B_{0_u} and $\partial B_{0_{\bar{D}}}$, respectively. As will be shown later, the micromorphic balance equation and its boundary conditions can be simplified, if further constitutive assumptions are made.

The PVW can equivalently be formulated in terms of quantities defined in the current configuration of the body. The interested reader may find details about this in Appendices 6.7.2 - 6.7.3.

6.3.2 Kinematics of finite deformation elastoplasticity with nonlinear kinematic hardening

For the sake of modeling elastoplastic material behavior, it is assumed that the deformation gradient can multiplicatively be decomposed into elastic ($\mathbf{F}_e$) and plastic ($\mathbf{F}_p$) parts according to

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \quad (6.5)$$

which is nowadays widely acknowledged (see, e. g., Asaro [1983], Eckart [1948], Kröner [1959], Lee [1969], Lee and Liu [1967] and Lubarda and Lee [1981]). Furthermore, in order to model nonlinear kinematic hardening, it is convenient to introduce an additional multiplicative split of the plastic part of the deformation gradient into recoverable ($\mathbf{F}_{p_e}$) and irrecoverable ($\mathbf{F}_{p_i}$) parts, i. e.,

$$\mathbf{F}_p = \mathbf{F}_{p_e} \mathbf{F}_{p_i} \quad (6.6)$$

The additional split of $\mathbf{F}_p$ is physically motivated. According to Lion [2000], $\mathbf{F}_{p_e}$ accounts for dislocation-induced lattice rotations and stretches on the microscale, whereas $\mathbf{F}_{p_i}$ results from

local plastic deformations coming from inelastic slip on crystallographic slip systems.

It is worth mentioning that each of the above decompositions leads naturally to the existence of an additional (local) intermediate plastic configuration, a kinematic concept which is schematically illustrated in Fig. 6.1.

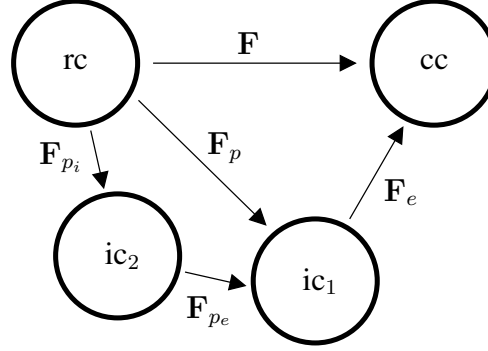


Figure 6.1: Configurations: rc - reference configuration, cc - current configuration, ic₁ - intermediate plastic configuration, ic₂ - intermediate configuration of kinematic hardening (image from Brepols et al. [2014])

6.3.3 State potential in terms of the Helmholtz free energy

The state potential of the model in terms of the Helmholtz free energy ψ is assumed to depend on the deformation only through the elastic right Cauchy-Green deformation tensors $\mathbf{C}_e$ and $\mathbf{C}_{pe}$ which are defined as

$$\mathbf{C}_e = \mathbf{F}_e^T \mathbf{F}_e = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}, \quad \mathbf{C}_{pe} = \mathbf{F}_{pe}^T \mathbf{F}_{pe} = \mathbf{F}_{pi}^{-T} \mathbf{C}_p \mathbf{F}_{pi}^{-1} \quad (6.7)$$

Here, $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and $\mathbf{C}_p = \mathbf{F}_p^T \mathbf{F}_p$ denote the right Cauchy-Green and plastic right Cauchy-Green tensor, respectively. The general form of the free energy per unit reference volume is assumed to be additively separable in the following way:

$$\psi = f_{\text{dam}}(D) (\psi_e(\mathbf{C}_e) + \psi_p(\mathbf{C}_{pe}, \xi_p)) + \psi_d(\xi_d) + \psi_{\bar{d}}(D - \bar{D}, \text{Grad}(\bar{D})) \quad (6.8)$$

The first term ψ_e is the elastic part of the free energy expressed in terms of $\mathbf{C}_e$. The second part ψ_p denotes the plastic energy stored due to kinematic and isotropic hardening which depends on both $\mathbf{C}_{pe}$ and ξ_p , the latter of which represents the isotropic hardening variable. The third term ψ_d accounts for stored energy due to damage hardening and depends on the variable ξ_d which is the damage hardening variable; technically, it plays a similar role as the isotropic hardening variable in plasticity. The last term $\psi_{\bar{d}}$ is the energy related to the micromorphic

extension of the model. It depends on both the gradient of $\bar{D}$ (here assumed with respect to the reference configuration) and on the difference between the micromorphic and the local damage variable which introduces a coupling between the two quantities in the formulation.

As indicated in (6.8), it is assumed that both the elastic and plastic energies are influenced by damage through a twice-differentiable positive and monotonically decreasing (but otherwise arbitrary) scalar-valued phenomenological function $f_{\text{dam}}(D)$, which is one for a virgin material ($D = 0$) and approaches zero, if damage attains a predefined critical value ($D = D_{\text{cr}}$).

6.3.4 State relations and thermodynamic conjugate forces derived from the Clausius-Duhem inequality

The constitutive relations of the model should not violate the second law of thermodynamics. Therefore, their derivation is based upon the isothermal local form of the Clausius-Duhem inequality which reads:

$$-\dot{\psi} + \mathbf{S} \cdot \frac{1}{2} \dot{\mathbf{C}} + \underbrace{a_{0_i} \dot{\bar{D}} + \mathbf{b}_{0_i} \cdot \text{Grad}(\dot{\bar{D}})}_{\text{micromorphic extension}} \stackrel{!}{\geq} 0 \quad (6.9)$$

In contrast to the conventional case, the micromorphic extension of the model leads, in a natural way, to two additional terms in the inequality which account for the contributions of the micromorphic damage and its gradient (see Forest [2009, 2016]).

Inserting the Helmholtz free energy (6.8) into the inequality and using the chain rule of differentiation yields

$$\begin{aligned} & -f_{\text{dam}}(D) \left(\frac{\partial \psi_e}{\partial \mathbf{C}_e} \cdot \dot{\mathbf{C}}_e + \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \cdot \dot{\mathbf{C}}_{p_e} + \frac{\partial \psi_p}{\partial \xi_p} \dot{\xi}_p \right) + \\ & - \left(\frac{df_{\text{dam}}(D)}{dD} (\psi_e + \psi_p) + \frac{\partial \psi_{\bar{d}}}{\partial D} \right) \dot{D} - \frac{\partial \psi_d}{\partial \xi_d} \dot{\xi}_d + \frac{\partial \psi_{\bar{d}}}{\partial \bar{D}} \dot{\bar{D}} - \frac{\partial \psi_{\bar{d}}}{\partial \text{Grad}(\bar{D})} \cdot \text{Grad}(\dot{\bar{D}}) + \\ & + \mathbf{S} \cdot \frac{1}{2} \dot{\mathbf{C}} + a_{0_i} \dot{\bar{D}} + \mathbf{b}_{0_i} \cdot \text{Grad}(\dot{\bar{D}}) \geq 0 \end{aligned} \quad (6.10)$$

In the following, this expression will be further reformulated.

By differentiating Eq. (6.7) and using the product rule of differentiation, the material time derivative of $\mathbf{C}_e$ can be expressed as

$$\dot{\mathbf{C}}_e = \dot{\mathbf{F}}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1} + \mathbf{F}_p^{-T} \dot{\mathbf{C}} \mathbf{F}_p^{-1} + \mathbf{F}_p^{-T} \mathbf{C} \dot{\mathbf{F}}_p^{-1} \quad (6.11)$$

Taking further into account the two identities

$$\dot{\mathbf{F}}_p^{-1} = -\mathbf{F}_p^{-1} \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}, \quad \dot{\mathbf{F}}_p^{-T} = -\mathbf{F}_p^{-T} \dot{\mathbf{F}}_p^T \mathbf{F}_p^{-T} \quad (6.12)$$

and proceeding analogously with $\mathbf{C}_{pe}$, the following expressions for the deformation rates $\dot{\mathbf{C}}_e$ and $\dot{\mathbf{C}}_{pe}$ are obtained:

$$\dot{\mathbf{C}}_e = -\mathbf{l}_p^T \mathbf{C}_e + \mathbf{F}_p^{-T} \dot{\mathbf{C}} \mathbf{F}_p^{-1} - \mathbf{C}_e \mathbf{l}_p, \quad \dot{\mathbf{C}}_{pe} = -\mathbf{l}_{pi}^T \mathbf{C}_{pe} + \mathbf{F}_{pi}^{-T} \dot{\mathbf{C}}_p \mathbf{F}_{pi}^{-1} - \mathbf{C}_{pe} \mathbf{l}_{pi} \quad (6.13)$$

Here, $\mathbf{l}_p := \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}$ and $\mathbf{l}_{pi} := \dot{\mathbf{F}}_{pi} \mathbf{F}_{pi}^{-1}$ are the plastic and plastic inelastic velocity gradient, respectively.

Next, by assuming that ψ_e is an isotropic function of $\mathbf{C}_e$ and ψ_{pe} an isotropic function of $\mathbf{C}_{pe}$, the coaxiality of the tensors $\mathbf{C}_e$ and $\partial\psi_e/\partial\mathbf{C}_e$ as well as $\mathbf{C}_{pe}$ and $\partial\psi_p/\partial\mathbf{C}_{pe}$ can be deduced, respectively. In other words, $\mathbf{C}_e (\partial\psi_e/\partial\mathbf{C}_e) \equiv (\partial\psi_e/\partial\mathbf{C}_e) \mathbf{C}_e$ and $\mathbf{C}_{pe} (\partial\psi_p/\partial\mathbf{C}_{pe}) \equiv (\partial\psi_p/\partial\mathbf{C}_{pe}) \mathbf{C}_{pe}$ and these products are themselves symmetric. Together with well-known rules for the scalar product of two second-order tensors (i. e., $\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{A} \mathbf{B}^T) = \text{tr}(\mathbf{A}^T \mathbf{B})$ and $\mathbf{A} \cdot \mathbf{C} = \text{sym}(\mathbf{A}) \cdot \mathbf{C}$ for general tensors $\mathbf{A}$, $\mathbf{B}$ and a symmetric tensor $\mathbf{C}$), the latter relations can be used to establish the identities

$$\frac{\partial\psi_e}{\partial\mathbf{C}_e} \cdot (\mathbf{C}_e \mathbf{l}_p) = \left(\mathbf{C}_e \frac{\partial\psi_e}{\partial\mathbf{C}_e} \right) \cdot \mathbf{l}_p = \left(\mathbf{C}_e \frac{\partial\psi_e}{\partial\mathbf{C}_e} \right) \cdot \mathbf{d}_p \quad (6.14)$$

where $\mathbf{d}_p = \text{sym}(\mathbf{l}_p)$ denotes the symmetric part of the plastic velocity gradient. Furthermore, since $\text{tr}(\mathbf{A} \mathbf{B}) = \text{tr}(\mathbf{B} \mathbf{A})$, it holds

$$\begin{aligned} \frac{\partial\psi_e}{\partial\mathbf{C}_e} \cdot (\mathbf{F}_p^{-T} \dot{\mathbf{C}} \mathbf{F}_p^{-1}) &= \text{tr} \left(\left(\frac{\partial\psi_e}{\partial\mathbf{C}_e} \right)^T \mathbf{F}_p^{-T} \dot{\mathbf{C}} \mathbf{F}_p^{-1} \right) = \text{tr} \left(\mathbf{F}_p^{-1} \frac{\partial\psi_e}{\partial\mathbf{C}_e} \mathbf{F}_p^{-T} \dot{\mathbf{C}} \right) = \\ &= \left(2 \mathbf{F}_p^{-1} \frac{\partial\psi_e}{\partial\mathbf{C}_e} \mathbf{F}_p^{-T} \right) \cdot \frac{1}{2} \dot{\mathbf{C}} \end{aligned} \quad (6.15)$$

Analogous results as in (6.11) – (6.15) are obtained, if one considers ψ_p and $\mathbf{C}_{pe}$ instead.

Finally, by inserting (6.13) into (6.10) and exploiting (6.14) - (6.15) together with the relationships

$$\mathbf{d}_p = \frac{1}{2} \mathbf{F}_p^{-T} \dot{\mathbf{C}}_p \mathbf{F}_p^{-1}, \quad \mathbf{d}_{pi} = \frac{1}{2} \mathbf{F}_{pi}^{-T} \dot{\mathbf{C}}_{pi} \mathbf{F}_{pi}^{-1} \quad (6.16)$$

(where $\mathbf{d}_{pi}$ is the symmetric part of the inelastic plastic velocity gradient), the final form of

the Clausius-Duhem inequality is obtained which reads:

$$\begin{aligned}
 & \left(\mathbf{S} - f_{\text{dam}}(D) 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-\text{T}} \right) \cdot \frac{1}{2} \dot{\mathbf{C}} + \left(\mathbf{b}_{0_i} - \frac{\partial \psi_{\bar{d}}}{\partial \text{Grad}(\bar{D})} \right) \cdot \text{Grad}(\dot{\bar{D}}) + \\
 & + \left(a_{0_i} - \frac{\partial \psi_{\bar{d}}}{\partial \bar{D}} \right) \dot{\bar{D}} + \left(f_{\text{dam}}(D) 2 \mathbf{C}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} - f_{\text{dam}}(D) 2 \mathbf{F}_{p_e} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_e}^{\text{T}} \right) \cdot \mathbf{d}_p + \\
 & + \left(f_{\text{dam}}(D) 2 \mathbf{C}_{p_e} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \right) \cdot \mathbf{d}_{p_i} - f_{\text{dam}}(D) \frac{\partial \psi_p}{\partial \xi_p} \dot{\xi}_p \\
 & - \left(\frac{df_{\text{dam}}(D)}{dD} (\psi_e + \psi_p) + \frac{\partial \psi_{\bar{d}}}{\partial D} \right) \dot{D} - \frac{\partial \psi_d}{\partial \xi_d} \dot{\xi}_d \geq 0
 \end{aligned} \tag{6.17}$$

A reasonable choice is now to assume that the expressions in the first three parentheses vanish identically. By doing this, the state relations of the model are obtained as

$$\mathbf{S} = f_{\text{dam}}(D) 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-\text{T}}, \quad a_{0_i} = \frac{\partial \psi_{\bar{d}}}{\partial \bar{D}}, \quad \mathbf{b}_{0_i} = \frac{\partial \psi_{\bar{d}}}{\partial \text{Grad}(\bar{D})} \tag{6.18}$$

The remaining part of the dissipation inequality can then be written in a more compact format as

$$(\mathbf{M} - \boldsymbol{\chi}) \cdot \mathbf{d}_p + \mathbf{M}_{\text{kin}} \cdot \mathbf{d}_{p_i} + Y \dot{D} - q_p \dot{\xi}_p - q_d \dot{\xi}_d \geq 0 \tag{6.19}$$

Here, several abbreviations were introduced for the thermodynamic conjugate forces of the model as follows. The second-order tensor

$$\mathbf{M} := f_{\text{dam}}(D) 2 \mathbf{C}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} \tag{6.20}$$

represents the Mandel stress tensor which is symmetric for reasons which were already explained above. Similar reasoning implies also the symmetries of the stress-like tensor

$$\mathbf{M}_{\text{kin}} := f_{\text{dam}}(D) 2 \mathbf{C}_{p_e} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \tag{6.21}$$

and of the back stress tensor in the intermediate configuration, respectively, defined as

$$\boldsymbol{\chi} := f_{\text{dam}}(D) 2 \mathbf{F}_{p_e} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_e}^{\text{T}} \tag{6.22}$$

Finally, the thermodynamic conjugate forces to damage (Y), isotropic hardening (q_p) as well

as damage hardening (q_d) are defined as

$$Y := -\frac{df_{\text{dam}}(D)}{dD} (\psi_e + \psi_p) - \frac{\partial \psi_d}{\partial D}, \quad q_p := f_{\text{dam}}(D) \frac{\partial \psi_p}{\partial \xi_p}, \quad q_d := \frac{\partial \psi_d}{\partial \xi_d} \quad (6.23)$$

6.3.5 Yield function and plastic evolution equations

A von Mises-type yield function / criterion is considered which is influenced by combined kinematic and isotropic hardening, viz.,

$$\Phi_p = \sqrt{\frac{3}{2}} \|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\| - (\sigma_0 + \tilde{q}_p) \quad (6.24)$$

The material parameter σ_0 represents the initial yield stress. Plasticity is assumed to act on the intact part of the material only, the reason for which the yield function is expressed in terms of effective (i. e., 'undamaged') quantities ($\tilde{\bullet}$) that are defined as

$$(\tilde{\bullet}) := \frac{(\bullet)}{f_{\text{dam}}(D)} \quad (6.25)$$

The model's evolution equations of the strain-like plastic internal variables are chosen as

$$\mathbf{d}_p = \dot{\lambda}_p \frac{\partial \Phi_p}{\partial \mathbf{M}} = \dot{\lambda}_p \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'}{\|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\|} \quad (6.26)$$

$$\mathbf{d}_{p_i} = \dot{\lambda}_p \frac{b/a}{f_{\text{dam}}(D)} \tilde{\mathbf{M}}'_{\text{kin}}, \quad \dot{\xi}_p = -\dot{\lambda}_p \frac{\partial \Phi_p}{\partial q_p} = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} \quad (6.27)$$

where $\dot{\lambda}_p$ is the plastic multiplier. Associative rules are chosen for $\mathbf{d}_p$ and $\dot{\xi}_p$ whereas the evolution equation for $\mathbf{d}_{p_i}$ is suitable for modeling nonlinear Armstrong-Frederick kinematic hardening with a and b being corresponding material parameters (Armstrong and Frederick [1966]). Finally, the loading / unloading conditions of plasticity need to be taken into account:

$$\dot{\lambda}_p \geq 0, \quad \Phi_p \leq 0, \quad \dot{\lambda}_p \Phi_p = 0 \quad (6.28)$$

Remark 1. The accumulated plastic strain κ (also referred to as the von Mises equivalent or effective plastic strain) can be defined and computed in view of Eq. (6.26) via the rate evolution equation

$$\dot{\kappa} := \sqrt{\frac{2}{3} \mathbf{d}_p \cdot \mathbf{d}_p} = \sqrt{\frac{2}{3}} \|\mathbf{d}_p\| = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} = \dot{\xi}_p \quad (6.29)$$

As such, the evolution of κ is equivalent to that of the isotropic hardening variable ξ_p in the present framework.

6.3.6 Damage loading function and damage evolution equations

A two-surface strategy for plasticity and damage is pursued in this work. This means that the model's damage behavior is characterized by a separate damage loading function / criterion as follows:

$$\Phi_d = Y - (Y_0 + q_d) \quad (6.30)$$

Formally, the analogy to the definition of the yield function (6.24) should be apparent. Damage hardening is taken into account by the term q_d and Y_0 represents the damage onset material parameter. Moreover, associative damage evolution equations are introduced, viz.,

$$\dot{D} = \dot{\lambda}_d \frac{\partial \Phi_d}{\partial Y} = \dot{\lambda}_d, \quad \dot{\xi}_d = -\dot{\lambda}_d \frac{\partial \Phi_d}{\partial q_d} = \dot{\lambda}_d \quad (6.31)$$

where $\dot{\lambda}_d$ denotes the damage multiplier. Finally, the loading / unloading conditions of damage need to be considered:

$$\dot{\lambda}_d \geq 0, \quad \Phi_d \leq 0, \quad \dot{\lambda}_d \Phi_d = 0 \quad (6.32)$$

Remark 2. Two things are worth mentioning at this point. Firstly, more complex or sophisticated expressions for Φ_d in (6.30) are possible, if desired. Secondly, by inspecting evolution equations (6.31) it becomes apparent that, in the present framework, the internal variables for damage (D) and damage hardening (ξ_d) develop in a completely equal manner. Assuming further that their initial values are the same (which is usually the case, namely zero), both internal variables are in fact equal to each other, such that ξ_d could be eliminated from the set of unknowns. This is a mere consequence of the assumed model's simplicity in which damage is characterized by a scalar variable D and due to the particular choices of Φ_d and $\dot{\xi}_d$, respectively. However, in more complex models, damage could, for example, be represented by a second- or fourth-order tensor. In such cases, ξ_d would represent a corresponding 'equivalent' scalar damage measure, similar to ξ_p in plasticity. In order to keep notational consistency with the available literature in the field and also to point out the formal analogy to plasticity, ξ_d is maintained as an autonomous variable in the theoretical framework.

6.3.7 Proof of the model's thermodynamic consistency

The model's thermodynamic consistency is demonstrated in the following. First of all, in view of (6.25) and (6.27)₁, and by considering a classical rule for the scalar product of two second-order tensors (i. e., $\mathbf{A} \cdot \mathbf{B}' = \mathbf{A}' \cdot \mathbf{B}$ where $\mathbf{A}$ and $\mathbf{B}$ are general second-order tensors), it holds for the second term in (6.19) that

$$\mathbf{M}_{\text{kin}} \cdot \mathbf{d}_{p_i} = \dot{\lambda}_p \frac{b/a}{f_{\text{dam}}(D)} \mathbf{M}_{\text{kin}} \cdot \tilde{\mathbf{M}}'_{\text{kin}} = \dot{\lambda}_p \frac{b}{a} \tilde{\mathbf{M}}_{\text{kin}} \cdot \tilde{\mathbf{M}}'_{\text{kin}} = \dot{\lambda}_p \frac{b}{a} \tilde{\mathbf{M}}'_{\text{kin}} \cdot \tilde{\mathbf{M}}'_{\text{kin}} \geq 0 \quad (6.33)$$

which is obviously always greater than or equal to zero. Next, consider the first and fourth term in (6.19). In view of relations (6.24) - (6.27)₂, it can be concluded that

$$\begin{aligned} (\mathbf{M} - \boldsymbol{\chi}) \cdot \mathbf{d}_p - q_p \dot{\xi}_p &= (\mathbf{M} - \boldsymbol{\chi}) \cdot \left(\dot{\lambda}_p \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'}{\|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\|} \right) - q_p \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)} = \\ \dot{\lambda}_p \left(\sqrt{\frac{3}{2}} (\tilde{\mathbf{M}} - \tilde{\boldsymbol{\chi}}) \cdot \frac{\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'}{\|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\|} - \tilde{q}_p \right) &= \dot{\lambda}_p \left(\sqrt{\frac{3}{2}} \|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\| - \tilde{q}_p \right) = \dot{\lambda}_p (\Phi_p + \sigma_0) \geq 0 \end{aligned} \quad (6.34)$$

The last step in the above can be understood by considering in addition the loading / unloading conditions of plasticity (6.28) together with $\sigma_0 \geq 0$. Finally, with (6.30) - (6.31) at hand, it holds for the third and fifth term in (6.19) that

$$Y \dot{D} - q_p \dot{\xi}_p = Y \dot{\lambda}_d - q_p \dot{\lambda}_d = \dot{\lambda}_d (Y - q_d) = \dot{\lambda}_d (\Phi_d + Y_0) \geq 0 \quad (6.35)$$

where the loading / unloading conditions of damage (6.32) and $Y_0 \geq 0$ are taken into account to establish the result.

6.3.8 Representation of the constitutive equations in the reference configuration

The constitutive equations of the model are not all defined in the same configuration. For example, the second-Piola Kirchhoff stress (6.18)₁ 'lives' in the reference configuration whereas evolution equations (6.26) and (6.27)₁ for $\mathbf{d}_p$ and $\mathbf{d}_{p_i}$ are defined in the plastic intermediate configuration and intermediate configuration of kinematic hardening, respectively. Of course, this is no problem from the theoretical point of view. However, pulling back the tensor-valued evolution equations of the model to the reference configuration and expressing all the scalar equations (as, for example, yield function (6.24)) in terms of quantities that are defined in the reference configuration has two advantages: On the one hand, the model then only depends on

a relatively low number of symmetric internal variables as will be shown below. On the other hand, it allows also for the development of an efficient exponential map algorithm to integrate the model's plastic evolution equations which automatically preserves both the symmetry of the internal variables and the plastic incompressibility, a topic which will be discussed in Sect. 6.4.2.

Consider the free energy ψ_e which is an isotropic function of $\mathbf{C}_e$. Therefore, its derivative $\partial\psi_e/\partial\mathbf{C}_e$ is an isotropic tensor-valued function of $\mathbf{C}_e$ as well and can, thus, be represented (see, e. g., Itskov [2009]) as

$$\frac{\partial\psi_e}{\partial\mathbf{C}_e} = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{C}_e + \alpha_2 \mathbf{C}_e^2 \quad (6.36)$$

Here, the factors α_i , $i = 0, 1, 2$, are scalar-valued functions of $\mathbf{C}_e$ which can be expressed in terms of the latter variable's invariants (or eigenvalues). By inserting (6.36) into (6.18)₁ and using relation $\mathbf{C}_e = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}$, the second Piola-Kirchhoff stress tensor becomes

$$\mathbf{S} = f_{\text{dam}}(D) 2 \mathbf{F}_p^{-1} \frac{\partial\psi_e}{\partial\mathbf{C}_e} \mathbf{F}_p^{-T} = f_{\text{dam}}(D) 2 \left(\alpha_0 \mathbf{C}_p^{-1} + \alpha_1 \mathbf{C}_p^{-1} \mathbf{C} \mathbf{C}_p^{-1} + \alpha_2 \mathbf{C}_p^{-1} (\mathbf{C} \mathbf{C}_p^{-1})^2 \right) \quad (6.37)$$

In other words, $\mathbf{S}$ is a function of $\mathbf{C}$, $\mathbf{C}_p$ and D only. Note that the factors α_i , $i = 0, 1, 2$ are themselves expressible in terms of $\mathbf{C}$ and $\mathbf{C}_p$, too (for details, see Appendix 6.7.4).

A similar observation can be made for the back stress tensor $\mathbf{X}$ in the reference configuration which is defined as the pull-back of $\boldsymbol{\chi}$, that is,

$$\mathbf{X} = \mathbf{F}_p^{-1} \boldsymbol{\chi} \mathbf{F}_p^{-T} = f_{\text{dam}}(D) 2 \mathbf{F}_p^{-1} \mathbf{F}_{pe} \frac{\partial\psi_p}{\partial\mathbf{C}_{pe}} \mathbf{F}_{pe}^T \mathbf{F}_p^{-T} = f_{\text{dam}}(D) 2 \mathbf{F}_{pi}^{-1} \frac{\partial\psi_p}{\partial\mathbf{C}_{pe}} \mathbf{F}_{pi}^{-T} \quad (6.38)$$

For the same reasons as above, $\partial\psi_p/\partial\mathbf{C}_{pe}$ is an isotropic tensor-valued function of $\mathbf{C}_{pe}$ which can be represented in the form

$$\frac{\partial\psi_p}{\partial\mathbf{C}_{pe}} = \beta_0 \mathbf{I} + \beta_1 \mathbf{C}_{pe} + \beta_2 \mathbf{C}_{pe}^2 \quad (6.39)$$

where the coefficients β_i , $i = 0, 1, 2$, are scalar-valued functions of $\mathbf{C}_{pe}$ that can be expressed in terms of the latter variable's invariants (or eigenvalues). Inserting this result into expression

(6.38) and considering that $\mathbf{C}_{p_e} = \mathbf{F}_{p_i}^{-T} \mathbf{C}_p \mathbf{F}_{p_i}^{-1}$ leads to

$$\begin{aligned} \mathbf{X} &= f_{\text{dam}}(D) 2 \mathbf{F}_{p_i}^{-1} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_i}^{-T} = \\ &= 2 f_{\text{dam}}(D) \left(\beta_0 \mathbf{C}_{p_i}^{-1} + \beta_1 \mathbf{C}_{p_i}^{-1} \mathbf{C}_p \mathbf{C}_{p_i}^{-1} + \beta_2 \mathbf{C}_{p_i}^{-1} (\mathbf{C}_p \mathbf{C}_{p_i}^{-1})^2 \right) \end{aligned} \quad (6.40)$$

which shows that $\mathbf{X}$ is a function of $\mathbf{C}_p$, $\mathbf{C}_{p_i}$ and D only.

Finally, by inserting (6.26) and (6.27)₁ into the pull back relations $\dot{\mathbf{C}}_p = 2 \mathbf{F}_p^T \mathbf{d}_p \mathbf{F}_p$ and $\dot{\mathbf{C}}_{p_i} = 2 \mathbf{F}_{p_i}^T \mathbf{d}_{p_i} \mathbf{F}_{p_i}$, respectively, one obtains after some transformations (mathematical details can be found in Appendix 6.7.5)

$$\dot{\mathbf{C}}_p = 2 \dot{\lambda}_p \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \mathbf{F}_p^T \frac{\tilde{\mathbf{M}}' - \tilde{\mathbf{X}}'}{\|\tilde{\mathbf{M}}' - \tilde{\mathbf{X}}'\|} \mathbf{F}_p = 2 \dot{\lambda}_p \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{Y}}' \mathbf{C}_p}{\sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^T}} \quad (6.41)$$

$$\dot{\mathbf{C}}_{p_i} = 2 \dot{\lambda}_p \frac{b/a}{f_{\text{dam}}(D)} \mathbf{F}_{p_i}^T \tilde{\mathbf{M}}'_{\text{kin}} \mathbf{F}_{p_i} = 2 \dot{\lambda}_p \frac{b/a}{f_{\text{dam}}(D)} \tilde{\mathbf{Y}}'_{\text{kin}} \mathbf{C}_{p_i} \quad (6.42)$$

which are the plastic evolution equations expressed in the reference configuration. Here, the stress-like second-order tensors

$$\mathbf{Y} := \mathbf{C} \mathbf{S} - \mathbf{C}_p \mathbf{X} \quad \mathbf{Y}_{\text{kin}} := \mathbf{C}_p \mathbf{X} \quad (6.43)$$

were introduced as auxiliary quantities. Both are defined in the reference configuration and are in general unsymmetric. However, the products $\mathbf{Y} \mathbf{C}_p$ and $\mathbf{Y} \mathbf{C}_{p_i}$ (and thus also $\mathbf{Y}' \mathbf{C}_p$ and $\mathbf{Y}' \mathbf{C}_{p_i}$) are symmetric which can be easily verified with the help of relations (6.37) and (6.40), respectively.

Considering further that yield function (6.24) can be expressed in terms of $\mathbf{Y}$ (for details, see Appendix 6.7.6), it can be concluded that all constitutive equations of the model can be represented solely in terms of the symmetric tensors $\mathbf{C}$, $\mathbf{C}_p$, $\mathbf{C}_{p_i}$ in the reference configuration, the micromorphic damage variable $\bar{D}$, the damage variable D as well as the plastic and damage multipliers $\dot{\lambda}_p$, $\dot{\lambda}_d$. The internal variables of the model are $\mathbf{C}_p$, $\mathbf{C}_{p_i}$, ξ_p , D and ξ_d which describe the evolution of plastic deformation, kinematic hardening, isotropic hardening, damage and damage hardening, respectively.

A summary of the model's constitutive equations in the reference configuration is given below:

- State laws

$$\mathbf{S} = f_{\text{dam}}(D) 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-\text{T}}, \quad a_{0_i} = \frac{\partial \psi_{\bar{d}}}{\partial \bar{D}}, \quad b_{0_i} = \frac{\partial \psi_{\bar{d}}}{\partial \text{Grad}(\bar{D})} \quad (6.44)$$

- Thermodynamic conjugate forces

$$\mathbf{X} = f_{\text{dam}}(D) 2 \mathbf{F}_{p_i}^{-1} \frac{\partial \psi_p}{\partial \mathbf{C}_{p_e}} \mathbf{F}_{p_i}^{-\text{T}}, \quad q_p = f_{\text{dam}}(D) \frac{\partial \psi_p}{\partial \xi_p} \quad (6.45)$$

$$Y = -\frac{df_{\text{dam}}(D)}{dD} (\psi_e + \psi_p) - \frac{\partial \psi_{\bar{d}}}{\partial \bar{D}}, \quad q_d = \frac{\partial \psi_d}{\partial \xi_d} \quad (6.46)$$

- Auxiliary stress tensors

$$\mathbf{Y} = \mathbf{C} \mathbf{S} - \mathbf{C}_p \mathbf{X}, \quad \mathbf{Y}_{\text{kin}} = \mathbf{C}_p \mathbf{X} \quad (6.47)$$

- Evolution equations

$$\dot{\mathbf{C}}_p = 2 \dot{\lambda}_p \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{Y}}' \mathbf{C}_p}{\sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^{\text{T}}}}, \quad \dot{\mathbf{C}}_{p_i} = 2 \dot{\lambda}_p \frac{b/a}{f_{\text{dam}}(D)} \tilde{\mathbf{Y}}'_{\text{kin}} \mathbf{C}_{p_i} \quad (6.48)$$

$$\dot{\xi}_p = \frac{\dot{\lambda}_p}{f_{\text{dam}}(D)}, \quad \dot{D} = \dot{\lambda}_d, \quad \dot{\xi}_d = \dot{\lambda}_d \quad (6.49)$$

- Yield and damage loading function

$$\Phi_p = \sqrt{\frac{3}{2}} \sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^{\text{T}}} - (\sigma_0 + \tilde{q}_p), \quad \Phi_d = Y - (Y_0 + q_d) \quad (6.50)$$

- Loading / unloading conditions

$$\dot{\lambda}_p \geq 0, \quad \Phi_p \leq 0, \quad \dot{\lambda}_p \Phi_p = 0 \quad (6.51)$$

$$\dot{\lambda}_d \geq 0, \quad \Phi_d \leq 0, \quad \dot{\lambda}_d \Phi_d = 0 \quad (6.52)$$

6.3.9 Particular choice of the Helmholtz free energy in the present study

Apart from nonlinear Armstrong-Fredrick kinematic hardening and isotropic gradient-extended damage, both of which were assumed to be fundamental ingredients of the model, the constitutive framework has so far been presented in a quite general manner and the Helmholtz

free energy of the model has not been specified in detail, yet. In order to allow for a meaningful discussion of the numerical results at the end of this study, the free energy is further particularized in what follows.

In the present study, a compressible Neo-Hookean-type elastic energy ψ_e is chosen which reads

$$\psi_e = \frac{\mu}{2} \left(\text{tr } \mathbf{C}_e - 3 - 2 \ln \left(\sqrt{\det \mathbf{C}_e} \right) \right) + \frac{\Lambda}{4} \left(\det \mathbf{C}_e - 1 - 2 \ln \left(\sqrt{\det \mathbf{C}_e} \right) \right) \quad (6.53)$$

where Λ and μ are the two Lamé material parameters. The plastic energy ψ_p is defined as

$$\psi_p = \frac{a}{2} \left(\text{tr } \mathbf{C}_{pe} - 3 - 2 \ln \left(\sqrt{\det \mathbf{C}_{pe}} \right) \right) + e \left(\xi_p + \frac{\exp(-f \xi_p) - 1}{f} \right) \quad (6.54)$$

Here, the first term is related to kinematic hardening with the stiffness-like parameter a (the second kinematic hardening parameter b is dimensionless and does not show up in the energy but only in evolution equation (6.27)₁ for $\mathbf{d}_{pi}$, or, alternatively, equation (6.42) for $\dot{\mathbf{C}}_{pi}$). The second term is used in order to model nonlinear Voce isotropic hardening with e and f being a corresponding stiffness-like and dimensionless material parameter, respectively (Voce [1955]). Keep in mind that, even though the energies ψ_e and ψ_p are here for consistency with (6.8) expressed in terms of the variables $\mathbf{C}_e$ and $\mathbf{C}_{pe}$, respectively, they can equivalently be expressed in terms of quantities that are defined in the reference configuration (i. e., $\mathbf{C}$, $\mathbf{C}_p$ and $\mathbf{C}_{pi}$).

With (6.53) and (6.54) at hand, Eqs. (6.18)₁, (6.27)₂ and (6.38) lead to the second Piola-Kirchhoff stress as well as the thermodynamic conjugate forces to isotropic and kinematic hardening, respectively, which read

$$\mathbf{S} = f_{\text{dam}}(D) \left(\mu (\mathbf{C}_p^{-1} - \mathbf{C}^{-1}) + \frac{\Lambda}{2} \left(\frac{\det \mathbf{C}}{\det \mathbf{C}_p} - 1 \right) \mathbf{C}^{-1} \right) \quad (6.55)$$

$$\mathbf{X} = f_{\text{dam}}(D) a (\mathbf{C}_{pi}^{-1} - \mathbf{C}_p^{-1}) \quad (6.56)$$

$$q_p = f_{\text{dam}}(D) e (1 - \exp(-f \xi_p)) \quad (6.57)$$

Furthermore, the energy ψ_d is defined as

$$\psi_d = r \left(\xi_d + \frac{\exp(-s \xi_d) - 1}{s} \right) \quad (6.58)$$

It represents nonlinear Voce damage hardening with the stiffness-like and dimensionless mate-

rial parameters r and s , respectively. The formal analogy to the energy of isotropic hardening shown in the above should be apparent. Finally, energy $\psi_{\bar{d}}$ related to the micromorphic extension of the model reads

$$\psi_{\bar{d}} = \frac{H}{2} (D - \bar{D})^2 + \frac{A}{2} \text{Grad}(\bar{D}) \cdot \text{Grad}(\bar{D}) \quad (6.59)$$

The first term penalizes the difference between the local and micromorphic damage and leads to a coupling between the two variables, the degree of which can be controlled via parameter H . The second term describes the influence of the gradient of $\bar{D}$ in the formulation. Parameter A represents the ‘internal length’ of the formulation. With (6.58) and (6.59) at hand, Eqs. (6.18)₂ - (6.18)₃, (6.23)₁ and (6.23)₃ lead to the the remaining state relations as well as the thermodynamic conjugate forces to damage and damage hardening, respectively, which read

$$a_{0_i} = -H (D - \bar{D}), \quad b_{0_i} = A \text{Grad}(\bar{D}) \quad (6.60)$$

$$Y = -\frac{df_{\text{dam}}(D)}{dD} (\psi_e + \psi_p) - H (D - \bar{D}) \quad (6.61)$$

$$q_d = r (1 - \exp(-s \xi_d)) \quad (6.62)$$

Via Y (sometimes loosely referred to as the ‘energy release rate’), which is used in the definition of the damage loading function (6.30), a ‘nonlocal’ character of damage comes into play at the constitutive level through the term $-H (D - \bar{D})$. Moreover, Y is influenced by both the elastic and plastic energies as can be seen from the first term in expression (6.61). This behavior is desired: several authors pointed out in the past that a purely elastic energy release rate might be too restrictive from a physical point of view (e. g., among others, see Chaboche [2003], Chow and Wang [1987], Ju [1989], Kachanov [1993], Saanouni et al. [1994]).

6.3.10 Weak form of the problem and its linearization

In the present study, further simplifying assumptions for the micromorphic balance equation (6.4) are applicable. Generalized contact and external forces are neglected (i. e., $a_{0_c} = a_{0_e} = 0$, $b_{0_e} = 0$), only Neumann boundary conditions are considered for the micromorphic damage variable (i. e., $\partial B_{0_c} \equiv \partial B_0$, $\partial B_{0_{\bar{D}}} \equiv \emptyset$) and, with expressions (6.60) for a_{0_i} and b_{0_i} at hand,

the micromorphic balance equation can be rewritten as

$$H (D - \bar{D}) + A \operatorname{Div} (\operatorname{Grad} (\bar{D})) = 0 \quad \text{in } B_0 \quad (6.63)$$

$$\operatorname{Grad} (\bar{D}) \cdot \mathbf{n}_0 = 0 \quad \text{on } \partial B_0 \quad (6.64)$$

In the usual way, the weak form of the problem can then be constructed by multiplying the linear momentum and micromorphic balance equations by appropriate vectorial and scalar test functions $\delta \mathbf{u}$ and $\delta \bar{D}$, respectively, and by integrating over the domain B_0 . Considering further the divergence theorem as well as abbreviation (6.3), and taking the boundary conditions into account, the weak form follows as:

$$g(\mathbf{u}, \bar{D}, \delta \mathbf{u}) := \int_{B_0} \mathbf{S} \cdot \delta \mathbf{E} \, dV - \int_{B_0} \mathbf{f}_0 \cdot \delta \mathbf{u} \, dV - \int_{\partial B_{0t}} \mathbf{t}_0 \cdot \delta \mathbf{u} \, dA = 0 \quad \forall \delta \mathbf{u} \quad (6.65)$$

$$h(\mathbf{u}, \bar{D}, \delta \bar{D}) := \int_{B_0} (H (D - \bar{D}) \delta \bar{D} - A \operatorname{Grad} (\bar{D}) \cdot \operatorname{Grad} (\delta \bar{D})) \, dV = 0 \quad \forall \delta \bar{D} \quad (6.66)$$

The weak form (6.65) - (6.66) is generally nonlinear. Thus, it is linearized with respect to the unknowns $\mathbf{u}$ and $\bar{D}$, leading to the following set of coupled equations which need to be solved iteratively for the increments $\Delta \mathbf{u}$ and $\Delta \bar{D}$ (mathematical details of the linearization can be found in Appendix 6.7.7):

$$\begin{aligned} \int_{B_0} \operatorname{Grad} (\delta \mathbf{u}) \cdot (\operatorname{Grad} (\Delta \mathbf{u}) \mathbf{S}) \, dV + \int_{B_0} \delta \mathbf{E} \cdot \frac{\partial \mathbf{S}}{\partial \mathbf{E}} [\Delta \mathbf{E}] \, dV + \int_{B_0} \delta \mathbf{E} \cdot \frac{\partial \mathbf{S}}{\partial D} \Delta \bar{D} \, dV = \\ - \left(\int_{B_0} \delta \mathbf{E} \cdot \mathbf{S} \, dV - \int_{B_0} \delta \mathbf{u} \cdot \mathbf{f}_0 \, dV - \int_{\partial B_{0t}} \delta \mathbf{u} \cdot \mathbf{t}_0 \, dA \right) \quad \forall \delta \mathbf{u} \end{aligned} \quad (6.67)$$

$$\begin{aligned} \int_{B_0} \delta \bar{D} H \frac{\partial D}{\partial \bar{D}} \cdot \Delta \mathbf{E} \, dV + \int_{B_0} \left(\delta \bar{D} H \left(\frac{\partial D}{\partial \bar{D}} - 1 \right) \Delta \bar{D} - \operatorname{Grad} (\delta \bar{D}) \cdot A \operatorname{Grad} (\Delta \bar{D}) \right) dV = \\ - \int_{B_0} (\delta \bar{D} H (D - \bar{D}) - \operatorname{Grad} (\delta \bar{D}) \cdot A \operatorname{Grad} (\bar{D})) \, dV \quad \forall \delta \bar{D} \end{aligned} \quad (6.68)$$

In the above, increment $\Delta \mathbf{E}$ is defined as

$$\Delta \mathbf{E} := \frac{1}{2} \left(\mathbf{F}^T \operatorname{Grad} (\Delta \mathbf{u}) + \operatorname{Grad} (\Delta \mathbf{u})^T \mathbf{F} \right) \quad (6.69)$$

It is well-known that the quadratic rate of convergence of the underlying Newton-Raphson scheme can usually only be preserved, if the material sensitivities $\partial \mathbf{S} / \partial \mathbf{E}$, $\partial \mathbf{S} / \partial \bar{D}$, $\partial D / \partial \mathbf{E}$ and $\partial D / \partial \bar{D}$ are computed consistently, i. e., in accordance with the numerical algorithm used to integrate the constitutive equations (for details, see, e. g., Simo and Taylor [1985], Wriggers [2008]). This topic will be further discussed in Sect. 6.4.4.

6.4 Algorithmic implementation

6.4.1 Finite element discretization of the global equations

The present section gives a brief overview of the finite element approximation of the linearized weak form and the corresponding matrix notation. To begin with, the geometry of the body in the reference configuration B_0 is approximated by n_{el} finite elements B_0^e as follows (from now on, a superscript e indicates that a quantity belongs to element e):

$$B_0 \approx \bigcup_{e=1}^{n_{\text{el}}} B_0^e \quad (6.70)$$

With this, the integrals over B_0 in (6.67) - (6.68) can be expressed as sums of individual element contributions. In the next step, finite element approximations of the exact displacement field $\mathbf{u}(\mathbf{X})$, the micromorphic damage field $\bar{D}(\mathbf{X})$ and the test functions on a typical finite element are introduced as

$$\begin{aligned} \mathbf{u}(\mathbf{X}) &\approx \mathbf{N}_u^e(\mathbf{X}) \mathbf{u}^e & \delta \mathbf{u}(\mathbf{X}) &\approx \mathbf{N}_u^e(\mathbf{X}) \delta \mathbf{u}^e \\ \bar{D}(\mathbf{X}) &\approx \mathbf{N}_{\bar{D}}^e(\mathbf{X}) \bar{D}^e & \delta \bar{D}(\mathbf{X}) &\approx \mathbf{N}_{\bar{D}}^e(\mathbf{X}) \delta \bar{D}^e \end{aligned} \quad \mathbf{X} \in B_0^e \quad (6.71)$$

where $\mathbf{u}^e$ and $\bar{D}^e$ denote the respective element nodal values (column vectors) and $\mathbf{N}_u^e(\mathbf{X})$ and $\mathbf{N}_{\bar{D}}^e(\mathbf{X})$ are corresponding element shape functions (matrices). As indicated, the finite element interpolations of the displacement and the micromorphic damage do not necessarily have to be the same. In a similar manner, the gradients of the above quantities can be approximated by

$$\begin{aligned} \text{Grad}(\mathbf{u}(\mathbf{X})) &\approx \mathbf{B}_{0u}^e(\mathbf{X}) \mathbf{u}^e & \text{Grad}(\delta \mathbf{u}(\mathbf{X})) &\approx \mathbf{B}_{0u}^e(\mathbf{X}) \delta \mathbf{u}^e \\ \text{Grad}(\bar{D}(\mathbf{X})) &\approx \mathbf{B}_{0\bar{D}}^e(\mathbf{X}) \bar{D}^e & \text{Grad}(\delta \bar{D}(\mathbf{X})) &\approx \mathbf{B}_{0\bar{D}}^e(\mathbf{x}) \delta \bar{D}^e \end{aligned} \quad \mathbf{X} \in B_0^e \quad (6.72)$$

where $\mathbf{B}_u^e(\mathbf{X}) := \text{Grad}(\mathbf{N}_u^e(\mathbf{X}))$ and $\mathbf{B}_{\bar{D}}^e(\mathbf{X}) := \text{Grad}(\mathbf{N}_{\bar{D}}^e(\mathbf{X}))$ are matrices which contain the respective derivatives of the element shape functions with respect to $\mathbf{X}$. Finally, the Green-

Lagrange strain $\mathbf{E}$ and test function $\delta\mathbf{E}$ can be approximated in terms of the nodal values $\mathbf{u}^e$ and $\delta\mathbf{u}^e$ as well:

$$\mathbf{E}(\mathbf{X}) \approx \mathbf{G}_{0u}^e(\mathbf{X}) \mathbf{u}^e \quad \delta\mathbf{E}(\mathbf{X}) \approx \mathbf{G}_{0u}^e(\mathbf{X}) \delta\mathbf{u}^e \quad \mathbf{X} \in B_0^e \quad (6.73)$$

Here, $\mathbf{G}_{0u}^e(\mathbf{X})$ is a matrix which contains products of the shape function derivatives with components of the deformation gradient $\mathbf{F}$ (the specific form can be found, for example, in one of the references given below).

The particular shape of the vectors and matrices shown above was not explicitly defined here because it strongly depends on the considered space dimension, element type and specific interpolation for both the displacements and micromorphic damage variable (which may differ from each other, if desired). Details can be found elsewhere, e. g., in any standard textbook on nonlinear finite element analysis (see, e. g., Belytschko et al. [2014] or Wriggers [2008]).

By inserting the finite element approximations above into the linearized weak form (6.67) - (6.68), and introducing usual matrix and vector representations of the second Piola-Kirchhoff stress ($\hat{\mathbf{S}}$), the Green-Lagrange strain ($\hat{\mathbf{E}}$), the body forces ($\mathbf{f}_0$) and tractions ($\mathbf{t}_0$) as well as the material sensitivities ($\partial\hat{\mathbf{S}}/\partial\hat{\mathbf{E}}$, $\partial\hat{\mathbf{S}}/\partial\bar{D}$, $\partial D/\partial\hat{\mathbf{E}}$), one obtains the following expressions:

$$\begin{aligned} \sum_{e=1}^{n_{el}} \delta\mathbf{u}^{eT} \left\{ \underbrace{\left(\int_{B_0^e} \mathbf{B}_{0u}^{eT} \mathcal{D}^e \mathbf{B}_{0u}^e dV + \int_{B_0^e} \mathbf{G}_{0u}^{eT} \left(\frac{\partial\hat{\mathbf{S}}}{\partial\hat{\mathbf{E}}} \right)^e \mathbf{G}_{0u}^e dV \right)}_{:=\mathbf{k}_{uu}^e} \Delta\mathbf{u}^e + \right. \\ \left. + \underbrace{\int_{B_0^e} \mathbf{G}_{0u}^{eT} \left(\frac{\partial\hat{\mathbf{S}}}{\partial\bar{D}} \right)^e \mathbf{N}_D^e dV}_{:=\mathbf{k}_{u\bar{D}}^e} \Delta\bar{D}^e \right\} = \\ - \sum_{e=1}^{n_{el}} \delta\mathbf{u}^{eT} \left\{ \underbrace{\int_{B_0^e} \mathbf{G}_{0u}^{eT} \hat{\mathbf{S}}^e dV - \int_{B_0^e} \mathbf{N}_u^{eT} \mathbf{f}_0 dV - \int_{\partial B_{0t}^e} \mathbf{N}_u^{eT} \mathbf{t}_0 dA}_{:=\mathbf{r}_u^e} \right\} \quad (6.74) \end{aligned}$$

$$\begin{aligned}
& \sum_{e=1}^{n_{el}} \delta \bar{\mathbf{D}}^e \mathbf{T} \left\{ \underbrace{\int_{B_0^e} H \mathbf{N}_D^{eT} \left(\frac{\partial D}{\partial \hat{\mathbf{E}}} \right)^{eT} \mathbf{B}_{0u}^e dV}_{:=\mathbf{k}_{Du}^e} \Delta \mathbf{u}^e + \right. \\
& \quad \left. + \left(\underbrace{\int_{B_0^e} H \left(\left(\frac{\partial D}{\partial \bar{D}} \right)^e - 1 \right) \mathbf{N}_D^{eT} \mathbf{N}_D^e dV - \int_{B_0^e} A \mathbf{B}_{0\bar{D}}^{eT} \mathbf{B}_{0\bar{D}}^e dV}_{:=\mathbf{k}_{\bar{D}\bar{D}}^e} \right) \Delta \bar{\mathbf{D}}^e \right\} = \\
& \quad - \sum_{e=1}^{n_{el}} \delta \bar{\mathbf{D}}^e \mathbf{T} \left\{ \underbrace{\int_{B_0^e} H \mathbf{N}_D^{eT} (D^e - \mathbf{N}_D^e \bar{\mathbf{D}}^e) dV - \int_{B_0^e} A \mathbf{B}_{0\bar{D}}^{eT} \mathbf{B}_{0\bar{D}}^e \bar{\mathbf{D}}^e dV}_{:=\mathbf{r}_D^e} \right\} \quad (6.75)
\end{aligned}$$

Here, $\mathcal{D}$ is the matrix representation of the fourth-order tensor (see, e. g., de Souza Neto et al. [2008])

$$\mathcal{D}_{ijkl} = S_{jl} \delta_{ik} \quad (6.76)$$

with δ_{ij} being the Kronecker delta. The corresponding integral term in (6.74) accounts for the geometric stiffness. Furthermore, the abbreviations $\mathbf{k}_{uu}^e, \mathbf{k}_{u\bar{D}}^e, \mathbf{k}_{\bar{D}u}^e, \mathbf{k}_{\bar{D}\bar{D}}^e, \mathbf{r}_u^e, \mathbf{r}_{\bar{D}}^e$ denote certain parts of the element stiffness matrix and the element residual vector, respectively, whereas $\Delta \mathbf{u}^e$ and $\Delta \bar{\mathbf{D}}^e$ are the element nodal increments of the displacement and micromorphic damage, respectively.

Finally, the individual element contributions are assembled in the usual way which leads, after taking into account the boundary conditions and considering the arbitrariness of $\delta \mathbf{u}$ and $\delta \bar{\mathbf{D}}$, to the following set of global finite element equations:

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\bar{D}} \\ \mathbf{K}_{\bar{D}u} & \mathbf{K}_{\bar{D}\bar{D}} \end{bmatrix} \begin{Bmatrix} \Delta \mathbf{u} \\ \Delta \bar{\mathbf{D}} \end{Bmatrix} = - \begin{Bmatrix} \mathbf{R}_u \\ \mathbf{R}_{\bar{D}} \end{Bmatrix} \quad (6.77)$$

In the above,

$$\begin{aligned}
\mathbf{K}_{uu} &= \mathbf{A}_{e=1}^{n_{el}} (\mathbf{k}_{uu}^e), \quad \mathbf{K}_{u\bar{D}} = \mathbf{A}_{e=1}^{n_{el}} (\mathbf{k}_{u\bar{D}}^e), \quad \mathbf{K}_{\bar{D}u} = \mathbf{A}_{e=1}^{n_{el}} (\mathbf{k}_{\bar{D}u}^e), \quad \mathbf{K}_{\bar{D}\bar{D}} = \mathbf{A}_{e=1}^{n_{el}} (\mathbf{k}_{\bar{D}\bar{D}}^e), \\
\mathbf{R}_u &= \mathbf{A}_{e=1}^{n_{el}} (\mathbf{r}_u^e), \quad \mathbf{R}_{\bar{D}} = \mathbf{A}_{e=1}^{n_{el}} (\mathbf{r}_{\bar{D}}^e) \quad (6.78)
\end{aligned}$$

are the assembled global parts of the stiffness matrix and the residual vector, respectively, where $\mathbf{A}_{e=1}^{n_{el}}(\bullet)$ denotes the classical finite element assembly operator. The coupled equation system (6.77) needs to be solved iteratively for the global nodal increments $\Delta \mathbf{u}$ and $\Delta \bar{\mathbf{D}}$ until convergence is achieved.

6.4.2 Implicit time integration of the evolution equations

A fully implicit time integration of the evolution equations at the integration point level is desired. In this context, care should be taken to maintain the model's plastic incompressibility (i. e., $\det \mathbf{C}_p = 1$) and to preserve also the existing symmetries of the tensorial internal variables $\mathbf{C}_p$ and $\mathbf{C}_{pi}$ during the course of the computation. A corresponding algorithm which fulfills the above mentioned requirements is reviewed below.

Consider first the plastic flow rule (6.48)₁ which can be rewritten as

$$\dot{\mathbf{C}}_p = \dot{\lambda}_p \mathbf{f}(\mathbf{C}, \mathbf{C}_p, \mathbf{C}_{pi}, D) = \dot{\lambda}_p \mathbf{g}(\mathbf{C}, \mathbf{C}_p, \mathbf{C}_{pi}, D) \mathbf{C}_p \quad (6.79)$$

with $\mathbf{f}$ and $\mathbf{g}$ being the second-order tensors

$$\mathbf{f} := 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{Y}}' \mathbf{C}_p}{\sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^T}}, \quad \mathbf{g} := \mathbf{f} \mathbf{C}_p^{-1} \quad (6.80)$$

Note that the tensor-valued function $\mathbf{f}$ is a symmetric quantity, whereas the same is not true for $\mathbf{g}$, i. e., $\mathbf{g} \neq \mathbf{g}^T$. If the term $\dot{\lambda}_p \mathbf{g}$ in (6.79) were constant, say $\dot{\lambda}_p \mathbf{g} \equiv \mathbf{g}_0$, the corresponding differential equation $\dot{\mathbf{C}}_p = \mathbf{g}_0 \mathbf{C}_p$ could be solved analytically as follows:

$$\mathbf{C}_p(t) = \exp \left(\int_{t_n}^t \mathbf{g}_0 d\tau \right) \mathbf{C}_p(t_n) = \exp((t - t_n) \mathbf{g}_0) \mathbf{C}_p(t_n) \quad (6.81)$$

Here, $\mathbf{C}_p(t_n)$ is the initial value of $\mathbf{C}_p$ at time t_n and

$$\exp(\bullet) := \sum_{k=0}^{\infty} \frac{1}{k!} (\bullet)^k \quad (6.82)$$

denotes the exponential function of a general second-order tensor $(\bullet)$. The analytical solution (6.81) naturally fulfills the symmetry condition, i. e.,

$$\exp((t - t_n) \mathbf{g}_0) \mathbf{C}_p(t_n) = \mathbf{C}_p(t_n) \exp^T((t - t_n) \mathbf{g}_0) \quad (6.83)$$

Unfortunately, the term $\dot{\lambda}_p \mathbf{g}$ is generally nonlinear and time-dependent, meaning that no analytical solution of (6.79) is available. In such cases, Eq. (6.81) can still serve as a starting point for developing an approximate implicit numerical time integration scheme. For this, $\dot{\lambda}_p \mathbf{g}$ is kept constant during a considered time interval $\Delta t := t_{n+1} - t_n$ and approximated by its (yet unknown) value at time t_{n+1} . By doing this, the unconditionally stable and first-order

accurate implicit exponential map is obtained, viz.,

$$\mathbf{C}_p = \exp(\Delta\lambda_p \mathbf{g}) \mathbf{C}_{p_n} \quad (6.84)$$

where $\mathbf{C}_{p_n} := \mathbf{C}_p(t_n)$ and $\Delta\lambda_p := \Delta t \dot{\lambda}_p$ is the incremental plastic multiplier (in order to prevent an excessive proliferation of notation, any quantity is referred to the current time t_{n+1} , if not explicitly denoted otherwise).

However, as noted by Dettmer and Reese [2004], update formula (6.84) is actually not a suitable integration rule in the present case since it violates the symmetry condition, meaning that

$$\exp(\Delta\lambda_p \mathbf{g}) \mathbf{C}_{p_n} \neq \mathbf{C}_{p_n} \exp^T(\Delta\lambda_p \mathbf{g}) \quad (6.85)$$

In other words, using the classical implicit exponential map above, the symmetry of $\mathbf{C}_p$ cannot be ensured during the course of the computation. To tackle this problem, the latter authors suggested a modified update formula which a priori guarantees symmetry:

$$\mathbf{C}_p \mathbf{C}_{p_n}^{-1} \mathbf{C}_p = \exp(\Delta\lambda_p \mathbf{g}) \mathbf{C}_p \quad (6.86)$$

Since the argument $\Delta\lambda_p \mathbf{g}$ is an unsymmetric tensor, no closed-form expression of the exponential term is available which requires the computation of a truncated series representation using definition (6.82).

Later, Reese and Christ [2008] and Vladimirov et al. [2008] proposed a further useful modification of (6.86) as follows. Having in mind the series representation (6.82) and using the definition $\mathbf{U}_p := \sqrt{\mathbf{C}_p}$ of the plastic right stretch tensor, the exponential term can be rewritten as follows:

$$\begin{aligned} \exp(\Delta\lambda_p \mathbf{g}) &= \mathbf{I} + \Delta\lambda_p \mathbf{g} + \frac{(\Delta\lambda_p)^2}{2} \mathbf{g}^2 + \dots \\ &= \mathbf{I} + \Delta\lambda_p \mathbf{f} \mathbf{C}_p^{-1} + \frac{(\Delta\lambda_p)^2}{2} (\mathbf{f} \mathbf{C}_p^{-1})^2 + \dots \\ &= \mathbf{U}_p \left(\mathbf{I} + \Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} + \frac{(\Delta\lambda_p)^2}{2} (\mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1})^2 + \dots \right) \mathbf{U}_p^{-1} \\ &= \mathbf{U}_p \exp(\Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1} \end{aligned} \quad (6.87)$$

The advantage here is that the product $\Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}$ represents a symmetric tensor, thus the exponential term on the right-hand side of the equation can be evaluated in closed-form by means of the spectral decomposition. By inserting (6.87) into (6.86), the final form of the

update formula reads:¹

$$\mathbf{C}_p \mathbf{C}_{p_n}^{-1} \mathbf{C}_p = \mathbf{U}_p \exp \left(\Delta \lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} \right) \mathbf{U}_p \Rightarrow \mathbf{C}_{p_n}^{-1} = \mathbf{U}_p^{-1} \exp \left(\Delta \lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} \right) \mathbf{U}_p^{-1} \quad (6.88)$$

It remains to show that this formula indeed preserves the plastic incompressibility. By applying the determinant operator on both sides of the above equation and by considering that $\det(\exp(\bullet)) = \exp(\text{tr}(\bullet))$ for any second-order tensor $(\bullet)$ (see Gurtin [1981]), it holds

$$\begin{aligned} \det \mathbf{C}_{p_n}^{-1} &= \det \mathbf{U}_p^{-1} \det \left(\exp \left(\Delta \lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} \right) \right) \det \mathbf{U}_p^{-1} \\ &= \det \mathbf{U}_p^{-1} \exp \left(\text{tr} \left(\Delta \lambda_p \mathbf{U}_p^{-1} \mathbf{g} \mathbf{U}_p \right) \right) \det \mathbf{U}_p^{-1} \\ &= \left(\det \mathbf{U}_p^{-1} \right)^2 = \det \mathbf{C}_p^{-1} \end{aligned} \quad (6.89)$$

where it has additionally been exploited that $\mathbf{g}$ is deviatoric (i. e., $\text{tr} \mathbf{g} = 0$). In other words, it holds also $\det \mathbf{C}_p = \det \mathbf{C}_{p_n} = 1$ which proves the assertion.

Proceeding analogously with the evolution equation of kinematic hardening (6.48)₂ leads to the update formula

$$\mathbf{C}_{p_{in}}^{-1} = \mathbf{U}_{p_i}^{-1} \exp \left(\Delta \lambda_p \mathbf{U}_{p_i}^{-1} \mathbf{f}_{\text{kin}} \mathbf{U}_{p_i}^{-1} \right) \mathbf{U}_{p_i}^{-1} \quad (6.90)$$

where

$$\mathbf{f}_{\text{kin}} := 2 \frac{b/a}{f_{\text{dam}}(D)} \tilde{\mathbf{Y}}'_{\text{kin}} \mathbf{C}_{p_i} \quad (6.91)$$

and $\mathbf{U}_{p_i} := \sqrt{\mathbf{C}_{p_i}}$ is the inelastic plastic right stretch tensor. Finally, the scalar evolution equations (6.49) of the model are integrated by means of the classical backward Euler algorithm, leading to

$$\xi_p = \xi_{p_n} + \frac{\Delta \lambda_p}{f_{\text{dam}}(D)}, \quad D = D_n + \Delta \lambda_d, \quad \xi_d = \xi_{d_n} + \Delta \lambda_d \quad (6.92)$$

where $\Delta \lambda_d := \Delta t \dot{\lambda}_d$ denotes the incremental damage multiplier.

Remark 3. Evolution equation (6.48)₂ for the kinematic hardening variable could, in principle, also be integrated by means of a simple backward Euler algorithm since the latter also preserves the symmetry of $\mathbf{C}_{p_i}$ and the determinant $\det \mathbf{C}_{p_i}$ is, from a physical point of view, not required to be equal to one. However, as mentioned by Dettmer and Reese [2004], no significant gain in computational efficiency could be obtained by using such an approach. Therefore, and for reasons of better consistency with the corresponding evolution equation

¹In a similar fashion, Arghavani et al. [2010, 2011] derived an alternative update formula based on a logarithmic mapping.

for $\mathbf{C}_p$, the authors of the present paper decided to use the exponential map formula (6.90) instead.

Remark 4. During the iteration process at the integration point level, the variables ξ_p , D and ξ_d do not need to be treated as additional unknowns in the above equation system but can be entirely expressed in terms of the incremental multipliers $\Delta\lambda_p$, $\Delta\lambda_d$ and known values at time t_n , as can be inspected from (6.92).

6.4.3 Possible solutions of the incremental problem and algorithmic approach at the integration point level

The discretized Eqs. (6.88), (6.90) and (6.92) are subject to the time-discrete version of the plastic and damage loading / unloading conditions (6.51) - (6.52). During a time interval $[t_n, t_{n+1}]$ of the computation, four mutually exclusive cases can occur at a respective integration point: elastic loading / unloading (or neutral loading), plastic loading, elastic-damage loading or elastoplastic-damage loading. The corresponding implications for the plastic and damage multiplier as well as the yield and damage function are shown in Table 6.1, respectively, and were described in detail in another of the authors' papers (see Brepols et al. [2017]).

	case	multiplier		function	
		plasticity	damage	plasticity	damage
1.)	elastic loading / unloading neutral loading	$\Delta\lambda_p = 0$	$\Delta\lambda_d = 0$	$\Phi_p \leq 0$	$\Phi_d \leq 0$
2.)	plastic loading	$\Delta\lambda_p > 0$	$\Delta\lambda_d = 0$	$\Phi_p = 0$	$\Phi_d \leq 0$
3.)	elastic-damage loading	$\Delta\lambda_p = 0$	$\Delta\lambda_d > 0$	$\Phi_p \leq 0$	$\Phi_d = 0$
4.)	elastoplastic-damage loading	$\Delta\lambda_p > 0$	$\Delta\lambda_d > 0$	$\Phi_p = 0$	$\Phi_d = 0$

Table 6.1: Possible scenarios at an integration point

As an example, having Remark 4 in mind, the equations which finally need to be solved in case of an elastoplastic-damage step (case 4 in Table 6.1) are given below in a residuum format (the corresponding residuals in case of plastic loading (case 2 in Table 6.1) or elastic-damage loading (case 3 in Table 6.1) are obtained by deleting either r_4 or $\mathbf{r}_1$, $\mathbf{r}_2$ and r_3 in

(6.93), respectively):

$$\begin{aligned}
\mathbf{r}_1 &= -\mathbf{C}_{p_n}^{-1} + \mathbf{U}_p^{-1} \exp(\Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1} = \mathbf{0} \\
\mathbf{r}_2 &= -\mathbf{C}_{p_{in}}^{-1} + \mathbf{U}_{p_i}^{-1} \exp(\Delta\lambda_p \mathbf{U}_{p_i}^{-1} \mathbf{f}_{\text{kin}} \mathbf{U}_{p_i}^{-1}) \mathbf{U}_{p_i}^{-1} = \mathbf{0} \\
r_3 &= \Phi_p = 0 \\
r_4 &= \Phi_d = 0
\end{aligned} \tag{6.93}$$

Owing to the symmetry of the internal variables, the symmetric tensors $\mathbf{r}_1$ and $\mathbf{r}_2$ can be represented in Voigt form as two six-dimensional arrays. Taking further r_3 and r_4 into account, this results in a system of 14 nonlinear scalar equations in 14 unknowns which needs to be solved iteratively, for instance, by means of Newton’s method. For this, a preceding linearization of the equations in (6.93) has to be carried out (for constant $\mathbf{C}$ and $\bar{D}$; details can be found in Appendix 6.7.8). In every time step, the iteration is performed until the root-mean-square value of the total residuum becomes smaller than a prescribed tolerance. The update variables during the iteration are $\mathbf{U}_p^{-1}$, $\mathbf{U}_{p_i}^{-1}$, $\Delta\lambda_p$ and $\Delta\lambda_d$.

Brepols et al. [2017] described in detail two different algorithmic (monolithic) approaches to compute the actual solution to problems of the same type as discussed in this section. The first was a predictor-corrector algorithm based on an active set search strategy, analogous to approaches known from multisurface-plasticity. In contrast to that, the second algorithm relied upon a reformulation of the original inequality-constrained problem as an unconstrained one in terms of the so-called Fischer-Burmeister complementarity function, thus rigorously avoiding any case differentiation which is conceptually appealing. Both algorithms are without modifications likewise applicable in the present case. Further details are omitted here for brevity but can be found in the just mentioned reference.

6.4.4 Consistent tangent operators

For the calculation of the tangential stiffness matrix in a finite element program, and in order to preserve the quadratic rate of convergence of the corresponding global Newton-Raphson scheme, the material sensitivities $\partial\mathbf{S}/\partial\mathbf{E}$, $\partial\mathbf{S}/\partial\bar{D}$, $\partial D/\partial\mathbf{E}$, $\partial D/\partial\bar{D}$ need to be computed in a ‘consistent’ manner, a point which was already mentioned in Sect. 6.3.10. The relationship

between the increments $\Delta \mathbf{S}$, ΔD and $\Delta \mathbf{E} = \frac{1}{2} \Delta \mathbf{C}$, $\Delta \bar{D}$ can be expressed as:

$$\Delta \mathbf{S} = \mathcal{K}_E \left[\frac{1}{2} \Delta \mathbf{C} \right] + \mathbf{K}_{\bar{D}} \Delta \bar{D} \quad (6.94)$$

$$\Delta D = \mathbf{L}_E \cdot \left(\frac{1}{2} \Delta \mathbf{C} \right) + L_{\bar{D}} \Delta \bar{D} \quad (6.95)$$

where $\mathcal{K}_E$ (fourth-order tensor), $\mathbf{K}_{\bar{D}}$, $\mathbf{L}_E$ (second-order tensors) and $L_{\bar{D}}$ (scalar) denote the consistent (or algorithmic) tangent operators of the model which, in fact, are the above mentioned sensitivities. In the following, it will be shown how these quantities can be computed.

Since the stress $\mathbf{S}$ is a function of $\mathbf{C}$, $\mathbf{C}_p$ and D , the increment $\Delta \mathbf{S}$ can be expressed by using the chain rule of differentiation as

$$\begin{aligned} \Delta \mathbf{S} &= 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} \left[\frac{1}{2} \Delta \mathbf{C} \right] + \frac{\partial \mathbf{S}}{\partial \mathbf{C}_p} [\Delta \mathbf{C}_p] + \frac{\partial \mathbf{S}}{\partial D} \Delta D = \\ &= \left(2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} + 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}_p} : \frac{\partial \mathbf{C}_p}{\partial \mathbf{C}} + 2 \frac{\partial \mathbf{S}}{\partial D} \otimes \frac{\partial D}{\partial \mathbf{C}} \right) \left[\frac{1}{2} \Delta \mathbf{C} \right] + \left(\frac{\partial \mathbf{S}}{\partial \mathbf{C}_p} \left[\frac{\partial \mathbf{C}_p}{\partial \bar{D}} \right] + \frac{\partial \mathbf{S}}{\partial D} \frac{\partial D}{\partial \bar{D}} \right) \Delta \bar{D} \end{aligned} \quad (6.96)$$

By comparing the latter equation with (6.94), the expressions in the round brackets are identified as the operators $\mathcal{K}_E$ and $\mathbf{K}_{\bar{D}}$, respectively. Here, the partial derivatives of $\mathbf{S}$ can directly be computed from relationship (6.55) (or, more generally, from (6.18)₁). The other partial derivatives can be computed by considering the relationships between the increments $\Delta \mathbf{C}_p$, ΔD and $\Delta \mathbf{C}$, $\Delta \bar{D}$ which are obtained after the local iteration at the integration point level for Eqs. (6.93) has converged:

$$\Delta \mathbf{C}_p = \frac{\partial \mathbf{C}_p}{\partial \mathbf{C}} [\Delta \mathbf{C}] + \frac{\partial \mathbf{C}_p}{\partial \bar{D}} \Delta \bar{D} = (-\mathcal{A}_p^{-1} : \mathcal{A}_C) [\Delta \mathbf{C}] + (-\mathcal{A}_p^{-1} [\mathbf{A}_{\bar{D}}]) \Delta \bar{D} \quad (6.97)$$

$$\Delta D = \frac{\partial D}{\partial \mathbf{C}} \cdot \Delta \mathbf{C} + \frac{\partial D}{\partial \bar{D}} \Delta \bar{D} = (-B_{\Delta \lambda_d}^{-1} \mathbf{B}_C) \cdot \Delta \mathbf{C} + (-B_{\Delta \lambda_d}^{-1} B_{\bar{D}}) \Delta \bar{D} \quad (6.98)$$

A comparison of (6.98) with (6.95) shows that $\mathbf{L}_E = -2 B_{\Delta \lambda_d}^{-1} \mathbf{B}_C$ and $L_{\bar{D}} = -B_{\Delta \lambda_d}^{-1} B_{\bar{D}}$. The interested reader may find the specific expressions for $\mathcal{A}_p$, $\mathcal{A}_C$ (fourth-order tensors), $\mathbf{A}_{\bar{D}}$, $\mathbf{B}_C$ (second-order tensors) and $B_{\Delta \lambda_d}$, $B_{\bar{D}}$ (scalars) in Appendix 6.7.9.

Summarizing, the consistent tangent operators can be computed as

$$\mathcal{K}_E = 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} - 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}_p} : \mathcal{A}_p^{-1} : \mathcal{A}_C - 2 \frac{\partial \mathbf{S}}{\partial D} \otimes B_{\Delta\lambda_d}^{-1} \mathbf{B}_C \quad (6.99)$$

$$\mathbf{K}_{\bar{D}} = -\frac{\partial \mathbf{S}}{\partial \mathbf{C}_p} [\mathcal{A}_p^{-1} [\mathbf{A}_{\bar{D}}]] - \frac{\partial \mathbf{S}}{\partial D} B_{\Delta\lambda_d}^{-1} B_{\bar{D}} \quad (6.100)$$

$$\mathbf{L}_E = -2 B_{\Delta\lambda_d}^{-1} \mathbf{B}_C \quad (6.101)$$

$$L_{\bar{D}} = -B_{\Delta\lambda_d}^{-1} B_{\bar{D}} \quad (6.102)$$

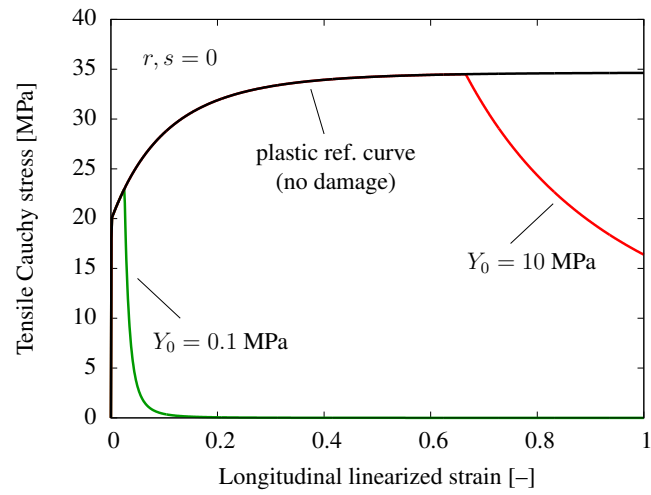
6.5 Numerical examples

6.5.1 Integration point study: Investigation of the model’s damage material parameters

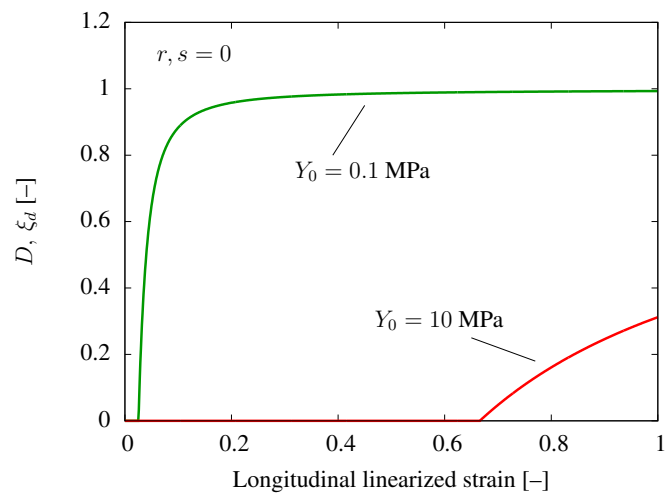
To begin with, the respective influence of the individual damage parameters Y_0 , r and s on the model’s behavior is investigated at a typical integration point. For this, a single 3D finite element of unit length is subjected to a state of uniaxial tension. The remaining model parameters in this example are chosen as $\Lambda = 5000$ MPa, $\mu = 7500$ MPa, $a = 12.5$ MPa, $b = 8.5$, $e = 12.5$ MPa, $f = 8.5$, $\sigma_0 = 20$ MPa, $H = 10^5$ MPa and $A = 10$ MPa mm², whereas the function introduced in Eq. (6.8) is set to $f_{\text{dam}}(D) = (1 - D)^2$. Note that the micromorphic parameters A and H have no real influence in the present case since uniaxial tension leads to a completely homogeneous (in other words ‘gradient-free’) state.

Fig. 6.2 is concerned with the influence of the damage threshold Y_0 only. For the time being, damage hardening is switched off, i. e., the parameters r and s are both set to zero. As can be seen, a higher damage threshold leads to a later onset of damage, as exemplarily shown for the values $Y_0 = 0.1$ MPa (green curve) and $Y_0 = 10$ MPa (red curve). As soon as the damage threshold is reached or exceeded in the simulation, the internal variables D and ξ_d start to develop, respectively, which can be inspected from Fig. 6.2b (as mentioned already in Remark 2, D and ξ_d are actually equal in the present model). They both approach one for increasing longitudinal strain. Due to the choice of the material parameters, the softening effect caused by damage in this example is stronger than the effect of plastic hardening, which in consequence leads to a reduction of the tensile stress, as can be seen in Fig. 6.2a. The particular choice of $f_{\text{dam}}(D)$ ensures a gradual transition of the tensile stress towards zero for increasing strain and damage. As a reference, the stress-strain response of a purely elastoplastic material is shown in Fig. 6.2a as well (black curve, obtained by letting $Y_0 \rightarrow \infty$).

The effect of damage hardening on the model’s behavior is studied in Fig. 6.3 in which



(a) Stress-strain response

(b) Evolution of D and ξ_d Figure 6.2: Influence of parameter Y_0 (assuming $r, s = 0$)

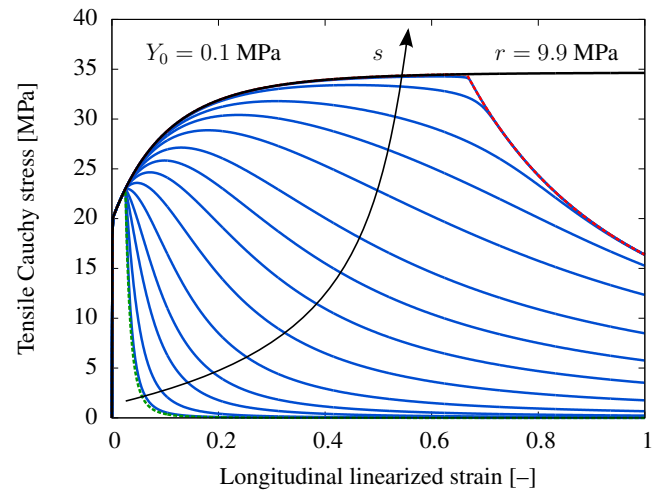
the parameter s is varied for constant values of the initial damage threshold $Y_0 = 0.1$ MPa and parameter $r = 9.9$ MPa. First of all, with the extreme choices $s = 0$ and $s \rightarrow \infty$, the same material responses are recovered as in the cases of no damage hardening and damage thresholds $Y_0 = 0.1$ MPa and $Y_0 = 10$ MPa, respectively (green and red dashed curves). This can be readily understood by inferring the particular expression for damage hardening $q_d = r(1 - \exp(-s\xi_d))$ in Eq. (6.62): On the one hand, if $s = 0$, the corresponding exponential term becomes one which results in $q_d = 0$ and $Y_0 = 0.1$ MPa. On the other hand, if $s \rightarrow \infty$, the exponential term vanishes completely, leading to a constant $q_d = r$ and $Y_0 = 10$ MPa. Both can be considered the ‘limit’ cases in which no damage hardening takes place at all. For any other value of s , a certain material response between those two ‘limits’ is obtained as shown by the blue curves in Figs. 6.3a and 6.3b (arrows indicate the change of the results for an increasing value of s). In this way, damage hardening allows for a greater applicability and adaptability of the model to different softening behaviors of the considered material. More practically speaking, damage hardening can be utilized for ‘slowing down’ the evolution of the damage variable D .

For completeness, Fig. 6.4 displays the calculated retention force during the computation. This plot indicates that, within a large deformation framework, a force decrease can in principle not only occur due to material softening (i. e., damage) but also due to geometric softening which can be clearly seen in case of the purely elastoplastic reference material (black curve). This happens whenever a force increase due to stress hardening becomes less significant than a force decrease due to a reducing cross section the stress is acting on. Such an effect could not be modeled within a geometrically linear theory. Besides, the present test can serve as a first indication that the user element for large deformations was correctly implemented.

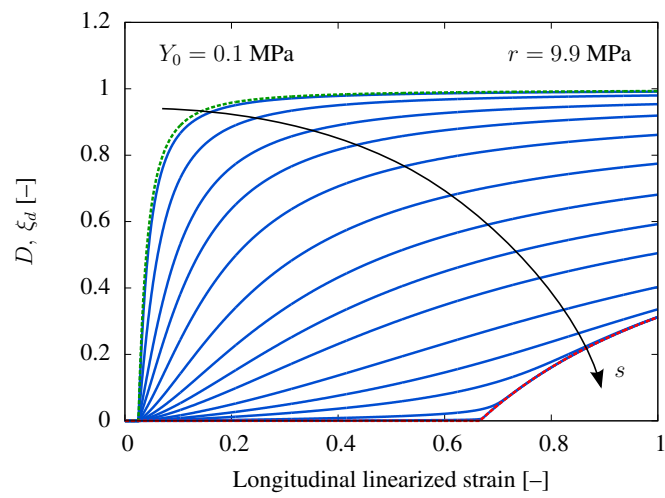
Of course, the damage behavior of the model is also strongly dependent upon the particular choice of the weakening function $f_{\text{dam}}(D)$. For brevity, this topic will not be further discussed here.

6.5.2 Structural example: Tensile specimen with imperfection

In the following, the mesh regularization properties of the proposed gradient-extended damage-plasticity model are tested in a finite element problem in which a 2D plane strain specimen is subjected to uniaxial tension by applying a tensile force $F(t)$ to its upper and lower edge, respectively. In order to trigger a strain localization process, a slight geometric imperfection is introduced at the specimen’s center (1.8% width reduction) which is linearly extended to the top and bottom. The idea for this specific example stems from Simo and Armero [1992] and the corresponding dimensions of the specimen are given in Fig. 6.5a. To gain efficiency,



(a) Stress-strain response

(b) Evolution of D and ξ_d Figure 6.3: Influence of parameters r and s

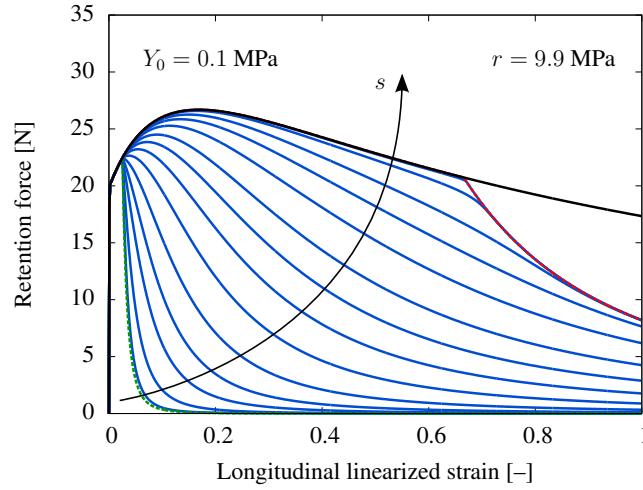


Figure 6.4: Illustration of geometric softening in large deformation problems

symmetry conditions are presumed which means that only a quarter of the sample is considered during the simulation (highlighted in gray in the figure; take also note of Remark 5. The actual boundary value problem is illustrated in Fig. 6.5b.

In the simulation, the specimen is firstly deformed up to the point of maximum load. Afterwards, further deformation occurs under a simultaneously decreasing global load which means that the applied force $F(t)$ is (pseudo-)time-dependent. The loaded edge at the top is constrained such that it remains straight and perpendicular to the loading direction throughout the simulation.

Some of the model's material parameters are identified with values given in the above mentioned reference: $\Lambda = 110700$ MPa, $\mu = 80190$ MPa, $\sigma_0 = 450$ MPa, $e = 265$ MPa and $f = 16.93$. The remaining parameters are freely chosen as follows: $a = 400$ MPa, $b = 4.25$, $Y_0 = 150$ MPa, $r = 10$ MPa, $s = 10$, $H = 10^5$ MPa and $A = 50$ MPa mm². The weakening function introduced in Eq. (6.8) is defined as $f_{\text{dam}}(D) = (1 - D)^2$ and linear finite element approximations of the displacement field and the micromorphic damage field are considered (see Eqs. (6.71) - (6.73)). A mesh convergence study is performed using different finite element meshes with 680, 1280, 2100, 4490, 9800, 19250, 38060 and 85040 elements. As exemplarily illustrated for both the coarsest and finest mesh in Fig. 6.6, respectively, all meshes are heavily refined in the region where damage is predominately expected to occur. Generally, standard quadrilateral elements with four integration points are used in the simulation, except for a few triangular elements which are necessary for the mesh refinement.

Fig. 6.7 illustrates the (normalized) load-displacement curves which are obtained in the simulation using the respective meshes. In the plot, the vertical displacement of the top edge

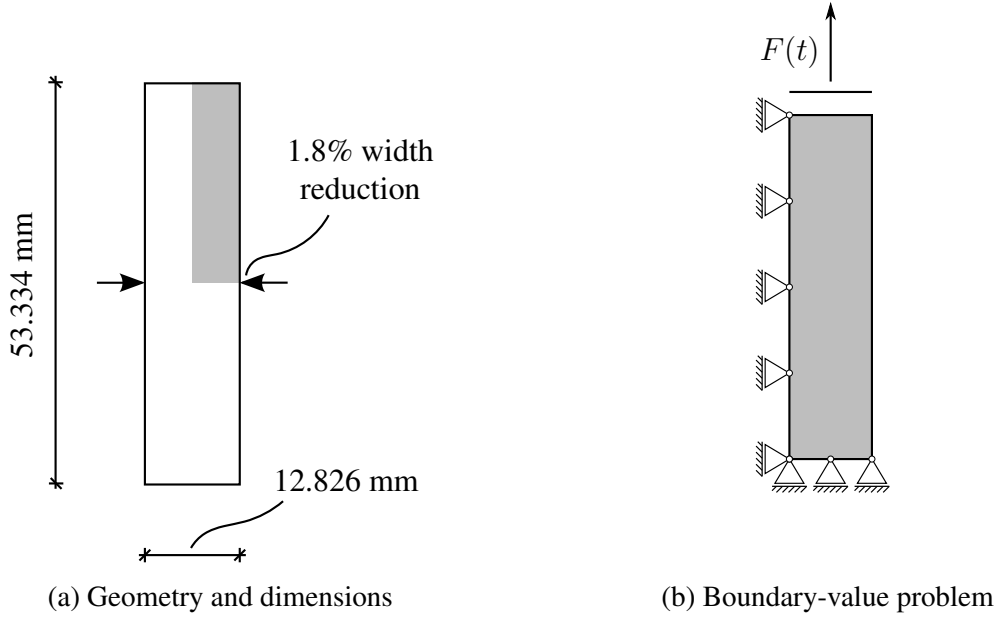
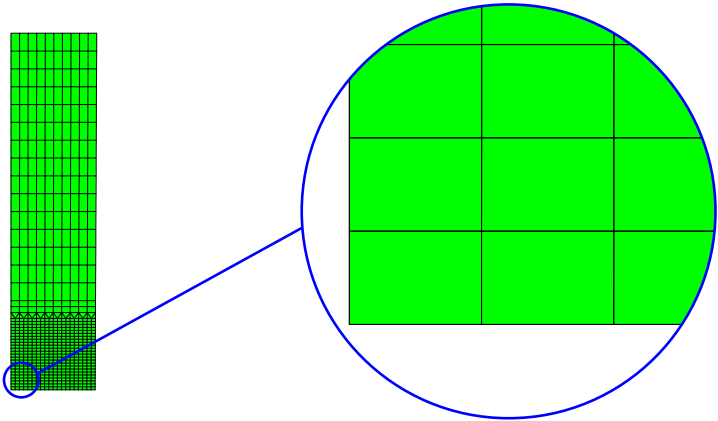


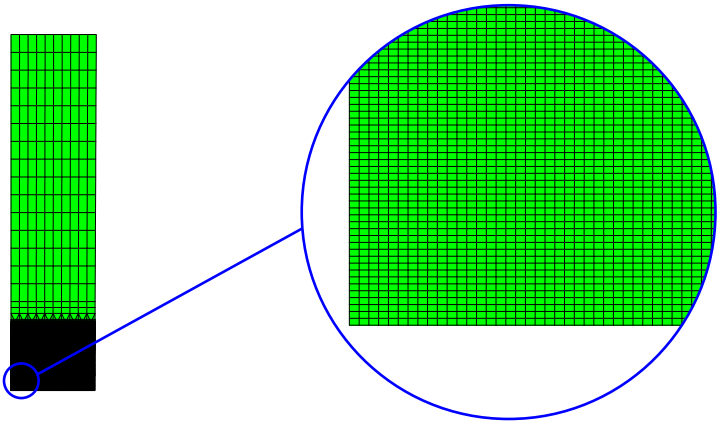
Figure 6.5: Tensile specimen with imperfection

is denoted by u whereas $F_{\max}$ is the maximum load attained in the simulation. During the process, the structure firstly undergoes a purely elastic deformation which is characterized by a steep and almost linear load-displacement curve (remember that a Neo-Hookean-type elastic energy is used in the model). Subsequently, a pronounced elastoplastic response of the structure is visible till the peak load is reached at a top edge displacement of $u \approx 3.7$ mm. Up to this point, the load-displacement curves for the different meshes are nearly indistinguishable from each other. As a consequence of the considered geometric nonlinearity, a gradual decrease in the force occurs afterwards: the softening effect due to a reduction of the structure's load-carrying area becomes more significant than the stress increase in the material due to plastic hardening. This effect was already described in Sect. 6.5.1. Finally, when damage sets in, a sudden and severe drop-down of the load-displacement curve occurs. From this point on, the differences between the results obtained for the respective meshes become apparent. However, though small differences can still be recognized between the load-displacement curves for the two finest meshes, a convergence towards an unambiguous solution with a finite amount of energy dissipation during the damage process is clearly visible. Fig. 6.8 further confirms the mesh convergence with respect to the specimen's deformed geometry and underlines the reason of using a model in the present example that is capable of representing large plastic deformations.

In order to study the convergence of the local fields, contour plots of the damage variable D and the accumulated plastic strain κ at the end of the simulation are exemplarily shown in



(a) Mesh with 680 elements



(b) Mesh with 85040 elements

Figure 6.6: Mesh refinement

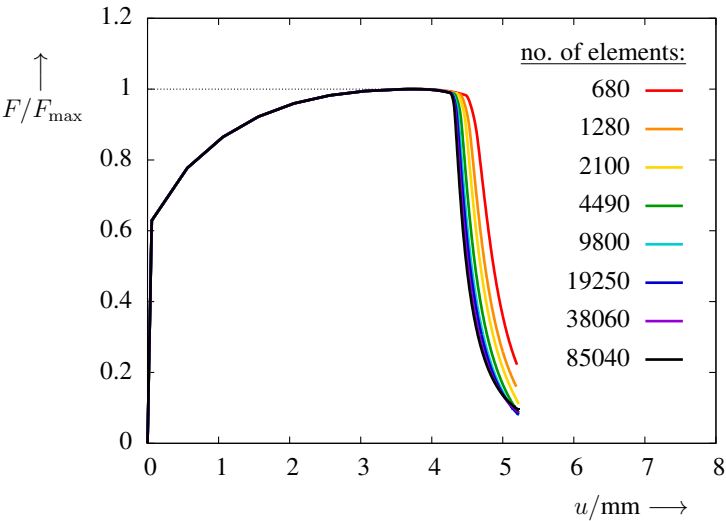


Figure 6.7: Convergence study: load-displacement curves

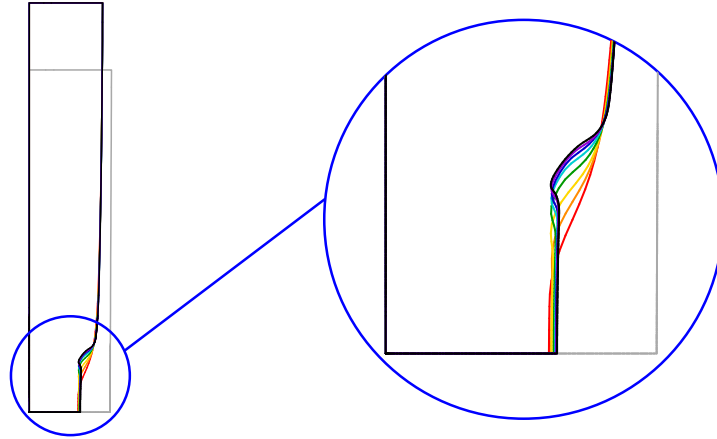


Figure 6.8: Convergence study: deformed geometry (gray: undeformed geometry; remaining colors as in Fig. 6.7)

Figs. 6.9 and 6.10 for the four finest meshes, respectively (the top and bottom values in the legends of the figures indicate the attained minimum and maximum value within the contour plots, respectively). The contours are plotted on the deformed geometry of the specimen, only the most interesting part of the structure is shown. It can be seen that a shear band and corresponding damage zone develop which run obliquely through the left corner of the considered quarter of the specimen.

Overall, the results show a satisfying agreement. The width of the damage zone in Fig. 6.9 remains finite and is nearly the same in all cases. Noticeable differences in the damage contours are only visible in the middle of this zone where D is highest. Here, it seems that not all details of the damage distribution are fully resolved yet, even in case of the finest mesh. Analogous observations can be made for the accumulated plastic strain contours shown in Fig. 6.10.

Nevertheless, a question remains as to why so many elements are needed in order to obtain a solution that can be regarded as ‘reasonably converged’. At the moment, it cannot be completely excluded that this is a kind of volumetric locking. Keep in mind that large deviatoric plastic strains occur in the present example but no special finite element technology is currently implemented in the applied finite elements which could eventually cause problems. It is a declared objective of the authors to investigate this issue in more detail in the future.

Remark 5. As shown in the example, a shear band and corresponding damage zone emerge during the process which run obliquely through the left corner of the considered quarter of the specimen. As a result of the assumed symmetry, this actually means that two mirrored shear bands are crossing each other in the middle of the complete sample. In reality, if dam-

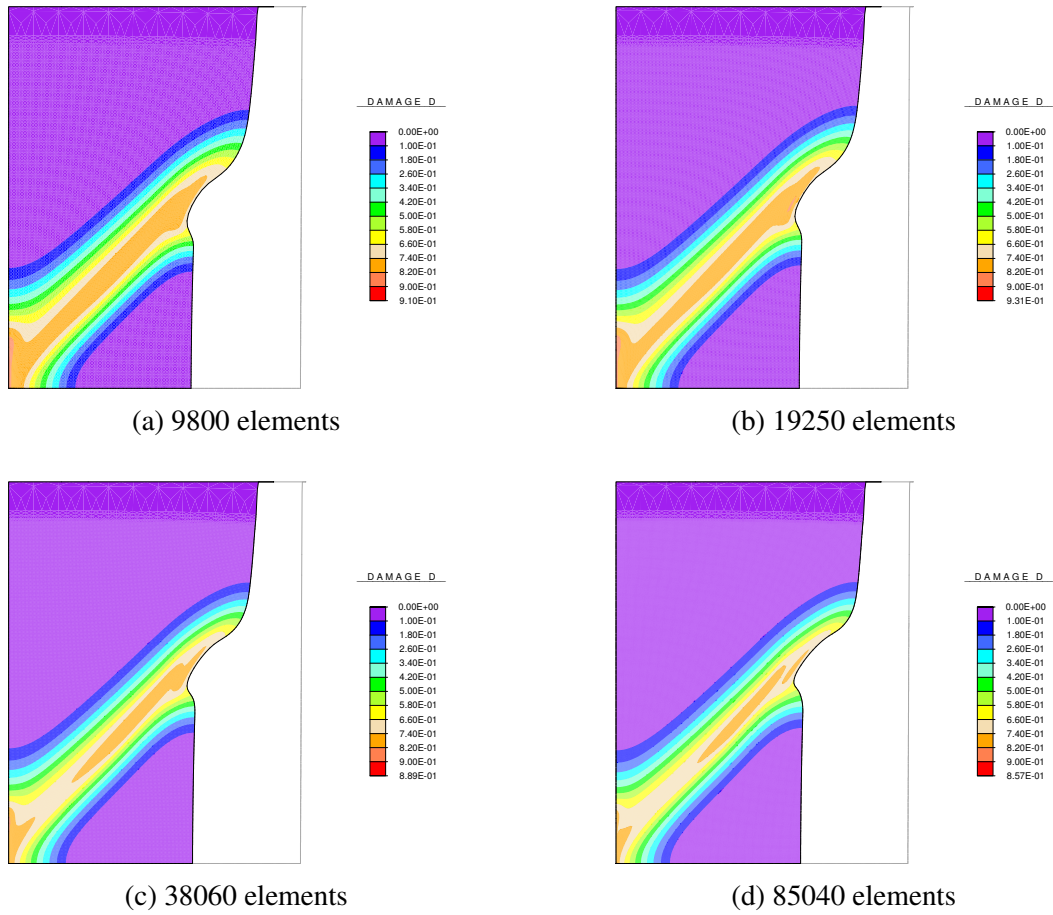


Figure 6.9: Contours of D at the end of the process for the four finest meshes

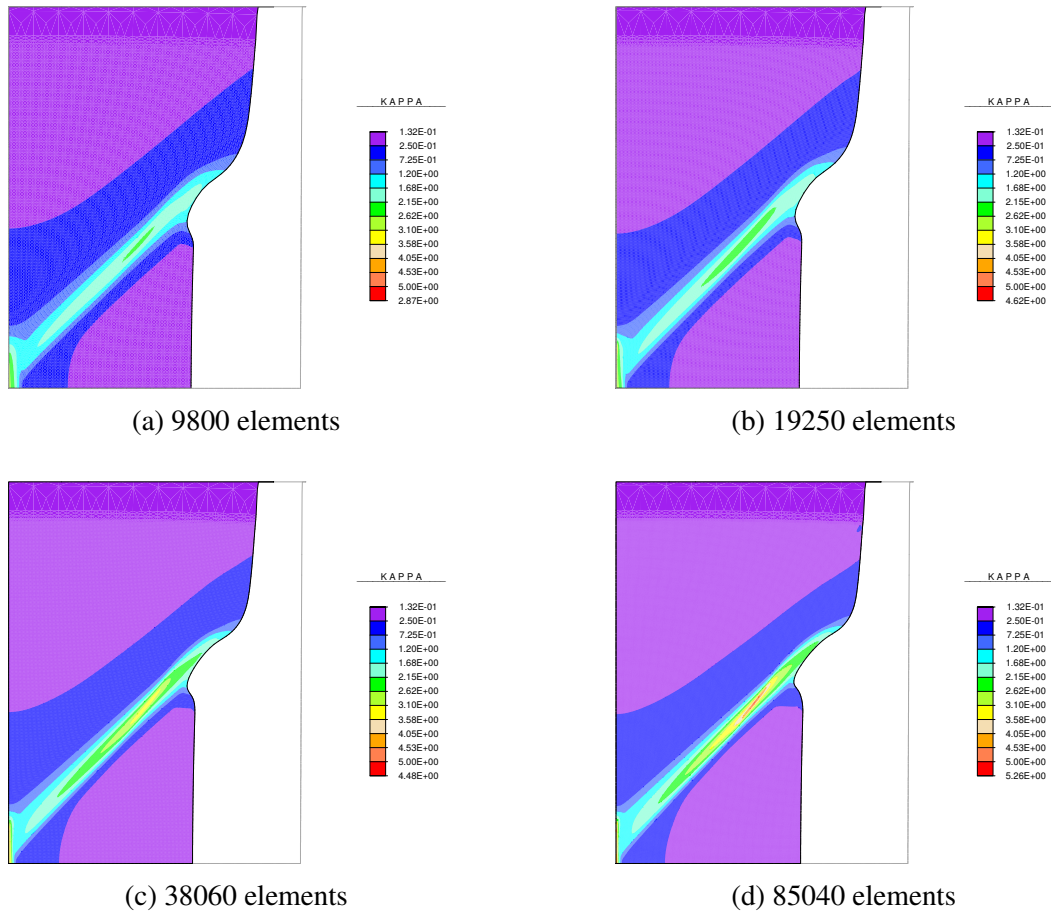


Figure 6.10: Contours of κ at the end of the process for the four finest meshes

age evolved sufficiently at some point of the process, an oblique shearing of the specimen would most likely be observable in the direction of either of the two shear bands, leading in consequence to complete failure of the sample. However, it is clear that this stage of the process cannot be modeled anymore by taking into account the symmetry conditions as shown in Fig. 6.5b. Instead, only the development of the shear band and corresponding damage zone up to this point can be simulated. Since the purpose of this example is mainly to successfully verify the mesh regularization properties of the proposed gradient-extended damage-plasticity model in the context of large plastic deformations, this modeling limitation is accepted.

6.6 Conclusions

In this work, a gradient-extended material model was presented which is able to deliver mesh-independent results in finite element simulations involving material softening in the context of large plastic deformations. It can be considered a geometrically nonlinear version of a corresponding model for small deformations proposed earlier by the same authors (Brepols et al. [2018]).

Damage and plasticity are treated in the model formulation as individual dissipative mechanisms, a technical feature which was realized by adopting a two-surface strategy that takes into account independent damage loading and plastic yield criteria as well as corresponding loading / unloading conditions, respectively. This allows for a quite versatile usage of the model, as it can be flexibly adapted to different modeling conditions in which the actual material is characterized by an either more brittle-like or more ductile-like damage behavior. Suitable yield and damage loading functions as well as thermodynamically consistent evolution equations for the strain-like damage and plastic internal variables were presented and discussed in detail.

The model's gradient-extension was derived on the basis of the micromorphic approach in the sense of Forest [2009, 2016]. Loosely speaking, the latter can be considered a general and systematic tool for incorporating gradient (i.e., 'nonlocal') effects into already existing 'local' constitutive models. Using the micromorphic approach, the modeling effort with regard to the gradient-extension usually reduces to the selection of appropriate internal variables of the model which are assumed to exert gradient effects, as well as to the formulation of an extended virtual work expression and an associated micromorphic energy function. The additional differential equation, which classically needs to be solved for gradient-extended material models, and further interdependencies between the gradient and other constitutive quantities of the model then follow more or less automatically by a standardized procedure. In

the present study, the damage variable was chosen as the one exerting gradient effects and all necessary steps to arrive at the micromorphic extension of a geometrically nonlinear model as the one discussed here were presented in great detail.

The proposed model was formulated in a well-established and thermodynamically motivated hyperelastic-based plasticity framework for large deformations which was co-developed earlier by one of the current authors (Vladimirov et al. [2008, 2009]). By assuming an additional physically motivated multiplicative split of the plastic part of the deformation gradient, this framework allows for the consideration of both nonlinear Armstrong-Frederick kinematic hardening as well as nonlinear Voce isotropic hardening in the model. It was shown in this work that, through a pull back of all constitutive equations of the model to the reference configuration, a quite condense and convenient formulation was finally obtained that depends exclusively on symmetric internal variables, which is appealing not only from the computational point view.

Important aspects regarding the numerics and implementation of the model were also highlighted. In linearizing the weak form of the underlying boundary value problem and subsequently introducing independent finite element interpolations of the unknown fields, it was demonstrated that a coupled system of algebraic finite element equations emerges which needs to be solved iteratively not only for the displacements but also for the micromorphic damage variable at every respective node of the finite element mesh. In order to retain the quadratic rate of convergence in a Newton-Raphson scheme at the global finite element level, it proves further necessary to compute four tangent operators (arisen from the prior linearization of the weak form) consistently, and corresponding formulas were provided in this study. Moreover, a special exponential map algorithm was described in detail to time-integrate the evolution equations of the model at the integration point level such that both the plastic incompressibility as well as the symmetry of the tensorial internal variables are preserved during the course of computations.

Finally, numerical calculations were carried out with the model. In a first example, a single finite element was subjected to a state of uniaxial tension in order to study the meaning of the model's damage parameters in the simplest context possible at a typical integration point. The influence of the initial damage threshold was practically illustrated and it was shown that the incorporated nonlinear damage hardening can offer a valueable additional flexibility regarding the model's damaging behavior. Afterwards, a structural example problem was considered in which a 2D plane strain tensile specimen with a slight imperfection in its middle was subjected to simple tension. A convergence study was carried out using several different mesh discretizations to assess the model's mesh regularization properties. Due to the chosen

material parameters in the example, a pronounced plastic deformation of the specimen at an increasing load firstly occurred during the simulation, especially in the area surrounding the imperfection. Up to the point of maximum load and even beyond, when a small load drop showed up due to geometric softening of the specimen, the results for the different meshes were almost identical. Only after damage set in, a severe drop-drown of the load occurred and the results obtained for the different meshes truly differed from each other. Even though quite a lot of elements were necessary to satisfactorily demonstrate it, a convergence towards an unambiguous result with a finite amount of energy dissipation during the damage process became visible, both with regard to the force-displacement curves and deformed geometry of the specimen. Careful investigations of the damage distribution and accumulated plastic strain field further indicated the occurrence of a shear band during the simulation and that the width of the damage zone remained finite also for the finest mesh discretizations.

Future work could, e. g., focus on extending the model to damage and plastic anisotropy. In the authors' opinion, especially the latter should be readily possible since a corresponding theoretical framework, compatible to the one used in this study, was already laid down (see, e. g., Pietryga et al. [2012] and Vladimirov et al. [2010]). Another very interesting point concretely planned by the current authors is the incorporation of the finite element technology developed by Reese [2002, 2003, 2005] into the formulation and the investigation of its effect in connection with the already implemented gradient-enhancement of the model. It is expected that this does not only cure possible locking effects but also leads to more efficient computations since the material model then only needs to be evaluated at a single integration point within corresponding elements. According to suggestions given in more recent works (see, e. g., Dimitrijevic and Hackl [2011], Miehe, Aldakheel and Raina [2016], Miehe, Teichtmeister and Aldakheel [2016], Saanouni and Hamed [2013]), the incorporation of a second internal length scale (i. e., a further gradient term) for plasticity would be worthwhile to consider, too. In this way, one could additionally account for plastic size effects or ensure that a developing damage zone remains inside of a plastic zone, for instance.

6.7 Appendix

6.7.1

Requiring that the internal and external virtual work are the same leads to

$$\begin{aligned} \int_{B_0} \mathbf{S} \cdot \delta \mathbf{E} \, dV - \int_{B_0} \mathbf{f}_0 \cdot \delta \mathbf{u} \, dV - \int_{\partial B_{0t}} \mathbf{t}_0 \cdot \delta \mathbf{u} \, dA + \\ + \int_{B_0} (a_{0i} \delta \bar{D} + \mathbf{b}_{0i} \cdot \text{Grad}(\delta \bar{D})) \, dV - \int_{B_0} (a_{0e} \delta \bar{D} + \mathbf{b}_{0e} \cdot \text{Grad}(\delta \bar{D})) \, dV + \\ - \int_{\partial B_{0c}} a_{0e} \delta \bar{D} \, dA = 0 \end{aligned}$$

By using the identity

$$\begin{aligned} \mathbf{S} \cdot \delta \mathbf{E} &= \mathbf{S} \cdot \frac{1}{2} \left(\mathbf{F}^T \text{Grad}(\delta \mathbf{u}) + \text{Grad}(\delta \mathbf{u})^T \mathbf{F} \right) = \\ &= \text{tr}(\mathbf{S}^T \mathbf{F}^T \text{Grad}(\delta \mathbf{u})) = (\mathbf{FS}) \cdot \text{Grad}(\delta \mathbf{u}) \end{aligned}$$

and the chain rule of differentiation

$$\begin{aligned} \text{Div}((\mathbf{FS})^T [\delta \mathbf{u}]) &= \text{Div}(\mathbf{FS}) \cdot \delta \mathbf{u} + (\mathbf{FS}) \cdot \text{Grad}(\delta \mathbf{u}) \\ \text{Div}(\mathbf{b}_{0i} \delta \bar{D}) &= \text{Div}(\mathbf{b}_{0i}) \delta \bar{D} + \mathbf{b}_{0i} \cdot \text{Grad}(\delta \bar{D}) \\ \text{Div}(\mathbf{b}_{0e} \delta \bar{D}) &= \text{Div}(\mathbf{b}_{0e}) \delta \bar{D} + \mathbf{b}_{0e} \cdot \text{Grad}(\delta \bar{D}) \end{aligned}$$

along with the divergence theorem

$$\begin{aligned} \int_{B_0} \text{Div}((\mathbf{FS})^T [\delta \mathbf{u}]) \, dV &= \int_{\partial B_0} (\mathbf{FS})^T [\delta \mathbf{u}] \cdot \mathbf{n}_0 \, dA \\ \int_{B_0} \text{Div}(\mathbf{b}_{0i} \delta \bar{D}) \, dV &= \int_{\partial B_0} (\mathbf{b}_{0i} \delta \bar{D}) \cdot \mathbf{n}_0 \, dA \\ \int_{B_0} \text{Div}(\mathbf{b}_{0e} \delta \bar{D}) \, dV &= \int_{\partial B_0} (\mathbf{b}_{0e} \delta \bar{D}) \cdot \mathbf{n}_0 \, dA \end{aligned}$$

and the fact that $(\mathbf{FS})^T [\delta \mathbf{u}] \cdot \mathbf{n}_0 = (\mathbf{FS}) [\mathbf{n}_0] \cdot \delta \mathbf{u}$, the expression can be reformulated as

$$\begin{aligned} & - \int_{B_0} (\text{Div}(\mathbf{FS}) + \mathbf{f}_0) \cdot \delta \mathbf{u} \, dV + \int_{\partial B_0} (\mathbf{FS}) [\mathbf{n}_0] \cdot \delta \mathbf{u} \, dA - \int_{\partial B_{0_t}} \mathbf{t}_0 \cdot \delta \mathbf{u} \, dA + \\ & - \int_{B_0} (\text{Div}(\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) - a_{0_i} + a_{0_e}) \delta \bar{D} \, dV + \int_{\partial B_0} (\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) \cdot \mathbf{n}_0 \delta \bar{D} \, dA + \\ & - \int_{\partial B_{0_c}} a_{0_c} \delta \bar{D} \, dA = 0 \end{aligned}$$

Finally, by considering that $\mathbf{u} = \hat{\mathbf{u}}$ on ∂B_{0_u} , $\bar{D} = \hat{\bar{D}}$ on $\partial B_{0_{\bar{D}}}$ as well as the fact that the test functions $\delta \mathbf{u}$ and $\delta \bar{D}$ vanish on ∂B_{0_u} and $\partial B_{0_{\bar{D}}}$, respectively, but are otherwise arbitrary and independent from each other, results in the statements

$$\begin{aligned} \text{Div}(\mathbf{FS}) + \mathbf{f}_0 &= \mathbf{0} & \text{in } B_0 & \quad \text{Div}(\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) - a_{0_i} + a_{0_e} = 0 & \text{in } B_0 \\ (\mathbf{FS}) [\mathbf{n}_0] &= \mathbf{t}_0 & \text{on } \partial B_{0_t} & \quad (\mathbf{b}_{0_i} - \mathbf{b}_{0_e}) \cdot \mathbf{n}_0 = a_{0_c} & \text{on } \partial B_{0_c} \\ \mathbf{u} &= \hat{\mathbf{u}} & \text{on } \partial B_{0_u} & \quad \bar{D} = \hat{\bar{D}} & \text{on } \partial B_{0_{\bar{D}}} \end{aligned}$$

which are valid in a point-wise sense.

6.7.2

The internal and external parts of the virtual work can equivalently be formulated with respect to quantities defined in the current configuration B of the body as follows (for more details, the reader is referred to Appendix 6.7.3):

$$\begin{aligned} g_{\text{int}} &= \int_B \boldsymbol{\sigma} \cdot \text{sym}(\text{grad}(\delta \mathbf{u})) \, dv + \underbrace{\int_B (a_i \delta \bar{D} + \mathbf{b}_i \cdot \text{grad}(\delta \bar{D})) \, dv}_{\text{micromorphic extension}} \\ g_{\text{ext}} &= \int_B \mathbf{f} \cdot \delta \mathbf{u} \, dv + \int_{\partial B_t} \mathbf{t} \cdot \delta \mathbf{u} \, da + \underbrace{\int_B (a_e \delta \bar{D} + \mathbf{b}_e \cdot \text{grad}(\delta \bar{D})) \, dv + \int_{\partial B_c} a_c \delta \bar{D} \, da}_{\text{micromorphic extension}} \end{aligned}$$

Here, $\boldsymbol{\sigma}$ is the Cauchy stress. All the other quantities and expressions were either already defined or should be clear from the context: they are simply the counterparts of those defined already in Sect. 6.3.1 but this time with respect to the current configuration. An application of the PVW leads to the balance of linear momentum, generalized balance equation and corresponding boundary conditions expressed in the current configuration, respectively (the proof

of this assertion is completely analogous that given in Appendix 6.7.1 for the formulation in the reference configuration):

$$\text{PVW : } g_{\text{int}} \stackrel{!}{=} g_{\text{ext}} \implies \left\{ \begin{array}{l} \text{linear momentum balance:} \\ \text{div}(\boldsymbol{\sigma}) + \mathbf{f} = \mathbf{0} \quad \text{in } B \\ \boldsymbol{\sigma}[\mathbf{n}] = \mathbf{t} \quad \text{on } \partial B_t \\ \mathbf{u} = \hat{\mathbf{u}} \quad \text{on } \partial B_u \\ \text{micromorphic balance equation:} \\ \text{div}(\mathbf{b}_i - \mathbf{b}_e) - a_i + a_e = 0 \quad \text{in } B \\ (\mathbf{b}_i - \mathbf{b}_e) \cdot \mathbf{n} = a_c \quad \text{on } \partial B_c \\ \bar{D} = \hat{\bar{D}} \quad \text{on } \partial B_{\bar{D}} \end{array} \right.$$

6.7.3

Expressed with respect to the reference configuration, the internal virtual work g_{int} is given by (6.1) as

$$g_{\text{int}} = \int_{B_0} \mathbf{S} \cdot \delta \mathbf{E} \, dV + \int_{B_0} (a_{0_i} \delta \bar{D} + \mathbf{b}_{0_i} \cdot \text{Grad}(\delta \bar{D})) \, dV$$

By considering $dV = J^{-1} dv$ (where $J := \det \mathbf{F}$), $\delta \mathbf{E} := \frac{1}{2} (\mathbf{F}^T \text{Grad}(\delta \mathbf{u}) + \text{Grad}(\delta \mathbf{u})^T \mathbf{F})$, $\text{Grad}(\delta \mathbf{u}) = \text{grad}(\delta \mathbf{u}) \mathbf{F}$ and $\text{Grad}(\delta \bar{D}) = \mathbf{F}^T [\text{grad}(\delta \bar{D})]$ one can rewrite the latter expression as

$$g_{\text{int}} = \int_B J^{-1} \mathbf{S} \cdot \underbrace{\left(\mathbf{F}^T \frac{1}{2} (\text{grad}(\delta \mathbf{u}) + \text{grad}(\delta \mathbf{u})^T) \mathbf{F} \right)}_{:= \text{sym}(\text{grad}(\delta \mathbf{u}))} dv + \int_B (J^{-1} a_{0_i} \delta \bar{D} + J^{-1} \mathbf{b}_{0_i} \cdot \mathbf{F}^T [\text{grad}(\delta \bar{D})]) dv$$

Now, exploiting that $\mathbf{S} \cdot (\mathbf{F}^T \text{sym}(\text{grad}(\delta \mathbf{u})) \mathbf{F}) = \text{tr}(\mathbf{F} \mathbf{S} \mathbf{F}^T \text{sym}(\text{grad}(\delta \mathbf{u}))) = (\mathbf{F} \mathbf{S} \mathbf{F}^T) \cdot \text{sym}(\text{grad}(\delta \mathbf{u}))$ and $\mathbf{b}_{0_i} \cdot \mathbf{F}^T [\text{grad}(\delta \bar{D})] = \mathbf{F} [\mathbf{b}_{0_i}] \cdot \text{grad}(\delta \bar{D})$, the above expression can further be rewritten as

$$g_{\text{int}} = \int_B (J^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T) \cdot \text{sym}(\text{grad}(\delta \mathbf{u})) dv + \int_B (J^{-1} a_{0_i} \delta \bar{D} + J^{-1} \mathbf{F} [\mathbf{b}_{0_i}] \cdot \text{grad}(\delta \bar{D})) dv$$

Finally, by introducing the abbreviations $a_i := J^{-1} a_{0_i}$, $\mathbf{b}_i := J^{-1} \mathbf{F} [\mathbf{b}_{0_i}]$ and by considering that $\boldsymbol{\sigma} = J^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T$, one obtains

$$g_{\text{int}} = \int_B \boldsymbol{\sigma} \cdot \text{sym}(\text{grad}(\delta \mathbf{u})) \, dv + \int_B (a_i \delta \bar{D} + \mathbf{b}_i \cdot \text{grad}(\delta \bar{D})) \, dv$$

which is the internal virtual work expression in the current configuration.

Next, the external virtual work g_{ext} is considered. In the reference configuration, it is given by (6.2) as

$$\begin{aligned} g_{\text{ext}} = & \int_{B_0} \mathbf{f}_0 \cdot \delta \mathbf{u} \, dV + \int_{\partial B_{0_t}} \mathbf{t}_0 \cdot \delta \mathbf{u} \, dA + \\ & + \int_{B_0} (a_{0_e} \delta \bar{D} + \mathbf{b}_{0_e} \cdot \text{Grad}(\delta \bar{D})) \, dV + \int_{\partial B_{0_c}} a_{0_c} \delta \bar{D} \, dA \end{aligned}$$

By considering $dV = J^{-1} dv$, $\mathbf{t}_0 \cdot \delta \mathbf{u} = \mathbf{F} \mathbf{S} [\mathbf{n}_0] \cdot \delta \mathbf{u} = (\mathbf{F} \mathbf{S})^T [\delta \mathbf{u}] \cdot \mathbf{n}_0$ on ∂B_{0_t} , Nanson's formula $\mathbf{n}_0 \, dA = J^{-1} \mathbf{F}^T [\mathbf{n}] \, da$ (which leads also to $dA = J^{-1} \|\mathbf{F}^{-T} [\mathbf{n}_0]\|^{-1} da$) and $\text{Grad}(\delta \bar{D}) = \mathbf{F}^T [\text{grad}(\delta \bar{D})]$, one can rewrite the latter expression as

$$\begin{aligned} g_{\text{ext}} = & \int_B J^{-1} \mathbf{f}_0 \cdot \delta \mathbf{u} \, dv + \int_{\partial B_t} J^{-1} (\mathbf{F} \mathbf{S})^T [\delta \mathbf{u}] \cdot \mathbf{F}^T [\mathbf{n}] \, da + \\ & + \int_B (J^{-1} a_{0_e} \delta \bar{D} + J^{-1} \mathbf{b}_{0_e} \cdot \mathbf{F}^T [\text{grad}(\delta \bar{D})]) \, dv + \int_{\partial B_c} J^{-1} \|\mathbf{F}^{-T} [\mathbf{n}_0]\|^{-1} a_{0_c} \delta \bar{D} \, da \end{aligned}$$

Finally, by considering that $J^{-1} (\mathbf{F} \mathbf{S})^T [\delta \mathbf{u}] \cdot \mathbf{F}^T [\mathbf{n}] = (J^{-1} \mathbf{F} \mathbf{S} \mathbf{F}^T) [\mathbf{n}] \cdot \delta \mathbf{u} = \boldsymbol{\sigma} [\mathbf{n}] \cdot \delta \mathbf{u}$ and $\boldsymbol{\sigma} [\mathbf{n}] = \mathbf{t}$ on ∂B_t as well as by introducing the abbreviations $a_e := J^{-1} a_{0_e}$, $a_c := J^{-1} \|\mathbf{F}^{-T} [\mathbf{n}_0]\|^{-1} a_{0_c}$, $\mathbf{b}_e := J^{-1} \mathbf{F} [\mathbf{b}_{0_e}]$ and $\mathbf{f} := J^{-1} \mathbf{f}_0$, one obtains

$$g_{\text{ext}} = \int_B \mathbf{f} \cdot \delta \mathbf{u} \, dv + \int_{\partial B_t} \mathbf{t} \cdot \delta \mathbf{u} \, da + \int_B (a_e \delta \bar{D} + \mathbf{b}_e \cdot \text{grad}(\delta \bar{D})) \, dv + \int_{\partial B_c} a_c \delta \bar{D} \, da$$

which is the external virtual work expression formulated in terms of quantities defined in the current configuration.

6.7.4

The three invariants of $\mathbf{C}_e$ are

$$I_{\mathbf{C}_e} := \text{tr}(\mathbf{C}_e), \quad II_{\mathbf{C}_e} := \frac{1}{2} (\text{tr}(\mathbf{C}_e)^2 - \text{tr}(\mathbf{C}_e^2)), \quad III_{\mathbf{C}_e} := \det(\mathbf{C}_e)$$

By using relation $\mathbf{C}_e = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}$ and well-known properties of the trace and determinant operators, it can be shown that

$$\begin{aligned}\text{tr}(\mathbf{C}_e) &= \text{tr}(\mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}) = \text{tr}(\mathbf{F}_p^{-1} \mathbf{F}_p^{-T} \mathbf{C}) = \text{tr}(\mathbf{C}_p^{-1} \mathbf{C}) \\ \text{tr}(\mathbf{C}_e^2) &= \text{tr}(\mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1} \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}) = \text{tr}(\mathbf{F}_p^{-1} \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1} \mathbf{F}_p^{-T} \mathbf{C}) = \text{tr}((\mathbf{C}_p^{-1} \mathbf{C})^2) \\ \det(\mathbf{C}_e) &= \det(\mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}) = \det(\mathbf{F}_p^{-1}) \det(\mathbf{F}_p^{-T}) \det(\mathbf{C}) = \det(\mathbf{C}_p^{-1} \mathbf{C})\end{aligned}$$

The above proves that the invariants of $\mathbf{C}_e$ can be expressed in terms of $\mathbf{C}$ and $\mathbf{C}_p$.

6.7.5

By considering the definition of the second Piola-Kirchhoff stress (6.18), the multiplicative split of the deformation gradient (6.5) and basic properties of the trace operator, the following transformation is obtained:

$$\begin{aligned}\mathbf{F}_p^T \tilde{\mathbf{M}}' \mathbf{F}_p &= \mathbf{F}_p^T \left(\tilde{\mathbf{M}} - \frac{1}{3} \text{tr}(\tilde{\mathbf{M}}) \mathbf{I} \right) \mathbf{F}_p \\ &= \mathbf{F}_p^T \tilde{\mathbf{M}} \mathbf{F}_p - \frac{1}{3} \text{tr}(\tilde{\mathbf{M}}) \mathbf{C}_p \\ &= \mathbf{F}_p^T 2 \mathbf{C}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p - \frac{1}{3} \text{tr} \left(2 \mathbf{C}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} \right) \mathbf{C}_p = \\ &= \mathbf{F}_p^T 2 \mathbf{F}_e^T \mathbf{F}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} (\mathbf{F}_p^{-T} \mathbf{F}_p^T) \mathbf{F}_p - \frac{1}{3} \text{tr} \left(2 \mathbf{F}_e^T \mathbf{F}_e \frac{\partial \psi_e}{\partial \mathbf{C}_e} \right) \mathbf{C}_p \\ &= \mathbf{F}^T \mathbf{F} 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-T} \mathbf{F}_p^T \mathbf{F}_p - \frac{1}{3} \text{tr} \left(\mathbf{F}^T \mathbf{F} 2 \mathbf{F}_p^{-1} \frac{\partial \psi_e}{\partial \mathbf{C}_e} \mathbf{F}_p^{-T} \right) \mathbf{C}_p \\ &= \mathbf{C} \tilde{\mathbf{S}} \mathbf{C}_p - \frac{1}{3} \text{tr}(\mathbf{C} \tilde{\mathbf{S}}) \mathbf{C}_p \\ &= (\mathbf{C} \tilde{\mathbf{S}})' \mathbf{C}_p\end{aligned}$$

Analogously, it can be shown that $\mathbf{F}_p^T \tilde{\chi}' \mathbf{F}_p = (\mathbf{C}_p \tilde{\mathbf{X}})' \mathbf{C}_p$ and $\mathbf{F}_{p_i}^T \tilde{\mathbf{M}}'_{\text{kin}} \mathbf{F}_{p_i} = (\mathbf{C}_p \tilde{\mathbf{X}})' \mathbf{C}_{p_i}$.

6.7.6

Using the relationship

$$\tilde{\mathbf{M}}' - \tilde{\chi}' = \mathbf{F}_p^{-T} \tilde{\mathbf{Y}}' \mathbf{C}_p \mathbf{F}_p^{-1} = \mathbf{F}_p^{-T} \tilde{\mathbf{Y}}' \mathbf{F}_p^T$$

as well as the properties of the scalar product and the trace operator, one can reformulate expression $\|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\|$ as:

$$\begin{aligned}
 \|\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}'\| &= \sqrt{(\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}') \cdot (\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}')} \\
 &= \sqrt{(\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}') \cdot (\tilde{\mathbf{M}}' - \tilde{\boldsymbol{\chi}}')^T} \\
 &= \sqrt{\text{tr}(\mathbf{F}_p^{-T} \tilde{\mathbf{Y}}' \mathbf{F}_p^T \mathbf{F}_p^{-T} \tilde{\mathbf{Y}}' \mathbf{F}_p^T)} \\
 &= \sqrt{\text{tr}(\tilde{\mathbf{Y}}' \tilde{\mathbf{Y}}')} \\
 &= \sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^T}
 \end{aligned}$$

6.7.7

The linearization of g in (6.65) about a known state $(\mathbf{u}^*, \bar{D}^*)$ can be written as

$$\begin{aligned}
 L_g(\Delta \mathbf{u}, \Delta \bar{D}, \delta \mathbf{u}) &\equiv g(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u}) \\
 &\quad + \mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] + \mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \bar{D}] \stackrel{!}{=} 0 \quad \forall \delta \mathbf{u}
 \end{aligned}$$

where the Gâteaux derivatives $\mathcal{D}g_u[\Delta \mathbf{u}]$ and $\mathcal{D}g_{\bar{D}}[\Delta \bar{D}]$ are defined as

$$\begin{aligned}
 \mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} g(\mathbf{u}^* + \epsilon \Delta \mathbf{u}, \bar{D}^*, \delta \mathbf{u}) \\
 \mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \bar{D}] &:= \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} g(\mathbf{u}^*, \bar{D}^* + \epsilon \Delta \bar{D}, \delta \mathbf{u})
 \end{aligned}$$

More precisely, the calculation of $\mathcal{D}g_u[\Delta \mathbf{u}]$ is carried out as

$$\begin{aligned}
\mathcal{D}g_u(\mathbf{u}^*, \bar{D}^*, \delta \mathbf{u})[\Delta \mathbf{u}] &= \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \left(\int_{B_0} ((\mathbf{F}(\epsilon) \mathbf{S}(\mathbf{E}(\mathbf{F}(\epsilon)), \bar{D}^*)) \cdot \text{Grad}(\delta \mathbf{u}) - \mathbf{f}_0 \cdot \delta \mathbf{u}) dV - \int_{\partial B_{0t}} \mathbf{t}_0 \cdot \delta \mathbf{u} dA \right) \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \int_{B_0} (\mathbf{F}(\epsilon) \mathbf{S}(\mathbf{E}(\mathbf{F}(\epsilon)), \bar{D}^*)) \cdot \text{Grad}(\delta \mathbf{u}) dV \\
&= \int_{B_0} \left(\frac{\partial \mathbf{F}}{\partial \epsilon} \mathbf{S}(\mathbf{E}(\mathbf{F}(\epsilon)), \bar{D}^*) + \mathbf{F}(\epsilon) \left(\frac{\partial \mathbf{S}}{\partial \mathbf{E}} \left[\frac{\partial \mathbf{E}}{\partial \mathbf{F}} \left[\frac{\partial \mathbf{F}}{\partial \epsilon} \right] \right] \right) \right) \bigg|_{\epsilon=0} \cdot \text{Grad}(\delta \mathbf{u}) dV \\
&= \int_{B_0} (\text{Grad}(\Delta \mathbf{u}) \underbrace{\mathbf{S}(\mathbf{E}(\mathbf{F}^*), \bar{D}^*)}_{:=\mathbf{S}^*}) \cdot \text{Grad}(\delta \mathbf{u}) dV + \\
&\quad + \int_{B_0} \mathbf{F}^* \left(\frac{\partial \mathbf{S}}{\partial \mathbf{E}} \left[\frac{1}{2} \underbrace{(\text{Grad}(\Delta \mathbf{u})^T \mathbf{F}^* + \mathbf{F}^{*T} \text{Grad}(\Delta \mathbf{u}))}_{:=\Delta \mathbf{E}^*} \right] \right) \cdot \text{Grad}(\delta \mathbf{u}) dV \\
&= \int_{B_0} (\text{Grad}(\Delta \mathbf{u}) \mathbf{S}^*) \cdot \text{Grad}(\delta \mathbf{u}) dV + \int_{B_0} \frac{\partial \mathbf{S}}{\partial \mathbf{E}} [\Delta \mathbf{E}^*] \cdot (\text{Grad}(\delta \mathbf{u})^T \mathbf{F}^*) dV \\
&= \int_{B_0} (\text{Grad}(\Delta \mathbf{u}) \mathbf{S}^*) \cdot \text{Grad}(\delta \mathbf{u}) dV + \\
&\quad + \int_{B_0} \frac{\partial \mathbf{S}}{\partial \mathbf{E}} [\Delta \mathbf{E}^*] \cdot \left(\frac{1}{2} \underbrace{(\text{Grad}(\delta \mathbf{u})^T \mathbf{F}^* + \mathbf{F}^{*T} \text{Grad}(\delta \mathbf{u}))}_{:=\delta \mathbf{E}^*} \right) dV \\
&= \int_{B_0} (\text{Grad}(\Delta \mathbf{u}) \mathbf{S}^*) \cdot \text{Grad}(\delta \mathbf{u}) dV + \int_{B_0} \frac{\partial \mathbf{S}}{\partial \mathbf{E}} [\Delta \mathbf{E}^*] \cdot \delta \mathbf{E}^* dV
\end{aligned}$$

with

$$\mathbf{F}(\epsilon) := \mathbf{I} + \text{Grad}(\mathbf{u}^* + \epsilon \Delta \mathbf{u}) = \mathbf{F}^* + \epsilon \text{Grad}(\Delta \mathbf{u})$$

Analogously, $\mathcal{D}g_{\bar{D}}[\Delta\bar{D}]$ is calculated as

$$\begin{aligned}
\mathcal{D}g_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta\mathbf{u})[\Delta\bar{D}] &= \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \left(\int_{B_0} (\mathbf{F}^* \mathbf{S}(\mathbf{F}^*, \bar{D}(\epsilon)) \cdot \text{Grad}(\delta\mathbf{u}) - \mathbf{f}_0 \cdot \delta\mathbf{u}) dV - \int_{B_{0t}} \mathbf{t}_0 \cdot \delta\mathbf{u} dA \right) \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \int_{B_0} (\mathbf{F}^* \mathbf{S}(\mathbf{F}^*, \bar{D}(\epsilon))) \cdot \text{Grad}(\delta\mathbf{u}) dV \\
&= \int_{B_0} \left(\mathbf{F}^* \frac{\partial \mathbf{S}}{\partial \bar{D}} \frac{\partial \bar{D}}{\partial \epsilon} \right) \bigg|_{\epsilon=0} \cdot \text{Grad}(\delta\mathbf{u}) dV \\
&= \int_{B_0} \left(\frac{\partial \mathbf{S}}{\partial \bar{D}} \Delta\bar{D} \right) \cdot \left(\text{Grad}(\delta\mathbf{u})^T \mathbf{F}^* \right) dV \\
&= \int_{B_0} \left(\frac{\partial \mathbf{S}}{\partial \bar{D}} \Delta\bar{D} \right) \cdot \underbrace{\left(\frac{1}{2} \left(\text{Grad}(\delta\mathbf{u})^T \mathbf{F}^* + \mathbf{F}^{*T} \text{Grad}(\delta\mathbf{u}) \right) \right)}_{:=\delta\mathbf{E}^*} dV \\
&= \int_{B_0} \left(\frac{\partial \mathbf{S}}{\partial \bar{D}} \Delta\bar{D} \right) \cdot \delta\mathbf{E}^* dV
\end{aligned}$$

where

$$\bar{D}(\epsilon) := \bar{D}^* + \epsilon \Delta\bar{D}$$

In the same manner, the linearization of h in (6.66) about a known state $(\mathbf{u}^*, \bar{D}^*)$ is carried out as

$$\begin{aligned}
L_h(\Delta\mathbf{u}, \Delta\bar{D}, \delta\bar{D}) &\equiv h(\mathbf{u}^*, \bar{D}^*, \delta\bar{D}) \\
&\quad + \mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta\bar{D})[\Delta\mathbf{u}] + \mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta\bar{D})[\Delta\bar{D}] \stackrel{!}{=} 0 \quad \forall \delta\bar{D}
\end{aligned}$$

with $\mathcal{D}h_u[\Delta\mathbf{u}]$ and $\mathcal{D}h_{\bar{D}}[\Delta\bar{D}]$ denoting the Gâteaux derivatives

$$\begin{aligned}
\mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta\bar{D})[\Delta\mathbf{u}] &:= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} h(\mathbf{u}^* + \epsilon \Delta\mathbf{u}, \bar{D}^*, \delta\bar{D}) \\
\mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta\bar{D})[\Delta\bar{D}] &:= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} h(\mathbf{u}^*, \bar{D}^* + \epsilon \Delta\bar{D}, \delta\bar{D})
\end{aligned}$$

In more detail, $\mathcal{D}h_u[\Delta \mathbf{u}]$ is computed as

$$\begin{aligned}
\mathcal{D}h_u(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \mathbf{u}] &= \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \left(\int_{B_0} (H(D(\mathbf{E}(\mathbf{F}(\epsilon)), \bar{D}^*) - \bar{D}^*) \delta \bar{D} - A \text{Grad}(\bar{D}^*) \cdot \text{Grad}(\delta \bar{D})) dV \right) \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \int_{B_0} H D(\mathbf{E}(\mathbf{F}(\epsilon)), \bar{D}^*) \delta \bar{D} dV \\
&= \int_{B_0} H \left(\frac{\partial D}{\partial \mathbf{E}} \cdot \frac{\partial \mathbf{E}}{\partial \mathbf{F}} \left[\frac{\partial \mathbf{F}}{\partial \epsilon} \right] \right) \bigg|_{\epsilon=0} \delta \bar{D} dV \\
&= \int_{B_0} H \frac{\partial D}{\partial \mathbf{E}} \cdot \left(\underbrace{\frac{1}{2} (\text{Grad}(\Delta \mathbf{u})^T \mathbf{F}^* + \mathbf{F}^{*T} \text{Grad}(\Delta \mathbf{u}))}_{:= \Delta \mathbf{E}^*} \right) \delta \bar{D} dV \\
&= \int_{B_0} H \left(\frac{\partial D}{\partial \mathbf{E}} \cdot \Delta \mathbf{E}^* \right) \delta \bar{D} dV
\end{aligned}$$

and $\mathcal{D}h_{\bar{D}}[\Delta \bar{D}]$ as

$$\begin{aligned}
\mathcal{D}h_{\bar{D}}(\mathbf{u}^*, \bar{D}^*, \delta \bar{D})[\Delta \bar{D}] &= \\
&= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \left(\int_{B_0} (H(D(\mathbf{E}(\mathbf{F}^*), \bar{D}(\epsilon)) - \bar{D}(\epsilon)) \delta \bar{D} - A \text{Grad}(\bar{D}(\epsilon)) \cdot \text{Grad}(\delta \bar{D})) dV \right) \\
&= \int_{B_0} \left(H \left(\frac{\partial D}{\partial \bar{D}} \frac{\partial \bar{D}}{\partial \epsilon} - \frac{\partial \bar{D}}{\partial \epsilon} \right) \bigg|_{\epsilon=0} \delta \bar{D} - A \frac{\partial \text{Grad}(\bar{D})}{\partial \epsilon} \bigg|_{\epsilon=0} \cdot \text{Grad}(\delta \bar{D}) \right) dV \\
&= \int_{B_0} \left(H \left(\frac{\partial D}{\partial \bar{D}} \Delta \bar{D} - \Delta \bar{D} \right) \delta \bar{D} - A \text{Grad}(\Delta \bar{D}) \cdot \text{Grad}(\delta \bar{D}) \right) dV \\
&= \int_{B_0} \left(H \Delta \bar{D} \left(\frac{\partial D}{\partial \bar{D}} - 1 \right) \delta \bar{D} - A \text{Grad}(\Delta \bar{D}) \cdot \text{Grad}(\delta \bar{D}) \right) dV
\end{aligned}$$

6.7.8

The equations in case of an elastoplastic-damage step which need to be linearized at the integration point level are repeated here for convenience:

$$\begin{aligned} \mathbf{r}_1 &= -\mathbf{C}_{p_n}^{-1} + \mathbf{U}_p^{-1} \exp(\Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) \mathbf{U}_p^{-1} = \mathbf{0} \\ \mathbf{r}_2 &= -\mathbf{C}_{p_{in}}^{-1} + \mathbf{U}_{p_i}^{-1} \exp(\Delta\lambda_p \mathbf{U}_{p_i}^{-1} \mathbf{f}_{\text{kin}} \mathbf{U}_{p_i}^{-1}) \mathbf{U}_{p_i}^{-1} = \mathbf{0} \\ r_3 &= \Phi_p = 0 \\ r_4 &= \Phi_d = 0 \end{aligned}$$

With the help of the abbreviations

$$\bar{\mathbf{Z}} := \Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}, \quad \mathbf{Z} := \exp(\Delta\lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1}) = \exp \bar{\mathbf{Z}}$$

the first residual can be rewritten as

$$\mathbf{r}_1 = -\mathbf{C}_{p_n}^{-1} + \mathbf{U}_p^{-1} \mathbf{Z} \mathbf{U}_p^{-1} = \mathbf{0}$$

Linearizing the latter equation and using the product rule of differentiation leads to

$$\Delta \mathbf{r}_1 = \underbrace{\Delta \mathbf{U}_p^{-1} \mathbf{Z} \mathbf{U}_p^{-1} + \mathbf{U}_p^{-1} \mathbf{Z} \Delta \mathbf{U}_p^{-1}}_{\mathcal{D}[\Delta \mathbf{U}_p^{-1}]} + \mathbf{U}_p^{-1} \Delta \mathbf{Z} \mathbf{U}_p^{-1}$$

where the fact has been exploited that $\Delta \mathbf{C}_{p_n}^{-1}$ vanishes and where the fourth-order tensor $\mathcal{D}$ is given in index notation as

$$\mathcal{D}_{ijkl} = \frac{1}{2} (\delta_{ik} Z_{ln} + \delta_{il} Z_{kn}) (U_p^{-1})_{nj} + \frac{1}{2} (\delta_{jl} Z_{mk} + \delta_{jk} Z_{ml}) (U_p^{-1})_{im}$$

Furthermore, under consideration of the spectral decomposition of the second-order tensor $\mathbf{Z}$, its derivative can be computed as

$$\Delta \mathbf{Z} = \Delta \left(\sum_{A=1}^3 \exp(\bar{Z}_{(A)}) \mathbf{n}_{(A)} \otimes \mathbf{n}_{(A)} \right) = \underbrace{\frac{\partial \mathbf{Z}}{\partial \bar{\mathbf{Z}}}}_{\mathcal{C}} [\Delta \bar{\mathbf{Z}}]$$

Here, $\bar{Z}_{(i)}$ and $\mathbf{n}_{(i)}$ ($i = 1, 2, 3$) denote the eigenvalues and eigenvectors of $\mathbf{Z}$, respectively. The fourth-order tensor $\mathcal{C}$ can be represented as (see, e. g., Ogden [1984])

$$\begin{aligned} \mathcal{C} = & \sum_{A=1}^3 \exp(\bar{Z}_{(A)}) \mathbf{n}_{(A)} \otimes \mathbf{n}_{(A)} \otimes \mathbf{n}_{(A)} \otimes \mathbf{n}_{(A)} \\ & + \sum_{A,B=1 \atop (A \neq B)}^3 \frac{1}{2} \frac{\exp(\bar{Z}_{(B)}) - \exp(\bar{Z}_{(A)})}{\bar{Z}_{(B)} - \bar{Z}_{(A)}} (\mathbf{n}_{(A)} \otimes \mathbf{n}_{(B)} \otimes \mathbf{n}_{(A)} \otimes \mathbf{n}_{(B)} \\ & \quad + \mathbf{n}_{(A)} \otimes \mathbf{n}_{(B)} \otimes \mathbf{n}_{(B)} \otimes \mathbf{n}_{(A)}) \end{aligned}$$

By introducing the abbreviations

$$\mathbf{f}_n := \mathbf{Y}' \mathbf{C}_p, \quad f_d := \sqrt{\mathbf{Y}' \cdot (\mathbf{Y}')^T}$$

the second-order tensor $\mathbf{f}$ can be written as

$$\mathbf{f} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\tilde{\mathbf{Y}}' \mathbf{C}_p}{\sqrt{\tilde{\mathbf{Y}}' \cdot (\tilde{\mathbf{Y}}')^T}} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\mathbf{Y}' \mathbf{C}_p}{\sqrt{\mathbf{Y}' \cdot (\mathbf{Y}')^T}} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\mathbf{f}_n}{f_d}$$

which in turn can be used to express $\bar{\mathbf{Z}}$ and its derivative $\Delta \bar{\mathbf{Z}}$ in the following way:

$$\begin{aligned} \bar{\mathbf{Z}} = & \Delta \lambda_p \mathbf{U}_p^{-1} \mathbf{f} \mathbf{U}_p^{-1} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\Delta \lambda_p}{f_d} \hat{\mathbf{Z}} \\ \Delta \bar{\mathbf{Z}} = & \underbrace{\left(2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\hat{\mathbf{Z}}}{f_d} \right) \Delta(\Delta \lambda_p)}_A + \underbrace{\left(2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\Delta \lambda_p}{f_d} \right) \Delta \hat{\mathbf{Z}}}_B + \\ & + \underbrace{\left(-2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{\Delta \lambda_p}{f_d^2} \right) \Delta f_d}_C + \underbrace{\left(-2 \frac{\sqrt{3/2}}{f_{\text{dam}}^2(D)} \frac{\Delta \lambda_p}{f_d} \frac{df_{\text{dam}}(D)}{dD} \bar{\mathbf{Z}} \right) \Delta(\Delta \lambda_d)}_D \end{aligned}$$

In the above, the definition $\hat{\mathbf{Z}} := \mathbf{U}_p^{-1} \mathbf{Y}' \mathbf{U}_p$ was utilized.

Now, the term $\mathbf{U}_p^{-1} \Delta \mathbf{Z} \mathbf{U}_p^{-1} = \mathbf{U}_p^{-1} \mathcal{C} [\Delta \bar{\mathbf{Z}}] \mathbf{U}_p^{-1}$ can be computed for the four summands above separately. A summary is given below without derivation:

A :

$$\mathbf{U}_p^{-1} (\mathcal{C} [\Delta \bar{\mathbf{Z}}]) \mathbf{U}_p^{-1} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{1}{f_d} \mathbf{U}_p^{-1} (\mathcal{C} [\hat{\mathbf{Z}}]) \mathbf{U}_p^{-1} \Delta(\Delta \lambda_p) = \mathbf{K} \Delta(\Delta \lambda_p)$$

$B :$

$$\begin{aligned} \mathbf{U}_p^{-1} (\mathcal{C} [\Delta \bar{\mathbf{Z}}]) \mathbf{U}_p^{-1} &= 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathcal{E}}_1 [\Delta \mathbf{U}_p^{-1}] \\ &\quad + 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathcal{E}}_2 [\Delta \mathbf{U}_{p_i}^{-1}] \\ &\quad + 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathcal{E}}_3 \Delta (\Delta \lambda_d) \end{aligned}$$

$C :$

$$\begin{aligned} \mathbf{U}_p^{-1} (\mathcal{C} [\Delta \bar{\mathbf{Z}}]) \mathbf{U}_p^{-1} &= \left(-\frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \otimes \mathcal{B}_1^T [(\mathbf{Y}')^T] \right) [\Delta \mathbf{U}_p^{-1}] \\ &\quad + \left(-\frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \otimes \mathcal{B}_2^T [(\mathbf{Y}')^T] \right) [\Delta \mathbf{U}_{p_i}^{-1}] \\ &\quad + \left(-\frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \left((\mathbf{Y}')^T \cdot \mathbf{B}_3 \right) \right) \Delta (\Delta \lambda_d) \end{aligned}$$

$D :$

$$\mathbf{U}_p^{-1} (\mathcal{C} [\Delta \bar{\mathbf{Z}}]) \mathbf{U}_p^{-1} = -\Delta \frac{\lambda_p}{f_{\text{dam}}(D)} \frac{df_{\text{dam}}(D)}{dD} \mathbf{K} \Delta (\Delta \lambda_d)$$

In the above, the following definitions were used:

$$\begin{aligned} (\mathcal{B}_1)_{ijkl} &:= \left(C_{im} \left(\frac{\partial \mathbf{S}}{\partial \mathbf{C}_p^{-1}} \right)_{mjno} - (C_p)_{im} \left(\frac{\partial \mathbf{S}}{\partial \mathbf{C}_p^{-1}} \right)_{mjno} \right) \frac{1}{2} \left(\delta_{nk} (U_p^{-1})_{lo} + \right. \\ &\quad \left. + \delta_{nl} (U_p^{-1})_{ko} + \delta_{ol} (U_p^{-1})_{nk} + \delta_{ok} (U_p^{-1})_{nl} \right) + \\ &\quad + \frac{1}{2} \left((U_p)_{ik} (C_p)_{ml} + (U_p)_{ml} (C_p)_{ik} + (U_p)_{il} (C_p)_{mk} + (U_p)_{mk} (C_p)_{il} \right) X_{mj} \\ (\mathcal{B}_2)_{ijkl} &:= - (C_p)_{im} \left(\frac{\partial \mathbf{X}}{\partial \mathbf{C}_{p_i}^{-1}} \right)_{mjno} \frac{1}{2} \left(\delta_{nk} (U_{p_i}^{-1})_{lo} + \delta_{nl} (U_{p_i}^{-1})_{ko} + \right. \\ &\quad \left. + \delta_{ol} (U_{p_i}^{-1})_{nk} + \delta_{ok} (U_{p_i}^{-1})_{nl} \right) \\ (B_3)_{ij} &:= C_{ik} \left(\frac{\partial \mathbf{S}}{\partial D} \right)_{kj} - (C_p)_{ik} \left(\frac{\partial \mathbf{X}}{\partial D} \right)_{kj} \\ (\hat{\mathcal{E}}_1)_{ijkl} &:= (U_p^{-1})_{im} \mathcal{C}_{mnop} \left((F_1)_{opkl} + E_{opkl} \right) (U_p^{-1})_{nj} \\ (\hat{\mathcal{E}}_2)_{ijkl} &:= (U_p^{-1})_{im} \mathcal{C}_{mnop} (F_2)_{opkl} (U_p^{-1})_{nj} \end{aligned}$$

$$\begin{aligned}
(\hat{E}_3)_{ij} &:= (U_p^{-1})_{ik} \mathcal{C}_{klmn} (F_3)_{mn} (U_p^{-1})_{lj} \\
(F_1)_{ijkl} &:= (U_p^{-1}) (U_p)_{nj} \mathcal{P}_{mnop} (\mathcal{B}_1)_{opkl} \\
(F_2)_{ijkl} &:= (U_p^{-1}) (U_p)_{nj} \mathcal{P}_{mnop} (\mathcal{B}_2)_{opkl} \\
(F_3)_{ij} &:= (U_p^{-1})_{im} (U_p)_{nj} \mathcal{P}_{mnop} (B_3)_{op} \\
E_{ijkl} &:= \frac{1}{2} (\delta_{ik} Y'_{lm} + \delta_{il} Y'_{km}) (U_p)_{mj} + \\
&\quad - \frac{1}{2} \left((U_p)_{nk} (U_p)_{jl} + (U_p)_{nl} (U_p)_{jk} \right) (U_p^{-1})_{im} Y'_{mn} \\
\mathcal{P}_{ijkl} &:= \delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{ij} \delta_{kl}
\end{aligned}$$

The fourth-order tensor $\mathcal{P}$ maps a general second-order tensor $\mathbf{A}$ onto its deviatoric part, i. e., $\mathbf{A}' = \mathbf{A} - \frac{1}{3} \text{tr}(\mathbf{A}) \mathbf{I} = \mathcal{P}[\mathbf{A}]$.

Residual $\mathbf{r}_2$ can be differentiated in an analogous manner. The resulting linearized system of equations reads:

$$\begin{aligned}
\Delta \mathbf{r}_1 &= \frac{\partial \mathbf{r}_1}{\partial \mathbf{U}_p^{-1}} [\Delta \mathbf{U}_p^{-1}] + \frac{\partial \mathbf{r}_1}{\partial \mathbf{U}_{pi}^{-1}} [\Delta \mathbf{U}_{pi}^{-1}] + \frac{\partial \mathbf{r}_1}{\partial \Delta \lambda_p} \Delta (\Delta \lambda_p) + \frac{\partial \mathbf{r}_1}{\partial \Delta \lambda_d} \Delta (\Delta \lambda_d) \\
\Delta \mathbf{r}_2 &= \frac{\partial \mathbf{r}_2}{\partial \mathbf{U}_p^{-1}} [\Delta \mathbf{U}_p^{-1}] + \frac{\partial \mathbf{r}_2}{\partial \mathbf{U}_{pi}^{-1}} [\Delta \mathbf{U}_{pi}^{-1}] + \frac{\partial \mathbf{r}_2}{\partial \Delta \lambda_p} \Delta (\Delta \lambda_p) + \frac{\partial \mathbf{r}_2}{\partial \Delta \lambda_d} \Delta (\Delta \lambda_d) \\
\Delta r_3 &= \frac{\partial r_3}{\partial \mathbf{U}_p^{-1}} \cdot \Delta \mathbf{U}_p^{-1} + \frac{\partial r_3}{\partial \mathbf{U}_{pi}^{-1}} \cdot \Delta \mathbf{U}_{pi}^{-1} + \frac{\partial r_3}{\partial \Delta \lambda_p} \Delta (\Delta \lambda_p) + \frac{\partial r_3}{\partial \Delta \lambda_d} \Delta (\Delta \lambda_d) \\
\Delta r_4 &= \frac{\partial r_4}{\partial \mathbf{U}_p^{-1}} \cdot \Delta \mathbf{U}_p^{-1} + \frac{\partial r_4}{\partial \mathbf{U}_{pi}^{-1}} \cdot \Delta \mathbf{U}_{pi}^{-1} + \frac{\partial r_4}{\partial \Delta \lambda_p} \Delta (\Delta \lambda_p) + \frac{\partial r_4}{\partial \Delta \lambda_d} \Delta (\Delta \lambda_d)
\end{aligned}$$

where the partial derivatives in the above can be computed as follows:

$$\begin{aligned}
\frac{\partial \mathbf{r}_1}{\partial \mathbf{U}_p^{-1}} &= \mathcal{D} + 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathcal{E}}_1 - \frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \otimes \mathcal{B}_1^T [(\mathbf{Y}')^T] \\
\frac{\partial \mathbf{r}_1}{\partial \mathbf{U}_{pi}^{-1}} &= 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathcal{E}}_2 - \frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \otimes \mathcal{B}_2^T [(\mathbf{Y}')^T] \\
\frac{\partial \mathbf{r}_1}{\partial \Delta \lambda_p} &= \mathbf{K} = 2 \frac{\sqrt{3/2}}{f_{\text{dam}}(D)} \frac{1}{f_d} \mathbf{U}_p^{-1} \left(\mathcal{C} [\hat{\mathbf{Z}}] \right) \mathbf{U}_p^{-1}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathbf{r}_1}{\partial \Delta \lambda_d} &= 2 \sqrt{\frac{3}{2}} \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{1}{f_d} \hat{\mathbf{E}}_3 - \frac{\Delta \lambda_p}{f_d^2} \mathbf{K} \left((\mathbf{Y}')^T \cdot \mathbf{B}_3 \right) - \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{df_{\text{dam}}(D)}{dD} \mathbf{K} \\
\frac{\partial \mathbf{r}_2}{\partial \mathbf{U}_p^{-1}} &= 2 \frac{b}{a} \frac{\Delta \lambda_p}{f_{\text{dam}}^2(D)} \hat{\boldsymbol{\varepsilon}}_{h_1} \\
\frac{\partial \mathbf{r}_2}{\partial \mathbf{U}_{p_i}^{-1}} &= \boldsymbol{\mathcal{D}}_h + 2 \frac{b}{a} \frac{\Delta \lambda_p}{f_{\text{dam}}^2(D)} \hat{\boldsymbol{\varepsilon}}_{h_2} \\
\frac{\partial \mathbf{r}_2}{\partial \Delta \lambda_p} &= \mathbf{K}_h = 2 \frac{b}{a} \frac{1}{f_{\text{dam}}^2(D)} \mathbf{U}_{p_i}^{-1} \left(\mathbf{C}_h \left[\hat{\mathbf{Z}}_h \right] \right) \mathbf{U}_{p_i}^{-1} \\
\frac{\partial \mathbf{r}_2}{\partial \Delta \lambda_d} &= 2 \frac{b}{a} \frac{\Delta \lambda_p}{f_{\text{dam}}^2(D)} \hat{\mathbf{E}}_{h_3} - 2 \frac{\Delta \lambda_p}{f_{\text{dam}}(D)} \frac{df_{\text{dam}}(D)}{dD} \mathbf{K}_h \\
\frac{\partial r_3}{\partial \mathbf{U}_p^{-1}} &= \sqrt{\frac{3}{2}} \frac{1}{f_{\text{dam}}(D)} \frac{1}{f_d} \mathcal{B}_1^T \left[(\mathbf{Y}')^T \right] \\
\frac{\partial r_3}{\partial \mathbf{U}_{p_i}^{-1}} &= \sqrt{\frac{3}{2}} \frac{1}{f_{\text{dam}}(D)} \frac{1}{f_d} \mathcal{B}_2^T \left[(\mathbf{Y}')^T \right] \\
\frac{\partial r_3}{\partial \Delta \lambda_p} &= -\frac{1}{f_{\text{dam}}(D)} e f \exp(-f \xi_p) \\
\frac{\partial r_3}{\partial \Delta \lambda_d} &= -\sqrt{\frac{3}{2}} \frac{df_{\text{dam}}(D)}{dD} \frac{f_d}{f_{\text{dam}}^2(D)} + \sqrt{\frac{3}{2}} \frac{1}{f_{\text{dam}}(D)} \frac{1}{f_d} \left((\mathbf{Y}')^T \cdot \mathbf{B}_3 \right) + \\
&\quad + \frac{\Delta \lambda_p}{f_{\text{dam}}^2(D)} \frac{df_{\text{dam}}(D)}{dD} e f \exp(-f \xi_p) \\
\frac{\partial r_4}{\partial \mathbf{U}_p^{-1}} &= -\frac{df_{\text{dam}}(D)}{dD} \left(\frac{\mu}{2} (\mathbf{C} \mathbf{U}_p^{-1} + \mathbf{U}_p^{-1} \mathbf{C} - 2 \mathbf{U}_p) + \frac{\Lambda}{4} \left(2 \frac{\det \mathbf{C}}{\det \mathbf{C}_p} \mathbf{U}_p - 2 \mathbf{U}_p \right) + \right. \\
&\quad \left. - \frac{a}{2} (\mathbf{U}_p \mathbf{C}_{p_i}^{-1} \mathbf{C}_p + \mathbf{C}_p \mathbf{C}_{p_i}^{-1} \mathbf{U}_p - 2 \mathbf{U}_p) \right) \\
\frac{\partial r_4}{\partial \mathbf{U}_{p_i}^{-1}} &= -\frac{df_{\text{dam}}(D)}{dD} \frac{a}{2} (\mathbf{C}_p \mathbf{U}_{p_i}^{-1} + \mathbf{U}_{p_i}^{-1} \mathbf{C}_p - 2 \mathbf{U}_{p_i}) \\
\frac{\partial r_4}{\partial \Delta \lambda_p} &= -\frac{df_{\text{dam}}(D)}{dD} \frac{1}{f_{\text{dam}}(D)} e (1 - \exp(-f \xi_p)) \\
\frac{\partial r_4}{\partial \Delta \lambda_d} &= -\frac{d^2 f_{\text{dam}}(D)}{dD^2} (\psi_e + \psi_p) - H + \frac{df_{\text{dam}}(D)}{dD} \left(\frac{\Delta \lambda_p}{f_{\text{dam}}^2(D)} \frac{df_{\text{dam}}(D)}{dD} e (1 - \exp(-f \xi_p)) \right)
\end{aligned}$$

The quantities $\mathcal{C}_h$, $\mathcal{D}_h$, $\hat{\mathcal{E}}_{h_1}$, $\hat{\mathcal{E}}_{h_2}$ and $\hat{\mathbf{Z}}_h$, resulting from the linearization of $\mathbf{r}_2$, can be derived analogously to the quantities $\mathcal{C}$, $\mathcal{D}$, $\hat{\mathcal{E}}_1$, $\hat{\mathcal{E}}_2$ and $\hat{\mathbf{Z}}$ which showed up during the linearization of $\mathbf{r}_1$.

6.7.9

After a somewhat lengthy calculation, the corresponding expressions in (6.97) - (6.98) are obtained as

$$\begin{aligned}\mathcal{A}_p &= \mathcal{S}_{1p} - \mathbf{S}_{1\Delta\lambda_d} \otimes (S_{4\Delta\lambda_d})^{-1} \mathbf{S}_{4p} \\ \mathcal{A}_c &= \mathcal{S}_{1c} - \mathbf{S}_{1\Delta\lambda_d} \otimes (S_{4\Delta\lambda_d})^{-1} \mathbf{S}_{4c} \\ \mathbf{A}_{\bar{D}} &= \mathbf{S}_{1\bar{D}} - \mathbf{S}_{1\Delta\lambda_d} (S_{4\Delta\lambda_d})^{-1} \mathbf{S}_{4\bar{D}} \\ \mathbf{B}_c &= \mathbf{S}_{4c} - (\mathcal{S}_{1p}^{-1} : \mathcal{S}_{1c})^T [\mathbf{S}_{4p}] \\ B_{\Delta\lambda_d} &= S_{4\Delta\lambda_d} - \mathbf{S}_{4p} \cdot \mathcal{S}_{1p}^{-1} [\mathbf{S}_{1\Delta\lambda_d}] \\ B_{\bar{D}} &= S_{4\bar{D}} - \mathbf{S}_{4p} \cdot \mathcal{S}_{1p}^{-1} [\mathbf{S}_{1\bar{D}}]\end{aligned}$$

in which the fourth-order tensors $\mathcal{S}_{1p}$, $\mathcal{S}_{1c}$, second-order tensors $\mathbf{S}_{1\Delta\lambda_d}$, $\mathbf{S}_{4p}$, $\mathbf{S}_{4c}$, $\mathbf{S}_{1\bar{D}}$ and scalars $S_{4\Delta\lambda_d}$, $S_{4\bar{D}}$ are given by

$$\begin{aligned}\mathcal{S}_{1p} &= \mathcal{T}_{1p} - \mathcal{T}_{1p_i} : \mathcal{T}_{2p_i}^{-1} : \mathcal{T}_{2p} \\ \mathcal{S}_{1c} &= \mathcal{T}_{1c} - \mathcal{T}_{1p_i} : \mathcal{T}_{2p_i}^{-1} : \mathcal{T}_{2c} \\ \mathbf{S}_{1\Delta\lambda_d} &= \mathbf{T}_{1\Delta\lambda_d} - (\mathcal{T}_{1p_i} : \mathcal{T}_{2p_i}^{-1}) [\mathbf{T}_{2\Delta\lambda_d}] \\ \mathbf{S}_{1\bar{D}} &= \mathbf{T}_{1\bar{D}} - (\mathcal{T}_{1p_i} : \mathcal{T}_{2p_i}^{-1}) [\mathbf{T}_{2\bar{D}}] \\ \mathbf{S}_{4p} &= \mathbf{T}_{4p} - (\mathcal{T}_{2p_i}^{-1} : \mathcal{T}_{2p})^T [\mathbf{T}_{4p_i}] \\ \mathbf{S}_{4c} &= \mathbf{T}_{4c} - (\mathcal{T}_{2p_i}^{-1} : \mathcal{T}_{2c})^T [\mathbf{T}_{4p_i}] \\ S_{4\Delta\lambda_d} &= T_{4\Delta\lambda_d} - \mathbf{T}_{4p_i} \cdot (\mathcal{T}_{2p_i}^{-1} [\mathbf{T}_{2\Delta\lambda_d}]) \\ S_{4\bar{D}} &= T_{4\bar{D}} - \mathbf{T}_{4p_i} \cdot (\mathcal{T}_{2p_i}^{-1} [\mathbf{T}_{2\bar{D}}])\end{aligned}$$

The latter quantities are themselves expressed in terms of the following derivatives of the residuals $\mathbf{r}_1$, $\mathbf{r}_2$, r_3 and r_4 as defined in (6.93):

$$\begin{aligned}\mathcal{T}_{1p} &= \frac{\partial \mathbf{r}_1}{\partial \mathbf{C}_p} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_p} \\ \mathcal{T}_{1p_i} &= \frac{\partial \mathbf{r}_1}{\partial \mathbf{C}_{p_i}} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_{p_i}}\end{aligned}$$

$$\begin{aligned}
\mathbf{T}_{1\Delta\lambda_d} &= \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_d} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \Delta\lambda_d} \\
\mathcal{T}_{1c} &= \frac{\partial \mathbf{r}_1}{\partial \mathbf{C}} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}} \\
\mathbf{T}_{1\bar{D}} &= \frac{\partial \mathbf{r}_1}{\partial \bar{D}} - \frac{\partial \mathbf{r}_1}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \bar{D}} \\
\mathcal{T}_{2p} &= \frac{\partial \mathbf{r}_2}{\partial \mathbf{C}_p} - \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_p} \\
\mathcal{T}_{2p_i} &= \frac{\partial \mathbf{r}_2}{\partial \mathbf{C}_{p_i}} - \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_{p_i}} \\
\mathbf{T}_{2\Delta\lambda_d} &= \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_d} - \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \Delta\lambda_d} \\
\mathcal{T}_{2c} &= \frac{\partial \mathbf{r}_2}{\partial \mathbf{C}} - \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_p} \otimes \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}} \\
\mathbf{T}_{2\bar{D}} &= \frac{\partial \mathbf{r}_2}{\partial \bar{D}} - \frac{\partial \mathbf{r}_2}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \bar{D}} \\
\mathbf{T}_{4p} &= \frac{\partial r_4}{\partial \mathbf{C}_p} - \frac{\partial r_4}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_p} \\
\mathbf{T}_{4p_i} &= \frac{\partial r_4}{\partial \mathbf{C}_{p_i}} - \frac{\partial r_4}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}_{p_i}} \\
T_{4\Delta\lambda_d} &= \frac{\partial r_4}{\partial \Delta\lambda_d} - \frac{\partial r_4}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \Delta\lambda_d} \\
\mathbf{T}_{4c} &= \frac{\partial r_4}{\partial \mathbf{C}} - \frac{\partial r_4}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \mathbf{C}} \\
T_{4\bar{D}} &= \frac{\partial r_4}{\partial \bar{D}} - \frac{\partial r_4}{\partial \Delta\lambda_p} \left(\frac{\partial r_3}{\partial \Delta\lambda_p} \right)^{-1} \frac{\partial r_3}{\partial \bar{D}}
\end{aligned}$$

7 | Conclusions and Outlook

The present cumulative dissertation was concerned with the theoretical development, algorithmic implementation and numerical investigation of novel material models that couple gradient damage with plasticity. From the very beginning, it was the goal to reach a high degree of flexibility with regard to the models' applicability which could be achieved by adopting a so-called 'two-surface' methodology. The latter means that damage and plasticity were modeled as truly distinct but coupled dissipative mechanisms in the formulation using separate yield and damage criteria as well as loading / unloading conditions, respectively. Due to that, the models are able to represent (quasi-)brittle-type, ductile-type or possibly a mixed-type damaging behavior of materials. Furthermore, nonlinear Armstrong-Frederick kinematic hardening, nonlinear Voce isotropic hardening as well as nonlinear damage hardening were incorporated into the models. In order to ease the development and study the behavior in a conceptually simpler context, the model formulation was firstly established for a geometrically linear framework, before it was at a later stage also extended to large deformations.

Since mainly two competing and inherently different formulations are available in the literature for geometrically nonlinear elastoplasticity (hypoelastic- and hyperelastic-based plasticity formulations), the dissertation began in Chaps. 2 and 3 with two of the author's (and his coauthors') published works that dealt with a preceding numerical comparison of both approaches in tests at the integration point level and in more application-oriented structural example problems. At that point, no damage material behavior was considered, yet. Instead, the intention was here to clarify whether one of the two plasticity formulations should generally be preferred, a question that was relevant for the later extension of the model formulation to the large deformation regime. By subjecting single finite elements to repeated closed-path deformation cycles (leading in consequence to a combined stretching and shearing of the respective element), it was demonstrated that, in principle, remarkable differences in the results can show up depending on the particular plasticity formulation used in the simulations. More precisely, while the hyperelastic-based plasticity model discussed in Chap. 3 (which relied upon an additional multiplicative split of the plastic part of the deformation gradient and a potential for kinematic hardening) led to physically reasonable results in all tests, the behav-

ior of the hypoelastic- and hyperelastic-based plasticity models considered in Chap. 2 (the latter of which made use of an objective rate equation for the backstress tensor of kinematic hardening) was strongly dependent upon the specific objective rate applied in the formulation, respectively. Only by using the self-consistent Eulerian model based on the logarithmic rate, spurious ‘elastic’ dissipation could be avoided. The reason for this was that the latter can actually be considered the equivalent rate form of a corresponding Hencky-type hyperelastic-based plasticity model and, thus, possesses an underlying potential structure which prevents the above mentioned issues. Interestingly enough, the application of the same models in finite element simulations of several complex forming processes delivered nearly congruent results which led to the conclusion that, in more application-oriented examples at the structural level, the particular modeling approach for large deformation elastoplasticity obviously plays a less significant role than originally expected. To some extent, this might also be understood as a justification for the still widespread usage of hypoelastic-based plasticity models in commercial finite element programs nowadays.

Chapter 4 represented a published work of the author (and his coauthors) in which the theory and numerics of the two-surface gradient-extended damage-plasticity model were thoroughly established. By considering at this point a geometrically linear, quasi-static and purely mechanical theory, the micromorphic approach was applied to achieve the gradient-enhancement of damage. The model’s development was further based on the effective stress concept and the assumption of a fictitious undamaged configuration of the material, defined such that the elastic and plastic energies of the damaged and undamaged configurations are equivalent to each other, respectively. A purely quadratic format of the Helmholtz free energy was chosen and thermodynamically consistent evolution equations of the strain-like internal variables were derived on the basis of two independent plastic and damage dissipation potentials in the formulation, respectively. The weak form of the underlying problem and its linearization were presented as well as the resulting finite element equation system. It was shown that the gradient-extension of the model in a natural way leads to an additional unknown at every node in the mesh (the nodal value of the micromorphic damage variable). Furthermore, the consistent computation of the tangent operators was discussed (necessary to preserve a quadratic rate of convergence in the Newton iteration at the global finite element level) as well as two algorithmic strategies to solve the discretized problem at the integration point level: a classical (local) active-set search strategy and an algorithm based on the so-called Fischer-Burmeister complementarity function. Subsequently, the model’s mesh regularizing properties were practically investigated and demonstrated in mesh convergence studies of several numerical 2D finite element example problems. In particular, it was shown that stable computations can be

performed with the model up to very high values of damage and that it can serve as a suitable tool to predict ‘cracks’ in a simple continuous sense.

Chapter 5 dealt with another of the author’s (and his coauthors’) published works in which a slightly different version of the two-surface gradient-extended damage-plasticity model was proposed. This time, the model was derived on the basis of the hypothesis of strain equivalence and an additional physically motivated split of the plastic strain into recoverable and irrecoverable parts was assumed to conveniently model nonlinear Armstrong-Frederick kinematic hardening. By considering a more complex format of the Helmholtz free energy instead, the necessity of using additional dissipation potentials to model nonlinear plastic and damage hardening could be avoided. Furthermore, a procedure was presented in this chapter to easily enforce stress constraints for general 3D gradient-extended material models at integration points of finite elements. The latter was finally utilized to perform a 2D plane stress example simulation with the model and mesh-independent results were obtained even for very high values of damage.

Finally, in Chap. 6 the preliminary version of an article of the author (and his coauthors) was presented which was concerned with the extension of the two-surface gradient-extended damage-plasticity model of Chap. 5 to the large deformation regime. As before, the model’s gradient-extension was achieved by using the micromorphic approach and a well-established and thermodynamically motivated hyperelastic-based plasticity framework for large deformations was utilized that was developed earlier by other members of the author’s workgroup. Based on an additional multiplicative decomposition of the plastic part of the deformation gradient, this framework allowed for a consistent incorporation of nonlinear Armstrong-Frederick kinematic hardening into the model and led to a formulation with only symmetric internal variables. Besides important aspects as, e. g., the linearization of the weak form of the underlying boundary value problem, the derivation of the resulting finite element equation system and a presentation of analytic expressions for the four consistent tangent operators, an exponential map algorithm was discussed to time-integrate the model’s evolution equations in such a way that both the plastic incompressibility and symmetry of the tensorial internal variables can be preserved during the course of computations. At the end of the study, the model was practically tested in two numerical example problems. Firstly, an integration point study was carried out to assess the meaning of the individual damage parameters in the formulation and it was shown that nonlinear damage hardening allows for a valuable higher flexibility and applicability of the model. Secondly, the mesh regularizing properties of the model were examined through a mesh convergence study of a 2D plain strain finite element test in which a tensile specimen with a slight geometric imperfection was subjected to tension. The convergence

of the results towards a solution with a finite amount of energy dissipation during the damaging process and a finite (and nearly similar) width of the damage zone for the finest mesh discretizations could be revealed.

The results that were obtained with the model for large deformations are promising. Once its practicability and functionality have been reconfirmed by further numerical tests (which are currently being conducted), the way will be clear for further improvements. Interesting points would be, for instance, the incorporation of damage and / or plastic anisotropy into the model. Damage and its evolution are by their very nature direction-dependent (i. e., anisotropic) phenomena. Thus, a more accurate model formulation should take account of that, e. g., by describing damage in terms of a higher-order tensor. In this regard, especially in the context of large deformations and a two-surface strategy, a formally correct and consistent modeling remains an intriguingly challenging task and further research in this field is beyond doubt necessary. The consideration of plastic anisotropy in the model formulation would be interesting, for example, for its usage in simulations of sheet metal forming processes in which the applied sheet metals usually show a pronounced directional dependence due to their manufacturing. It is supposed that such an extension of the large deformation model should be, in principle, ‘easily’ achievable since a suitable framework was already developed earlier by other members of the author’s workgroup. Another important issue concerns the consideration of special finite element technology. Due to the gradient-extension of the damage-plasticity models presented in this dissertation, it was necessary to perform the simulations using a self-developed user element in the academic finite element software FEAP, which was, for simplicity, based on standard interpolations for the unknown displacements and micromorphic damage variable, respectively. However, it is actually well-known that the usage of standard finite elements in the context of simulations with volume-preserving deformations (as was the case, for instance, in the numerical problem of Chap. 6 in which large deviatoric plastic strains of the considered structure occurred) can lead to volumetric locking. It seems therefore scientifically interesting to investigate the influence of suitable finite element technology, as, e. g., reduced integration with hourglass stabilization, on the mesh convergence behavior, which should additionally lead to an increased computational efficiency since the complex material model would then need to be evaluated in a reduced number of integration points. Finally, the incorporation of a separate internal length scale for plasticity (via an additional gradient term) could be a valuable improvement of the model. In this way, one could not only take plastic size effects into account but one could also ensure, for example, that damage occurs (and remains) within a developing plastic zone, which might physically and numerically be plausible in certain situations, as recent studies in the literature have revealed.

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