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Solution of Elastoplastic Problems based on Moreau-Yosida Theorem

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Abstract

The quasi-static problem of elastoplasticity with isotropic hardening is considered, with particular emphasis on its numerical solution by means of a Newton-like method. The smoothness properties necessary for such method can be ensured by Moreau-Yosida's theorem. After time discretization, the classical formulation of the elastoplastic problem is transformed to a minimization problem. The convex minimization functional depends on the displacement smoothly and on the plastic part of the strain non-smoothly. The minimization problem implicitly defines the plastic part of the strain as a function depending on the total strain tensor. Furthermore, this function may be calculated analytically. That way, the minimization problem depends on the displacement only. The Moreau-Yosida theorem, well-known in convex analysis, states that the minimization functional is smooth and also provides the Fréchet derivative of the functional. Hence, a method of the field of smooth optimization may be applied. After discretization in space, a Newton-like method is used to solve the discrete minimization problem. This method requires the Hesse matrix of the discrete minimization functional, which may be calculated in all material points apart from the elastoplastic interface. Numerical experiments in two dimensions show super-linear convergence of the Newton-like method. From the moment that elastic and plastic zones freeze, even quadratic convergence can be observed.

Zusammenfassung

Betrachtet wird das quasistatische Problem in der Elastoplastizität, und insbesondere dessen numerische Lösung mittels eines Newton-ähnlichen Verfahrens. Die dafür benötigten Glattheitseigenschaften können durch den Satz von Moreau-Yosida gewährleistet werden. Nach einer Zeitdiskretisierung wird die klassische Formulierung des Problems in ein Minimierungsproblem übergeführt. Das konvexe Minimierungsfunktional ist zwar differenzierbar bezüglich der Verschiebung, aber nicht bezüglich des plastischen Anteils des Verzerrungstensors. Durch das Minimierungsproblem wird aber der plastische Anteil des Verzerrungstensors implizit als Funktion nach dem Verzerrungstensor definiert, sodass das Minimierungsproblem insgesamt nur mehr von der Verschiebung abhängt. Der Satz von Moreau-Yosida sagt aus, dass das Minimierungsfunktional glatt ist, und liefert ferner die Fréchet-Ableitung in expliziter Form. Aus diesem Grund kann nun ein Verfahren aus dem Gebiet der glatten Optimierung angewandt werden. Nach einer Diskretisierung des Raumes wird ein Newton-ähnliches Verfahren zur Lösung des Minimierungsproblems verwendet. Für dieses Verfahren wird die Hessematrix des diskreten Minimierungsfunktionals benötigt, welche in allen Punkten, die nicht am elastoplastischen Interface liegen, berechnet werden kann. Numerische Beispiele in zwei Dimensionen deuten auf superlineare Konvergenz hin. Sobald sich die Form der elastischen und plastischen Zonen nicht mehr verändert, kann sogar quadratische Konvergenz beobachtet werden.

Contents

Chapter 1

Preliminaries

1.1 Introduction

The aim of this thesis is to provide a new solver for elastoplastic problems with hardening. We will show, that the elastoplastic initial-boundary value problem can be formulated as a minimization of a functional depending on the displacement smoothly. Numerically this minimum may be found by means of a Newton-like method. The main contribution of this thesis will be to show, that the functional is Fréchet differentiable.

The classical formulation of the elastoplastic initial-boundary value problem with hardening consists of the well known equalities for the elastic problem plus an inequality, describing the coherence of the stress and the plastic part of the strain with respect to the hardening law. Existence and uniqueness of a solution for the variational formulation of elastoplasticity with hardening have been proofed, e.g. see [HR95, HR99]. Variational formulation and time discretization lead us to a one time-step problem as in [AC00]. This problem may also be equivalently formulated as a minimization problem in three variables, namely displacement, plastic part of the strain, and a hardening parameter.

We will show, that minimization with respect to the plastic part of the strain and the hardening parameter may be realized in an analytic way, such that finally a minimization problem in only one variable has to be solved numerically.

Analytical minimization with respect to the hardening parameter depends on which hardening law we use. In this thesis we focus on isotropic hardening only, allthough it can be shown, that such minimizers can be found for other hardening laws too (see e.g. [ACFK02]).

A fact of crucial importance is, that the minimizer of the plastic part of the strain can be calculated in an analytic way. It may be expressed explicitly as a function depending on the displacement. A proof and the explicit formula can be found e.g. in [AC00]. It turns out, that the minimizing function for the plastic part does not depend on the displacement explicitly, but on the (total) strain only. This fact will allow for application of Moreau-Yosida's theorem.

After finding the two minimizers with respect to the hardening parameter and the plastic part of the strain, a minimizing problem with respect to only one variable, namely the displacement, is left to solve. The main theoretical contribution of this thesis is to find that this functional is smooth and that the Fréchet derivative can be calculated explicitly. All this is obtained by means of the Moreau-Yosida theorem and the special structure of the problem which allows for the application of the theorem.

Typically, Moreau-Yosida's theorem is applied in the field of convex analysis, representing one possibility of regularizing a convex but not smooth function by adding a special regularizing term to the function (see e.g. [Mor65, Yos94]). In this thesis, the theorem is applied not to regularize, but to verify that the given minimization functional has already a regularized structure and hence it is smooth. Even the second derivative may be calculated for displacements, which are not satisfying the elastoplastic interface condition, but it is not continuous on the interface.

Numerical solution of the minimization problem with respect to the displacement u may be achieved by means of finding the root first derivative $De(u)$ of the minimizing functional $e(u)$ by a Newton-like method. For spacial discretization we use h-FEM with first order nodal ansatz functions for the displacement u and piecewise constant ansatz functions for the plastic part p of the strain ε. Discretization is made for the two dimensional case only. A Newton-like method is applied to solve the nonlinear but finite dimensional problem.

This thesis does not contain any theoretical results concerning the convergence analysis of the solvers. Any statements about the speed of the solvers or about convergence rates must, without any exceptions, be understood as a guess which arose by the observation of the numerical testing results. It is left to further work on this subject to verify those expectations by a rigorous analysis.

Numerical examples in two dimensions implemented in Matlab© are shown in Chapter 5. The Tables presented in that chapter report on the convergence of the solver. Test examples for the interesting perfect plastic case ($H = 0$) are presented as well (e.g., Problem *Plate with a hole*, which has also been tested in [ea02], serves as a benchmark problem in computational plasticity). Both the following two statements characterize the convergence behaviour of the solver:

- If the hardening parameter H is positive, the Newton-like method converges super-linearly and even quadratically as long as the elastoplastic interface has been detected properly.
- In the perfect plastic case ($H = 0$), the Newton-like method may oscillate and another techniques are required in order to obtain convergence (see Section 4.4).

The thesis is organized as follows:

- Section 1.2 in this chapter includes a short collection of just a few theoretical results of the field of convex analysis.
- Those results will be required in Chapter 2, where the elastic-plastic and variational models are presented. After discretization in time, a dual minimization problem is deduced.
- Chapter 3 represents the main contribution of this thesis, since herein it is shown that the minimization functional is in fact Fréchet differentiable.
- In Chapter 4 we accomplish discretization in space (2D only) and discuss a Newton-like method, the explicit formulae of the derivatives in discrete form respectively.
- Numerical results are presented in Chapter 5, where graphical output is shown and tables on the convergence behaviour of the Newton-like method are reported.

- A short review on the most important results and contents of this thesis is given in Chapter 6. Moreover, some aspects about further work on this subject are suggested.
- One can find a list summarizing the used notation in the appendix.

1.2 Results from Convex Analysis

In this section some definitions and results from the field of convex analysis are presented (see [HR95, Kos91] for more detailed information). Those will play an important role in Chapter 2. Let X be a normed vector space over $\mathbb{R}$, with topological dual X^*, and with action $\langle x^*, x\rangle \in \mathbb{R}$ for all $x^* \in X^*$ and $x \in X$.

The definitions of convex sets and functions are the very basics of convex analysis.

Definition 1 (convex set)**.** *Let Y be a subset of X. Y is called* convex *if*

$$\forall x, y \in Y \ \forall t \in (0,1): \quad (tx + (1-t)\, y) \in Y.$$

Definition 2 (convex function)**.** *Let Y be a convex subset of X. A function $f : Y \to \mathbb{R}$ is called* convex *if*

$$\forall x, y \in Y \ \forall t \in (0,1): \quad f(tx + (1-t)y) \leq t f(x) + (1-t)\, f(y).$$

Moreover, we call f strictly convex *if the inequality holds with $<$ for $x \neq y$.*

The following two definitions are especially important for the formulation of Prandtl Reußnormality law occurring in Section 2.1.

Definition 3 (normal cone)**.** *Let Y be a convex subset of X and $x \in Y$. The set*

$$N_Y(x) := \{x^* \in X^* \ \mid \ \forall y \in Y : \ \langle x^*, y - x\rangle \leq 0\}$$

is called normal cone of Y in x.

Definition 4 (subdifferential)**.** *Let f be a convex function on X. For any $x \in X$ the* sub-differential $\partial f(x)$ *of x is the possibly empty subset of X^* defined by*

$$\partial f(x) = \{x^* \in X^* : \langle x^*, y - x\rangle \leq f(y) - f(x) \quad \forall y \in X\}.$$

There exist two dual classical formulations of the elastoplastic problem. One of them makes use of *conjugate* functions, which are defined as follows:

Definition 5 (conjugate function)**.** *For a function* $f : X \to [-\infty, \infty]$ *we define the* conjugate function $f^* : X^* \to [-\infty, \infty]$ *by*

$$f^*(x^*) = \sup_{x \in X}(\langle x^*, x\rangle - f(x)).$$

Theorem 1 will be important for the formulation of the dual classical formulation of elastoplasticity in Section 2.1. Therefore, the properties *lower semi-continuous* and *proper* are required.

Definition 6 (lower semicontinuity)**.** *A function* $f : X \to [-\infty, +\infty]$ *is called* lower semi-continuous *if*

$$(x_n)_{n\in\mathbb{N}} \to x \;\Rightarrow\; \liminf_{n\to\infty} f(x_n) \geq f(x).$$

Definition 7 (proper function)**.** *A function* $f : X \to [-\infty, +\infty]$ *is called* proper *if, first, there exists a point* $x \in X$ *such that* $f(x) < \infty$ *and, second,* $f(x) > -\infty$ *for all* $x \in X$*.*

Theorem 1. *Let* $f : X \to [-\infty, \infty]$ *be a proper, convex, lower semi-continuous function. Then*

$$x^* \in \partial f(x) \Leftrightarrow x \in \partial f^*(x^*).$$

Proof. See [Kos91]. □

Chapter 2

Mathematical Modelling

Let $d \in \mathbb{N}$ be the space dimension (let us consider, that typically $d \in \{2, 3\}$), $\Omega \in \mathbb{R}^d$ be an open domain with a Lipschitz-continuous boundary, i.e. $\Gamma := \partial\Omega \in C^{0,1}$. Further let Γ be split into two distinct parts Γ_D (*Dirichlet boundary*) and Γ_N (*Neumann boundary*), such that $\Gamma_D \cup \Gamma_N = \Gamma$. The set Θ be some time interval, and $\mathbb{R}^+ := \{x \in \mathbb{R} \mid x > 0\}$. The *matrix-scalar-product* $:$ is defined for two equal size matrices $A = (a_{ij})_{ij}$ and $B = (b_{ij})_{ij}$ as $A : B = \sum_{ij} a_{ij} b_{ij}$. The *Frobenius-norm* of matrix A reads $\|A\|_F := \sqrt{A : A}$. Let I denote the (square) identity matrix. The *trace* and the *deviator* of a matrix $A \in \mathbb{R}^{d \times d}$ are defined by $\operatorname{tr} A := A : I$ and $\operatorname{dev} A := A - \frac{\operatorname{tr} A}{d} I$.

2.1 Classical Formulation of Elastoplasticity

The equilibrium of forces reads

$$-\operatorname{div}(\sigma) = f \quad \text{in } \Omega \,, \tag{2.1}$$

where σ denotes the stress tensor and f describes volume forces acting in each material point $x \in \Omega$. The (linearized) strain ε describes the local deformation defined as

$$\varepsilon(u) := \frac{1}{2}\left(\nabla u + (\nabla u)^T\right), \tag{2.2}$$

where u denotes the body displacement. The plastic part of the strain is denoted by p. We assume the total strain ε to be the sum over its plastic and elastic part, such that the elastic part of the strain can be expressed by $(\varepsilon - p)$. The relation between stress and strain is given by Hook's law

$$\sigma = \mathbb{C}\,(\varepsilon - p)\,, \tag{2.3}$$

where the fourth-order *elasticity tensor* $\mathbb{C} \in \mathbb{R}^{d\times d}_{d\times d}$ is defined by $\mathbb{C}_{ijkl} := \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. Here, $\lambda, \mu \in \mathbb{R}^+$ denote the *Lamé-constants*, and δ_{ij} denotes the *Kronecker-symbol*. As an alternative, one uses another material parameters *Young's modulus* $E = \mu\frac{3\lambda+2\mu}{\lambda+\mu}$ and the *Poisson ratio* $\nu = \frac{\lambda}{2(\lambda+\mu)}$. Notice, that there also hold $\lambda = \frac{E\nu}{(1-2\nu)(1+\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$. Further we assume the initial conditions

$$\begin{array}{rcl} u(x,0) & = & 0 \\ \sigma(x,0) & = & 0 \end{array} \quad \text{on } \Omega, \tag{2.4}$$

and boundary conditions

$$u = u_D \qquad \text{on } \Gamma_D, \tag{2.5}$$

$$\sigma \cdot n = g \qquad \text{on } \Gamma_N, \tag{2.6}$$

where n denotes the exterior unit normal, u_D denotes a prescribed displacement and g denotes a prescribed surface tension.

Perfect elastic behaviour of a body is given by the expressions (2.1) - (2.6) and $p \equiv 0$. In order to model plasticity we need another two restrictions, which incorporate the time development of p. We introduce the hardening parameter α. In case of isotropic hardening [ACFK02] there holds that α is scalar. The tuple (σ, α) is called *generalized stress*. A generalized stress is called *admissible*, if a *dissipation functional* φ with

$$\varphi(\sigma,\alpha) := \begin{cases} 0 & \text{if } \phi(\sigma,\alpha) \leq 0, \\ \infty & \text{if } \phi(\sigma,\alpha) > 0, \end{cases} \tag{2.7}$$

satisfies

$$\varphi(\sigma,\alpha) < \infty. \tag{2.8}$$

The function ϕ is convex and called the *yield function*. In case of isotropic hardening it is defined

$$\phi(\sigma,\alpha) := \begin{cases} \|\operatorname{dev}\sigma\|_F - \sigma_y(1 + H\alpha) & \text{if } \alpha \geq 0\,, \\ \infty & \text{if } \alpha < 0\,, \end{cases} \tag{2.9}$$

The material constants $\sigma_y > 0$ and $H > 0$ are called *yield stress* and *modulus of hardening*. All admissible generalized stresses are characterized by

$\phi(\sigma,\alpha) \le 0$. Thus, the hardening parameter α in $\varphi(\sigma,\alpha) < \infty$ controls the (convex) set of admissible stresses σ. Finally the Prandtl-Reuss normality law states, that for all generalized stresses (τ,β) there holds

$$\dot p : (\tau - \sigma) - \dot\alpha\,(\beta - \alpha) \;\le\; \varphi(\tau,\beta) - \varphi(\sigma,\alpha), \tag{2.10}$$

where $\dot p$ and $\dot\alpha$ denote the first time derivative of p and α.

Problem 1 (classical formulation). *Find (u,p,α) such that*

$$\begin{aligned}
-\operatorname{div}(\sigma) &= f \quad \text{in } \Omega,\\
\sigma &= \mathbb{C}\,(\varepsilon(u) - p)\,,\\
\varepsilon(u) &= \frac{1}{2}\left(\nabla u + (\nabla u)^T\right),\\
u(x,0) &= p(x,0) \;=\; 0 \quad \text{in } \Omega,\\
\sigma \cdot n &= g \quad \text{on } \Gamma_N,\\
u &= u_D \quad \text{on } \Gamma_D,\\
\varphi(\sigma,\alpha) &< \infty,\\
\dot p : (\tau - \sigma) - \dot\alpha\,(\beta - \alpha) &\le \varphi(\tau,\beta) - \varphi(\sigma,\alpha) \qquad (\forall \tau,\beta).
\end{aligned}$$

We will reformulate Problem 1 as a dual classical formulation. In order to do so, we apply results from Convex Analysis theory. Due to Theorem 1, inequality (2.10) may be transformed by means of the following equivalences:

$$\begin{aligned}
& \dot p : (\tau - \sigma) - \dot\alpha\,(\beta - \alpha) &\le\;& \varphi(\tau,\beta) - \varphi(\sigma,\alpha) \qquad (\forall \tau,\beta)\\
\Leftrightarrow\;& \langle(\dot p, -\dot\alpha), (\tau,\beta) - (\sigma,\alpha)\rangle &\le\;& \varphi(\tau,\beta) - \varphi(\sigma,\alpha) \qquad (\forall \tau,\beta)\\
\Leftrightarrow\;& (\dot p, -\dot\alpha) &\in\;& \partial\varphi(\sigma,\alpha)\\
\Leftrightarrow\;& (\sigma,\alpha) &\in\;& \partial\varphi^*(\dot p, -\dot\alpha)\\
\Leftrightarrow\;& \langle(\sigma,\alpha), (q,\beta) - (\dot p, -\dot\alpha)\rangle &\le\;& \varphi^*(q,\beta) - \varphi^*(\dot p, -\dot\alpha) \quad (\forall q,\beta)\\
\Leftrightarrow\;& \sigma : (q - \dot p) + \alpha\,(\beta + \dot\alpha) &\le\;& \varphi^*(q,\beta) - \varphi^*(\dot p, -\dot\alpha) \quad (\forall q,\beta).
\end{aligned}$$

Thus Problem 1 is equivalent to

Problem 2 (dual classical formulation). *Find (u,p,α), such that*

$$-\operatorname{div}(\sigma) = f \quad \text{in } \Omega, \tag{2.11}$$

$$\begin{aligned}
\sigma &= \mathbb{C}\,(\varepsilon(u) - p)\,,\\
\varepsilon(u) &= \frac{1}{2}\left(\nabla u + (\nabla u)^T\right),
\end{aligned}$$

$$u(x,0) = p(x,0) \;=\; 0 \quad \text{in } \Omega, \tag{2.12}$$

$$\begin{aligned}
\sigma \cdot n &= g \quad \text{on } \Gamma_N,\\
u &= u_D \quad \text{on } \Gamma_D,\\
\varphi(\sigma,\alpha) &< \infty,
\end{aligned}$$

$$\sigma : (q - \dot p) + \alpha\,(\beta + \dot\alpha) \le \varphi^*(q,\beta) - \varphi^*(\dot p, -\dot\alpha) \qquad (\forall q,\beta). \tag{2.13}$$

2.2 Variational Formulation of Elastoplasticity

Let $V := [H^1(\Omega)]^d$, $V_D := [H^1_D(\Omega)]^d$, $V_0 := [H^1_0(\Omega)]^d$, and $W := [L_2(\Omega)]^{d\times d}_{\mathrm{sym}} \times L_2(\Omega)$. We multiply (2.11) with test functions $v \in V_0$, integrate (2.11) and (2.13) over Ω, partial integrate (2.11), and obtain a variational problem

Problem 3 (Variational formulation)**.** *Find $(u, p, \alpha) \in V_D \times W$, such that for all $(v, q, \beta) \in V_0 \times W$ there hold*

$$\int_\Omega \mathbb{C}\left(\varepsilon(u) - p\right) : \varepsilon(v)\,\mathrm{d}x = \int_\Omega f \cdot v\,\mathrm{d}x + \int_{\Gamma_N} g \cdot v\,\mathrm{d}S(x)$$

and

$$\int_\Omega \mathbb{C}\left(\varepsilon(u) - p\right) : (q - \dot{p}) + \alpha\left(\beta + \dot{\alpha}\right)\,\mathrm{d}x \leq \int_\Omega \varphi^*(q,\beta) - \varphi^*(\dot{p}, -\dot{\alpha})\,\mathrm{d}x.$$

We discretize in time by backward Euler with the discretization parameter k, precisely by the substitution of

$$u = u_1,\ p = p_1,\ \alpha = \alpha_1,\ \dot{p} = \frac{p_1 - p_0}{k},\ \dot{\alpha} = \frac{\alpha_1 - \alpha_0}{k},$$

where the initial value α_0 has to satisfy $\varphi(\cdot, \alpha_0) < \infty$, such that due to the definition of φ and ϕ there must hold $\alpha_0 \geq 0$. We obtain a one time-step problem

Problem 4 (One time-step)**.** *Find $(u_1, p_1, \alpha_1) \in V_D \times W$, such that for all $(v, q, \beta) \in V_0 \times W$ there holds*

$$\int_\Omega \mathbb{C}\left(\varepsilon(u_1) - p_1\right) : \varepsilon(v)\,\mathrm{d}x = \int_\Omega f \cdot v\,\mathrm{d}x + \int_{\Gamma_N} g \cdot v\,\mathrm{d}S(x),$$

and

$$\int_\Omega \left[\mathbb{C}\left(\varepsilon(u_1) - p_1\right) : (kq - p_1 + p_0) + \alpha_1\left(k\beta + \alpha_1 - \alpha_0\right)\right]\,\mathrm{d}x$$
$$\leq k\int_\Omega \varphi^*(q,\beta)\,\mathrm{d}x - k\int_\Omega \varphi^*(\frac{p_1 - p_0}{k}, \frac{\alpha_0 - \alpha_1}{k})\,\mathrm{d}x.$$

Problem 4 can be expressed in a more abstract way. Therefore, let $x_1 \in V$, $y_1 \in V$, $(x_2, x_3) \in W$, $(y_2, y_3) \in W$, $X := (x_1, x_2, x_3)$ and $Y := (y_1, y_2, y_3)$. Further let

$$\begin{aligned}
a_1(X,Y) &:= \int_\Omega \mathbb{C}\,(\varepsilon(x_1) - x_2) : \varepsilon(y_1)\, \mathrm{d}x, \\
a_2(X,Y) &:= \int_\Omega \left[x_3 y_3 - \mathbb{C}\,(\varepsilon(x_1) - x_2) : y_2\right] \mathrm{d}x, \\
a(X,Y) &:= a_1(X,Y) + a_2(X,Y), &(2.14)\\
L(X) &:= \int_\Omega f \cdot x_1 \,\mathrm{d}x + \int_{\Gamma_N} g \cdot x_1 \,\mathrm{d}S(x), &(2.15)\\
\Psi(X) &:= k \int_\Omega \varphi^*(\frac{x_2 - p_0}{k}, \frac{\alpha_0 - x_3}{k})\, \mathrm{d}x. &(2.16)
\end{aligned}$$

Notice, that $a(X,Y) = \int_\Omega \mathbb{C}\,(\varepsilon(x_1) - x_2) : (\varepsilon(y_1) - y_2) + x_3 y_3 \,\mathrm{d}x$ is a symmetric, positive definite bi-linear-form. Further L is linear and Ψ is convex in X. With the special choice of $x_1 := u_1$, $x_2 := p_1$, $x_3 := \alpha_1$, $y_1 := u_1 - v$, $y_2 := p_0 + kq$ and $y_3 := \alpha_0 - k\beta$ Problem 4 reads

Problem 5. *Find $X \in V_D \times W$, such that for all $Y \in V_D \times W$ there holds:*

$$\begin{aligned}
a_1(X, X - Y) &= L(X - Y), &(2.17)\\
a_2(X, X - Y) &\leq \Psi(Y) - \Psi(X). &(2.18)
\end{aligned}$$

Summation of (2.17) and (2.18) leads to

Problem 6. *Find $X \in V_D \times W$, such that for all $Y \in V_D \times W$ there holds:*

$$a(X, X - Y) \leq L(X - Y) + \Psi(Y) - \Psi(X). \tag{2.19}$$

Lemma 1. *Problems 5 and 6 are equivalent.*

Proof. Problem 5 $\Rightarrow$ Problem 6: trivial by adding (2.17) and (2.18).
Problem 6 $\Rightarrow$ Problem 5: We have to show that if X solves (2.19), it also solves (2.17) and (2.18). Let us first show that X solves (2.18). Let $X := (x_1, x_2, x_3)$ solve (2.19) for all $Y = (y_1, y_2, y_3)$. Particularly, for the choice $Y := (x_1, y_2, y_3)$ there follows that X solves (2.18) for all $Y := (x_1, y_2, y_3)$. Since the bi-linear form $a_2(\cdot,\cdot)$ and $\Psi(\cdot)$ are independent of y_1, X also solves (2.18) for arbitrary $Y \in V_D \times W$. Similarly, X solves

$$a_1(X, Y - X) \leq L(Y - X). \tag{2.20}$$

for the special choice $Y := (y_1, x_2, x_3)$. Since $a_1(\cdot,\cdot)$ and $L(\cdot)$ are independent of y_2 and y_3, X solves (2.20) for arbitrary $Y \in V_D \times W$. By the substitution $Z = Y - X$ in (2.20) one obtains the inequality

$$a_1(X, Z) \leq L(Z)$$

for all $Z \in V_0 \times W$. The reversed inequality is then formulated by replacing Z by $-Z$. Thus the equality (2.17) must be satisfied. □

Definition 8 (energy functional in elastoplasticity)**.** *Let $X \in V_D \times W$, and let $a(\cdot,\cdot)$, $\Psi(\cdot)$ and $L(\cdot)$ be defined as in (2.14)–(2.16). Then we define*

$$e(X) := \frac{1}{2}a(X, X) + \Psi(X) - L(X)$$

which is called the energy functional in elastoplasticity*.*

Lemma 2. *Let $a(\cdot,\cdot)$, $L(\cdot)$ and $\Psi(\cdot)$ be defined as in (2.14)–(2.16). Further let $e(\cdot)$ be defined as in Definition 8. Then expressions (i) and (ii) are equivalent:*
(i) *Find $X \in V_D \times W$ such that for all $Y \in V_D \times W$ there holds*

$$L(Y - X) \leq a(X, Y - X) + \Psi(Y) - \Psi(X)\ .$$

(ii) *Find $X \in V_D \times W$ such that*

$$e(X) = \min_{Y \in V_D \times W} e(Y).$$

Proof. $(ii) \Rightarrow (i)$: Let $Y \in V_D \times W$ and $\theta \in (0, 1)$ be arbitrary and fixed. Expression (ii) implies

$$e(X + \theta(Y - X)) \geq e(X). \tag{2.21}$$

Due to the definition of functional e and the convexity of Ψ, (2.21) yields

$$\theta a(X, Y - X) + \frac{1}{2}\theta^2 a(Y - X, Y - X) + \theta(\Psi(Y) - \Psi(X)) - \theta L(Y - X) \geq 0,$$

and thus

$$a(X, Y - X) + \frac{1}{2}\theta a(Y - X, Y - X) + \Psi(Y) - \Psi(X) - L(Y - X) \geq 0.$$

Taking the limit $\theta \downarrow 0$ leads to expression (i).

$(i) \Rightarrow (ii)$: Let $X \in V_D \times W$ solve (i), and $Y \in V_D \times W$ be arbitrary and fixed.

$$\begin{aligned} e(Y) &= e(X + (Y - X)) \\ &= \frac{1}{2}a(X,X) + a(X, Y-X) + \frac{1}{2}a(Y-X, Y-X) + \Psi(X + Y - X) \\ &\quad - L(X) - L(Y-X) \\ &= e(X) + \underbrace{a(X, Y-X) + \Psi(Y) - \Psi(X) - L(Y-X)}_{\geq 0} \geq e(X). \end{aligned}$$

Hence, there holds $e(X) = \min_{Y \in V_D \times W} e(Y)$. □

2.3 Minimization Problem

Thanks to Lemma 2, Problem 6 is equivalent to

Problem 7 (Minimization problem)**.** *Find $(u_1, p_1, \alpha_1) \in V_D \times W$, such that*

$$\begin{aligned} e(u_1, p_1, \alpha_1) = \frac{1}{2}\int_\Omega \Big[\mathbb{C}\,(\varepsilon(u_1) - p_1) : (\varepsilon(u_1) - p_1) + \alpha_1^2 \\ + 2k\,\varphi^*(\frac{p_1 - p_0}{k}, \frac{\alpha_0 - \alpha_1}{k})\Big]\,\mathrm{d}x \\ - \int_\Omega f \cdot u_1 \,\mathrm{d}x - \int_{\Gamma_N} g \cdot u_1 \,\mathrm{d}S(x) \to \; \mathit{min}. \end{aligned}$$

Lemma 3. *Let $\mathcal{R} := \mathbb{R}^{d\times d} \times \mathbb{R}$, the tuple $(p, \alpha) \in \mathcal{R}$, and the convex yield function ϕ be defined as in (2.9). Then there holds*

$$\varphi^*(p,\alpha) = \begin{cases} \sigma_y \|p\|_F & \mathit{if} \quad (\operatorname{tr} p = 0) \wedge (\alpha + H\sigma_y\|p\|_F \leq 0)\,, \\ \infty & \mathit{else.} \end{cases} \tag{2.22}$$

Proof. Let $\mathcal{M} := \{(q, \beta) \in \mathcal{R} \mid (\beta \geq 0) \wedge (\|\operatorname{dev} q\|_F - \sigma_y\,(1 + H\beta) \leq 0)\}$. The definition of a conjugate function (Definition 5) yields

$$\varphi^*(p,\alpha) = \sup_{(q,\beta)\in\mathcal{R}} (q : p + \beta\alpha - \varphi(q,\beta))\,. \tag{2.23}$$

If the supremum differs from $-\infty$, it can only be attained if $\varphi(q, \beta) < \infty$. Thus, due to the definitions of φ in (2.7) and ϕ in (2.9) there holds

$$\varphi^*(p,\alpha) = \sup_{(q,\beta)\in\mathcal{M}} (q : p + \beta\alpha)\ .$$

In the first instance, we will show

$$\varphi^*(p,\alpha) \geq \begin{cases} \sigma_y \|p\|_F & \text{if} \quad (\operatorname{tr} p = 0) \wedge (\alpha + H\sigma_y\|p\|_F \leq 0) \ , \\ \infty & \text{else} \ , \end{cases}$$

and then finally,

$$(\operatorname{tr} p = 0) \wedge (\alpha + H\sigma_y\|p\|_F \leq 0) \quad \Rightarrow \quad \varphi^*(p,\alpha) \leq \sigma_y\|p\|_F \ .$$

Let $c \in \mathbb{R}$. We choose $(q,\beta) = (cI, 0)$, which is element in $\mathcal{M}$, since

$$\|\operatorname{dev}(cI)\|_F = 0 \quad \text{and} \quad \sigma_y \geq 0 \ .$$

The choice of (q,β) yields

$$\varphi^*(p,\alpha) \geq \sup_{c\in\mathbb{R}} \ c \underbrace{p : I}_{=\operatorname{tr} p} \ ,$$

and thus there holds

$$\varphi^*(p,\alpha) \geq \begin{cases} 0 & \text{if } \operatorname{tr} p = 0 \ , \\ +\infty & \text{else} \ . \end{cases}$$

Let $\theta := \frac{\sigma_y(1+H\beta)}{\|p\|_F}$ and $\operatorname{tr} p = 0$. We choose $(q,\beta) = (\theta p, \beta)$, which is element in $\mathcal{M}$, since

$$\|\operatorname{dev}(\theta p)\|_F = \theta\|\operatorname{dev} p\|_F = \theta\|p\|_F = \sigma_y(1 + H\beta) \ .$$

The certain choice of (q,β) yields

$$\begin{aligned} \varphi^*(p,\alpha) &\geq \sup_{\beta\geq 0} (p : \theta p + \alpha\beta) = \sup_{\beta\geq 0} (\sigma_y (1 + H\beta) \|p\|_F + \alpha\beta) \\ &= \sigma_y\|p\|_F + \sup_{\beta\geq 0} ((\sigma_y H\|p\|_F + \alpha)\beta) \ , \end{aligned}$$

and thus there holds

$$\varphi^*(p,\alpha) \geq \begin{cases} \sigma_y\|p\|_F & \text{if } (\operatorname{tr} p = 0) \wedge (\sigma_y H\|p\|_F + \alpha \leq 0) \ , \\ +\infty & \text{else} \ . \end{cases}$$

Let $\operatorname{tr} p = 0$ and $\sigma_y H\|p\|_F + \alpha \leq 0$. There holds

$$\begin{aligned} \varphi^*(p,\alpha) &= \sup_{(q,\beta)\in\mathcal{M}} (p : q + \alpha\beta) = \sup_{(q,\beta)\in\mathcal{M}} \left((\operatorname{dev} q) : p + \frac{\operatorname{tr} q}{\dim(q)} \underbrace{I : p}_{=0} + \alpha\beta \right) \\ &\leq \sup_{(q,\beta)\in\mathcal{M}} (\|\operatorname{dev} q\|_F\|p\|_F + \alpha\beta) \\ &\leq \sup_{\beta\geq 0} (\sigma_y (1 + H\beta) \|p\|_F + \alpha\beta) \\ &= \sigma_y\|p\|_F + \sup_{\beta\geq 0} ((\sigma_y H\|p\|_F + \alpha)\beta) = \sigma_y\|p\|_F \ , \end{aligned}$$

so the proposition is true. □

Combining the definition of φ^* in (2.22) and the minimal value condition of the energy functional in Problem 7 it is necessary to guarantee the condition

$$\varphi^*(\frac{p_1 - p_0}{k}, \frac{\alpha_0 - \alpha_1}{k}) < +\infty.$$

Due to Lemma 3 we have to determine p_1 and α_1 such that $\operatorname{tr}(p_1 - p_0) = 0$ and $\alpha_1 \geq \alpha_0 + \sigma_y H \|p_1 - p_0\|_F$. Under this condition we can find the minimizer of α_1 in Problem 7 by setting $\alpha_1 = \alpha_0 + \sigma_y H \|p_1 - p_0\|_F$, which leads to a minimization problem in u_1 and p_1.

Problem 8. *Find* $(u_1, p_1) \in V_D \times [L_2(\Omega)]^{d\times d}_{sym}$ *such that*

$$\begin{aligned} e(u_1, p_1) = \frac{1}{2} \int_\Omega \mathbb{C}(\varepsilon(u_1) - p_1) : (\varepsilon(u_1) - p_1) + (\alpha_0 + \sigma_y H \|p_1 - p_0\|_F)^2 \,\mathrm{d}x \\ + \int_\Omega \sigma_y \|p_1 - p_0\|_F \,\mathrm{d}x - \int_\Omega f \cdot u_1 \,\mathrm{d}x - \int_{\Gamma_N} g \cdot u_1 \,\mathrm{d}S(x) \to \mathit{min}. \end{aligned} \tag{2.24}$$

Chapter 3

Fréchet Derivative of the Minimization Functional

3.1 Minimization in one Variable

We define

$$P := p_1 - p_0. \tag{3.1}$$

Finding the minimizer of p_1 in (2.24) for arbitrary and fixed u_1 is equivalent to finding P with $\operatorname{tr} P = 0$ such that

$$\begin{aligned} &\int_\Omega \frac{1}{2}\left(\mathbb{C}P : P + \sigma_y^2 H^2 P : P\right) - \mathbb{C}(\varepsilon(u_1) - p_0) : P \,\mathrm{d}x \\ &\qquad + \int_\Omega \sigma_y \left(1 + \alpha_0 H\right) \|P\|_F \,\mathrm{d}x \;\to\; \min. \end{aligned} \tag{3.2}$$

Since all of the integrands are positive, minimization of the integral is equivalent to point wise minimization of the integrands. Defining

$$A := \mathbb{C}\left[\varepsilon(u_1) - p_0\right],\ \beta := \sigma_y \left(1 + \alpha_0 H\right),\ \eta := \sigma_y^2 H^2 \tag{3.3}$$

and skipping all integrals in (3.2), we have to find P with $\operatorname{tr} P = 0$ such that

$$\frac{1}{2}\left(\mathbb{C} + \eta\right) P : P - A : P + \beta \|P\|_F \;\to\; \min. \tag{3.4}$$

Indeed, there exists a unique minimizer for P in (3.4) depending on u_1.

Lemma 4. *Let $d \in \mathbb{N}$, $A \in \mathbb{R}^{d\times d}$ and $\beta \in \mathbb{R}^+$. There holds*

$$\left[\forall Q \in \mathbb{R}^{d\times d}, \operatorname{tr} Q = 0 : \quad A : Q \leq \beta \|Q\|_F\right] \quad \Rightarrow \quad \|\operatorname{dev} A\|_F \leq \beta.$$

Proof. Let $A : Q \leq \beta\|Q\|_F$ for all Q with $\operatorname{tr} Q = 0$. Choosing $Q = \operatorname{dev} A$ implies $A : \operatorname{dev} A \leq \beta\|\operatorname{dev} A\|_F$. Hence $\operatorname{dev}\operatorname{dev} A = \operatorname{dev} A$, we obtain $\operatorname{dev} A : \operatorname{dev} A \leq \beta\|\operatorname{dev} A\|_F$ when substituting A by $\operatorname{dev} A$. □

The following theorem was yet formulated and proofed e.g. in [ACZ99]. Due to its crucial importance for this thesis it is shown here in detail as well.

Theorem 2. *Let $A \in \mathbb{R}^{d\times d}_{sym}$ and $\beta \in \mathbb{R}^+$. There exists exactly one $P \in \mathbb{R}^{d\times d}_{sym}$ with $\operatorname{tr} P = 0$ that satisfies*

$$(A - (C + \eta)\, P) : (Q - P) \leq \beta\, (\|Q\|_F - \|P\|_F) \tag{3.5}$$

for all $Q \in \mathbb{R}^{d\times d}$ with $\operatorname{tr} Q = 0$. This P is characterized as the minimizer of

$$\frac{1}{2}\,(\mathbb{C} + \eta)\, P : P - A : P + \beta\|P\|_F \ \rightarrow \ min \tag{3.6}$$

amongst trace-free symmetric $d \times d$-matrices, and equals

$$\frac{(\|\operatorname{dev} A\|_F - \beta)_+}{2\mu + \eta}\frac{\operatorname{dev} A}{\|\operatorname{dev} A\|_F}\,, \tag{3.7}$$

where $(\cdot)_+ := \max\{0, \cdot\}$ denotes the non-negative part. The minimal value of (3.6), attained for P as in (3.7), is

$$-\frac{1}{2}\,(\|\operatorname{dev} A - \beta\|_F)_+^2 \,/\, (2\mu + \eta)\,. \tag{3.8}$$

Proof. Due to Definition 4, expression (3.5) states that

$$A - (\mathbb{C} + \eta)\, P \in \beta\partial\|\cdot\|_F(P) \tag{3.9}$$

where only trace-free arguments are under consideration. The norm function $\|\cdot\|_F$ is convex and so is (3.6). Identity (3.9) is equivalent to 0 belonging to the sub-gradient of (3.6), which characterizes the minimizers of (3.6). If $P = 0$, (3.5) states

$$A : Q \leq \beta\|Q\|_F$$

for all $Q \in \mathbb{R}^{d\times d}$ with $\operatorname{tr} Q = 0$. Due to Lemma 4 there holds $\|\operatorname{dev} A\|_F \leq \beta$. If $\|\operatorname{dev} A\|_F > \beta$ we conclude $P \neq 0$ and obtain $\partial\|\cdot\|_F(P) = \{P/\|P\|_F\}$. Hence, (3.9) yields

$$\operatorname{dev} A - (\mathbb{C} + \eta)\, P = \beta P/\|P\|_F.$$

Notice that $\operatorname{tr} \mathbb{C}P = 0$ as $\operatorname{tr} P = 0$, and only trace-fee arguments are under consideration. Since then $\mathbb{C}P = 2\mu P$ we obtain

$$\operatorname{dev} A = (\beta + (2\mu + \eta)\, \|P\|_F)\, P/\|P\|_F \tag{3.10}$$

and so

$$\|\operatorname{dev} A\| = \beta + (2\mu + \eta)\, \|P\|_F,$$

whence

$$\|P\|_F = (\|\operatorname{dev} A\| - \beta)\, /\, (2\mu + \eta)\, .$$

Using this in (3.10) we deduce (3.7). Taking (3.7) in (3.6) we calculate the minimal value (3.8). □

Minimizing (2.24) with respect to p_1 for fixed u_1 may be accomplished by

$$p_1 = \frac{(\|\operatorname{dev} A\|_F - \beta)_+}{2\mu + \sigma_y^2 H^2} \frac{\operatorname{dev} A}{\|\operatorname{dev} A\|_F} + p_0, \tag{3.11}$$

where

$$A = \mathbb{C}\,[\varepsilon(u_1) - p_0] \quad \text{and} \quad \beta = \sigma_y(1 + \alpha_0 H). \tag{3.12}$$

A variety of established solvers in elastoplasticity (see [SH98, HR95]) are based on solving Problem 8. One possibility is to alternate minimize functional $e(\cdot,\cdot)$ with repsect to u_1 and p_1, which is done as follows:

Choose u_1^0
j := 1
while some termination criterion **do**
  Find p_1^j such that $e(u_1^{j-1}, p_1^j) \to \min$
  Find u_1^j such that $e(u_1^j, p_1^j) \to \min$
  j := j + 1
end while

Since $e(\cdot,\cdot)$ is smooth with respect to to its first component, minimization regarding u_1 may be realized by numerical methods of the field of smooth optimization, e.g., a Newton-like method. Minimization concerning p_1^j may be acoomplished in an analytical way utilizing Theorem 2, that is, by (3.11) and (3.12).

The new approach in this thesis is, that we substitute (3.11) for p_1 in Problem 8. Then we will show that this functional (depending on u_1 only) is smooth, such that, without having to minimize alternate, the minimization may be accomplished by a method of the field of smooth optimization.

Problem 8 is equivalent to the following minimization problem, which depends on the displacement u_1 only.

Problem 9. *Find $u_1 \in V_D$ such that*

$$
\begin{aligned}
e(u_1) = \frac{1}{2}\int_\Omega & \mathbb{C}(\varepsilon(u_1) - p_1(\varepsilon(u_1))) : (\varepsilon(u_1) - p_1(\varepsilon(u_1)))\,\mathrm{d}x \\
&+ \frac{1}{2}\int_\Omega (\alpha_0 + \sigma_y H \|p_1(\varepsilon(u_1)) - p_0\|_F)^2 + \sigma_y \|p_1(\varepsilon(u_1)) - p_0\|_F\,\mathrm{d}x \\
&- \int_\Omega f\cdot u_1\,\mathrm{d}x - \int_{\Gamma_N} g\cdot u_1\,\mathrm{d}S(x) \to \mathit{min},
\end{aligned}
\tag{3.13}
$$

with

$$
p_1(\varepsilon(u_1)) = \frac{(\|\operatorname{dev} A\|_F - \beta)_+}{2\mu + \sigma_y^2 H^2}\frac{\operatorname{dev} A}{\|\operatorname{dev} A\|_F} + p_0, \tag{3.14}
$$

where

$$
A = \mathbb{C}\,[\varepsilon(u_1) - p_0] \quad \mathit{and} \quad \beta = \sigma_y(1 + \alpha_0 H).
$$

3.2 The Moreau-Yosida Theorem

We will make use of an abstract formulation of (3.13). Let

$$
\begin{aligned}
\|B\|_{\mathbb{C}} &:= \left(\int_\Omega \mathbb{C}B(x) : B(x)\,\mathrm{d}x\right)^{\frac{1}{2}}, \text{ and} \\
\psi(p_1) &:= \frac{1}{2}\int_\Omega (\alpha_0 + \sigma_y H\|p_1 - p_0\|_F)^2\,\mathrm{d}x + \int_\Omega \sigma_y\|p_1 - p_0\|_F\,\mathrm{d}x
\end{aligned}
$$

define a new matrix scalar product and a (convex) functional. Expression (3.13) then rewrites as

$$
e(u_1) = \frac{1}{2}\|\varepsilon(u_1) - p_1(\varepsilon(u_1))\|_{\mathbb{C}}^2 + \psi(p_1(\varepsilon(u_1))) - L(u_1) \;\to\; \min. \tag{3.15}
$$

Minimizing functional $e(u_1)$ can be done by finding the root of its first derivative $De(u_1)$. The next theorem shows, that $e(u_1)$ is indeed smooth, no matter the dependency ψ on p is non-smooth.

Theorem 3 (Moreau-Yosida)**.** *Let H be a Hilbert space with scalar product $\langle\cdot,\cdot\rangle_H$, H^* its dual space, $\psi : H \to \mathbb{R}$ convex, and function f be defined as*

$$f : H \to \mathbb{R},\ y \mapsto \min_{x\in H} \left[\frac{1}{2}\|y-x\|_H^2 + \psi(x)\right] .$$

Further let $\tilde{x}(y)$ denote the (unique) function, which yields

$$f(y) = \frac{1}{2}\|y-\tilde{x}(y)\|_H^2 + \psi(\tilde{x}(y)) .$$

for all $y \in H$. Then there holds:

1. *f is convex.*
2. *f is Fréchet-differentiable with $Df(y) = y - \tilde{x}(y)\ \in H^*$.*

Proof. ad 1 (convexity): Let $y_1, y_2 \in H$, $t \in (0,1)$ be arbitrary and fixed. Further let $\overline{x} := \tilde{x}((1-t)y_1 + ty_2)$, $\overline{x}_1 := \tilde{x}(y_1)$ and $\overline{x}_2 := \tilde{x}(y_2)$. Due to the definition of f there holds

$$f((1-t)y_1 + ty_2) = \frac{1}{2}\|(1-t)y_1 + ty_2 - \overline{x}\|_H^2 + \psi(\overline{x}) .$$

Since $\overline{x}$ is the minimizer, the expression is certainly not getting any lower if $\overline{x}$ is substituted by any other element in H. Thus

$$f((1-t)y_1+ty_2) \le \frac{1}{2}\|(1-t)y_1+ty_2-(1-t)\overline{x}_1-t\overline{x}_2\|_H^2+\psi((1-t)\overline{x}_1+t\overline{x}_2) .$$

Triangle inequality and convexity of ψ yield

$$f((1-t)y_1+ty_2) \le (1-t)\left[\frac{1}{2}\|y_1-\overline{x}_1\|_H^2+\psi(\overline{x}_1)\right]+t\left[\frac{1}{2}\|y_2-\overline{x}_2\|_H^2+\psi(\overline{x}_2)\right],$$

and thus

$$f((1-t)y_1+ty_2) \le (1-t)f(y_1) + tf(y_2).$$

ad 2 (differentiability): Let $y \in H$ and $\Delta y \in H$ be arbitrary and fixed. All sub-gradients $g \in H^*$ of f yield

$$f(y+\Delta y) \ge f(y) + \langle g(y), \Delta y\rangle_H . \tag{3.16}$$

On the other hand there holds

$$\begin{aligned} f(y+\Delta y) &= \min_{x\in H}\left[\frac{1}{2}\|y+\Delta y-x\|_H^2+\psi(x)\right] \\ &\leq \frac{1}{2}\|y+\Delta y-\tilde{x}(y)\|_H^2+\psi(\tilde{x}(y)) \\ &= \frac{1}{2}\langle y+\Delta y-\tilde{x}(y),\ y+\Delta y-\tilde{x}(y)\rangle_H+\psi(\tilde{x}(y))\ . \end{aligned}$$

Hence,

$$f(y+\Delta y)\leq f(y)+\langle y-\tilde{x}(y),\ \Delta y\rangle_H+\frac{1}{2}\|\Delta y\|_H^2\ . \tag{3.17}$$

Subtracting expression (3.16) from (3.17) one obtains

$$0\leq \langle y-\tilde{x}(y),\Delta y\rangle_H-\langle g(y),\Delta y\rangle_H+\frac{1}{2}\|\Delta y\|_H^2\ .$$

The same inequality must be valid, if we replace Δy by $-\Delta y$, such that there holds

$$-\frac{1}{2}\|\Delta y\|_H^2\leq \langle y-\tilde{x}(y)-g(y),\Delta y\rangle_H\leq \frac{1}{2}\|\Delta y\|_H^2\ .$$

Hence, one obtains $y-\tilde{x}(y)-g(y)=0$ resp. $g(y)=y-\tilde{x}(y)$ (proof by contradiction, draft: assume, that $z:=y-\tilde{x}(y)-g(y)$ would not equal zero; choose $\gamma\in(0,1)$; choose $\Delta y=\gamma z$; contradiction). The sub-differential $g(y)$ is uniquely defined for all $y\in H$, thus a Fréchet-derivative, which is denoted by the symbol $Df:=g$, or explicitly

$$Df(y)=\langle y-\tilde{x}(y),\ \cdot\ \rangle_H\ .$$

□

Theorem 3 is essential in the so called *Moreau-Yosida regularization* (see [Mor65] and [Yos94]), which has its origin in convex analysis. Hence in this paper we are calling it the *Moreau-Yosida theorem*. Applying Theorem 3 and the chain rule to the energy function (3.15), we can now build its Gâteaux-differential.

$$\begin{aligned} De(u_1,v) &= \langle\varepsilon(u_1)-p_1(\varepsilon(u_1))\,,\,\varepsilon(v)\rangle_{\mathbb{C}}-L(v) \\ &= \int_\Omega \mathbb{C}\left(\varepsilon(u_1)-p_1(\varepsilon(u_1))\right):\varepsilon(v)\ \mathrm{d}x-L(v), \end{aligned} \tag{3.18}$$

with p_1 and L defined as in (3.14) and (2.15).

Chapter 4

Discretization and Implementation

Sections 4.1 and 4.3 are based on [ACFK02].

4.1 Discretization in Space

We decompose the polygonal 2D domain Ω into a triangulation with $\mathrm{N}_{\mathcal{T}} \sim h^{-d}$ triangles and $\mathrm{N}_{\mathcal{N}}$ nodes $x_i \in \{1, \ldots, \mathrm{N}_{\mathcal{N}}\}$. Here $\mathrm{N}_{\mathcal{T}}$ means *number of elements* and $\mathrm{N}_{\mathcal{N}}$ means *number of nodes*. Let $\mathcal{T}$ be such a domain decomposition in 2D where all $T \in \mathcal{T}$ are triangles with nodes x_i for $i \in \{1, \ldots, \mathrm{N}_{\mathcal{N}}\}$. Let $\mathcal{E}$ be a set of edges $E \in \mathcal{E}$ and let $\mathcal{E}_N$ be its intersection with the Neumann boundary Γ_N. We approximate the infinite-dimensional space V by a finite-dimensional subspace $V_h := \{u_{1h} \in V \mid u_{1h|_T}$ is a linear polynomial $\forall T \in \mathcal{T}\}$. The base functions $\eta_{i,j} \in V_h$, $i \in \{1, \ldots, \mathrm{N}_{\mathcal{N}}\}$, $j \in \{1, 2\}$ are of the form $\eta_{i,j}(x) := \varphi_i(x) e_j$, where $\varphi_i(x)$ is a 1D linear nodal shape (hut) function and e_j is the j-th unit vector. Therefore, u_h can be expressed $u_h(x) := \sum_{i,j} u_{i,j} \eta_{i,j}(x)$, where $u_{i,j} := (u(x_i))_j$. We are interested in finding $u_{1h} \in V_{hD} := V_h \cap V_D$ such that $De(u_{1h}) = 0$. For implementation, u_{1h} is stored as a vector $\mathbf{u} = ((u_{i,j})_{j=1}^2)_{i=1}^{\mathrm{N}_{\mathcal{N}}} \in \mathbb{R}^{2\mathrm{N}_{\mathcal{N}}}$. Analogously a test function v_h is represented by the vector $\mathbf{v}$. Let $(k_1, k_2, k_3) := ((x_1, y_1), (x_2, y_2), (x_3, y_3))$

be the vertices of one single element $T \in \mathcal{T}$. For linear elements there holds

$$\nabla \begin{pmatrix} \varphi_{k1} \\ \varphi_{k2} \\ \varphi_{k3} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{pmatrix}^{-1} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

4.2 Vector Representation

We consider the so called *plain model*, which assumes the strain ε or the stress σ to have zero components in direction, where the domain Ω is thin (*plain strain model* or *plain stress model*). The following formulations hold for the plain strain model only, a modification for the plain stress model can be done as well. We assume the total strain ε, the plastic strain p and the stress tensor σ in forms

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{12} & \varepsilon_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad p = \begin{pmatrix} p_{11} & p_{12} & 0 \\ p_{12} & p_{22} & 0 \\ 0 & 0 & p_{33} \end{pmatrix}, \quad \sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix}.$$

The information about ε can be saved in the vector $\overrightarrow{\varepsilon} := (\varepsilon_{11}, \varepsilon_{22}, 2\varepsilon_{12})^T$. Since p is trace-free, there must hold $p_{33} = -p_{11} - p_{22}$. Therefore it is sufficient to store p in the vector $\overrightarrow{p} := (p_{11}, p_{22}, p_{12})^T$. Due to $\sigma_{33} = \sigma_{11} + \sigma_{22}$ the stress σ can be saved in the vector $\overrightarrow{\sigma} := (\sigma_{11}\sigma_{22}, \sigma_{12})^T$ too. For the calculation of the energy functional derivative we will make an extent use of identifiers in vector representation. Table 4.1 summarizes in which way these identifiers will transform.

Common (Tensor) Representation	Vector Representation
$\varepsilon := \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{12} & \varepsilon_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\overrightarrow{\varepsilon} := \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\,\varepsilon_{12} \end{pmatrix}$
$p := \begin{pmatrix} p_{11} & p_{12} & 0 \\ p_{12} & p_{22} & 0 \\ 0 & 0 & -(p_{11} + p_{22}) \end{pmatrix}$	$\overrightarrow{p} := \begin{pmatrix} p_{11} \\ p_{22} \\ p_{12} \end{pmatrix}$ with $\lVert p \rVert_F^2 = \overrightarrow{p}^T N \overrightarrow{p}$ where $N := \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

Common (Tensor) Representation	Vector Representation
$\sigma_\varepsilon := \mathbb{C}\,\varepsilon = \begin{pmatrix} \sigma_{\varepsilon,11} & \sigma_{\varepsilon,12} & 0 \\ \sigma_{\varepsilon,12} & \sigma_{\varepsilon,22} & 0 \\ 0 & 0 & \sigma_{\varepsilon,33} \end{pmatrix}$ with $\mathbb{C} := \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$	$\vec{\sigma}_\varepsilon := \begin{pmatrix} \sigma_{\varepsilon,11} \\ \sigma_{\varepsilon,22} \\ \sigma_{\varepsilon,12} \end{pmatrix} = C\,\vec{\varepsilon}$ with $\quad C := \begin{pmatrix} \lambda + 2\,\mu & \lambda & 0 \\ \lambda & \lambda + 2\,\mu & 0 \\ 0 & 0 & \mu \end{pmatrix}$ and $\quad \sigma_{\varepsilon,33} = \underbrace{\frac{\lambda}{2\;(\lambda+\mu)}}_{=\nu} \begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \vec{\sigma}_\varepsilon$
$\sigma_p := \mathbb{C}\,p = 2\,\mu\,p + \lambda\,\underbrace{\mathrm{tr}(p)}_{=0}\,I = 2\,\mu\,p$	$\vec{\sigma}_p := \begin{pmatrix} \sigma_{p,11} \\ \sigma_{p,22} \\ \sigma_{p,12} \end{pmatrix} = 2\,\mu\,\vec{p}$ and $\quad \sigma_{p,33} = -\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} \vec{\sigma}_p$
$\sigma := \mathbb{C}\;(\varepsilon - p) = \sigma_\varepsilon - \sigma_p$	$\vec{\sigma} = \vec{\sigma}_\varepsilon - \vec{\sigma}_p$ and $\sigma_{33} = \sigma_{\varepsilon,33} - \sigma_{p,33}$
$\mathrm{tr}\,\sigma_\varepsilon := \sum_i \sigma_{\varepsilon,ii}$	$\mathrm{tr}\,\sigma_\varepsilon = \frac{\nu+1}{\nu}\,\sigma_{\varepsilon,33}$
$\mathrm{dev}\,\sigma_\varepsilon := \sigma_\varepsilon - \frac{\mathrm{tr}\,\sigma_\varepsilon}{\dim(\sigma_\varepsilon)}\,I$	$\overrightarrow{\mathrm{dev}\,\sigma_\varepsilon} := \begin{pmatrix} (\mathrm{dev}\,\sigma_\varepsilon)_{11} \\ (\mathrm{dev}\,\sigma_\varepsilon)_{22} \\ (\mathrm{dev}\,\sigma_\varepsilon)_{12} \end{pmatrix}$ $= \vec{\sigma}_\varepsilon - \frac{\mathrm{tr}\,\sigma_\varepsilon}{\dim(\sigma_\varepsilon)} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ $= \underbrace{\left(I - \frac{\nu+1}{\dim(\sigma_\varepsilon)} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right)}_{=:K} \vec{\sigma}_\varepsilon$ and

Common (Tensor) Representation	Vector Representation
	$(\operatorname{dev}\sigma_\varepsilon)_{33} = \sigma_{33} - \frac{\operatorname{tr}\sigma_\varepsilon}{\dim(\sigma_\varepsilon)}$ $= \underbrace{\left(\nu - \frac{1+\nu}{\dim(\sigma_\varepsilon)}\right) d^T}_{=:e^T} \sigma_{\varepsilon,V}$
$\operatorname{dev}\sigma = \operatorname{dev}\sigma_\varepsilon - \underbrace{\operatorname{dev}\sigma_p}_{=\sigma_p}$	$\overrightarrow{\operatorname{dev}\sigma} = \overrightarrow{\operatorname{dev}\sigma_\varepsilon} - \overrightarrow{\sigma}_p$ $(\operatorname{dev}\sigma)_{33} = -\begin{pmatrix}1 & 1 & 0\end{pmatrix} \overrightarrow{\sigma}$
$\|\operatorname{dev}\sigma\|_F^2 := \sum_{i,j} (\operatorname{dev}\sigma)_{ij}^2$	$\|\operatorname{dev}\sigma\|_F^2 = \left(\overrightarrow{\operatorname{dev}\sigma}\right)^T N \, \overrightarrow{\operatorname{dev}\sigma}$

Table 4.1: Table of Vector Representation

It follows for instance $\sigma_\varepsilon : \varepsilon = (\overrightarrow{\sigma}_\varepsilon)^T \overrightarrow{\varepsilon}$ and $\sigma_p : \varepsilon = (\overrightarrow{\sigma}_p)^T \overrightarrow{\varepsilon}$. Let R_T and R_E be element and edge restriction operators which map the global vector $\mathbf{u}$ on the local element $\mathbf{u}_T$ or edge $\mathbf{u}_E$ vectors

$$\mathbf{u}_T = R_T \mathbf{u} \, , \quad \mathbf{u}_E = R_E \mathbf{u} \, . \tag{4.1}$$

Since $\varepsilon(u_{1h})$ is constant on each element T there holds

$$\varepsilon_V(u_{1h}(x)_{|T}) = \begin{pmatrix} \partial_x\varphi_{k_1} & 0 & \partial_x\varphi_{k_2} & 0 & \partial_x\varphi_{k_3} & 0 \\ 0 & \partial_y\varphi_{k_1} & 0 & \partial_y\varphi_{k_2} & 0 & \partial_y\varphi_{k_3} \\ \partial_y\varphi_{k_1} & \partial_x\varphi_{k_1} & \partial_y\varphi_{k_2} & \partial_x\varphi_{k_2} & \partial_y\varphi_{k_3} & \partial_x\varphi_{k_3} \end{pmatrix} \begin{pmatrix} u_{k_1,x} \\ u_{k_1,y} \\ u_{k_2,x} \\ u_{k_2,y} \\ u_{k_3,x} \\ u_{k_3,y} \end{pmatrix}$$

or, in a more compact way,

$$\varepsilon_V(u_{1h}(x)_{|T}) = B_T \, \mathbf{u}_T \, . \tag{4.2}$$

The implementation of B_T in Matlab© reads:

```
function [B,area] = elem_B(vertices)
```

```
F = [ones(1,3);vertices'];
area = det(F)/2;
phiGrad = F\[zeros(1,2);eye(2)];
B([1,3],[1,3,5]) = phiGrad'; B([3,2],[2,4,6]) = phiGrad';
end
```

Integration over body and surface forces may be realized by the midpoint rule. We approximate f and g by

$$f_T := f(\overline{x}_T) \quad \text{and} \quad g_E := g(\overline{x}_E),$$

where $\overline{x}_T$, and $\overline{x}_E$ respectively, denote the center of mass of the element T, and the edge E respectively. Defining

$$\mathbf{f}_T := \frac{|T|}{3} R_T^T f_T \ , \quad \text{and} \quad \mathbf{g}_E := \frac{|E|}{2} R_E^T g_E \ ,$$

on each $T \in \mathcal{T}$ and on each $E \in \mathcal{E}$ there hold

$$\int_T f \cdot v \, \mathrm{d}x \approx \mathbf{f}_T^T \mathbf{v} \ , \quad \text{and} \quad \int_E g \cdot v \, \mathrm{d}S(x) \approx \mathbf{g}_E^T \mathbf{v} \ . \tag{4.3}$$

This can be realized by the following two Matlab© functions:

```
function f_ = elem_volumeforce(vertices)
T = det([ones(3,1),vertices]);
fs = f(sum(vertices)/3)';
f_ = [fs; fs; fs]*T/6;
end

function g_ = elem_surfaceforce(vertices)
n = (vertices(2,:) - vertices(1,:))*[0,-1; 1,0];
T = norm(n);
gs = g_neumann(sum(vertices)/2,n/norm(n))';
g_ = [gs; gs]*T/2;
end
```

4.3 Discrete Formulation and Newton Like Method

The Gâteaux-derivative in (3.18) will now be lead into its discrete analogon. First, the whole integral over Ω will be split into a sum of integrals on single finite elements. Combining (4.1), (4.2) and (4.3) we obtain the discrete formulation of the Gâteaux-differential

$$De(\mathbf{u},\mathbf{v}) = \sum_{T\in\mathcal{T}} \left[|T|\ \left(C\,B_T\mathbf{u}_T - 2\mu\,\overrightarrow{p_1}(B_T\mathbf{u}_T)\right)^T\ B_T\,R_T - \mathbf{f}_T^T\right]\mathbf{v} - \sum_{E\in\mathcal{E}_N} \mathbf{g}_E^T\,\mathbf{v}$$

with

$$\overrightarrow{p_1}(B_T\mathbf{u}_T) = \begin{cases} \overrightarrow{p_0} & \text{if } \|\operatorname{dev} A\| < \beta, \\ \frac{1}{\delta}\,\overrightarrow{\operatorname{dev} A}\left(1 - \frac{\beta}{\|\operatorname{dev} A\|}\right) + \overrightarrow{p_0} & \text{else,} \end{cases}$$

where

$$\begin{aligned} \overrightarrow{\operatorname{dev} A} &= KC\,B_T\,\mathbf{u}_T - 2\,\mu\,\overrightarrow{p_0}\,, \\ \|\operatorname{dev} A\| &= \left(\left(\overrightarrow{\operatorname{dev} A}\right)^T N\,\overrightarrow{\operatorname{dev} A}\right)^{\frac{1}{2}} =: \|\overrightarrow{\operatorname{dev} A}\|_N, \\ \beta &= \sigma_y\,(1+\alpha_0 H)\,, \\ \delta &= 2\mu + \sigma_y^2 H^2. \end{aligned}$$

Since $De(\mathbf{u},\mathbf{v})$ is linear in $\mathbf{v}$ we can obtain the Fréchet-derivative

$$De(\mathbf{u}) = \sum_{T\in\mathcal{T}} \left(|T|\ \left(CB_T\mathbf{u}_T - 2\mu\,\overrightarrow{p_1}(B_T\mathbf{u}_T)\right)^T\ B_T\,R_T - \mathbf{f}_T\right) - \sum_{E\in\mathcal{E}_N} \mathbf{g}_E, \quad (4.4)$$

which represent the discrete form of (3.18). Notice that the second derivative $D^2e(\mathbf{u})$ can be calculated everywhere appart from the the material points satisfying the condition $\|\operatorname{dev} A\| \neq \beta$ and reads

$$\begin{aligned} D^2e(\mathbf{u}) &= D\left(\sum_{T\in\mathcal{T}} |T|\ \left(CB_T\mathbf{u}_T - 2\mu\,\overrightarrow{p_1}(B_T\mathbf{u}_T)\right)^T B_T\,R_T\right) \\ &= \sum_{T\in\mathcal{T}} |T|\,R_T^T\,B_T^T\left(C - 2\mu\,D\,\overrightarrow{p_1}(B_T\mathbf{u}_T)\right)^T B_T\,R_T\ , \end{aligned} \quad (4.5)$$

with

$$D\ \overrightarrow{p_1}(B_T\mathbf{u}_T) = \begin{cases} 0 & \text{if } \|\operatorname{dev} A\| < \beta \\ \frac{1}{\delta}\,w' - \frac{\beta}{\delta}\left(\frac{w'}{(w^TNw)^{\frac{1}{2}}} - \frac{w\,w^TNw'}{(w^TNw)^{\frac{3}{2}}}\right) & \text{if } \|\operatorname{dev} A\| > \beta, \end{cases} \quad (4.6)$$

where $w := \overrightarrow{\operatorname{dev} A} = KC\,B_T\,\mathbf{u}_T - 2\,\mu\,\overrightarrow{p_0}$ and $w' := D_{B_T\mathbf{u}_T}\overrightarrow{\operatorname{dev} A} = K\,C$.

Remark 1. In order to obtain (4.6) it is necessary to calculate following identities before:
Let $f : \mathbb{R}^n \to \mathbb{R}^n$, $x \mapsto f(x)$ and $N \in \mathbb{R}^{n\times n}$ symmetric. In Einstein's summation convention, there holds

$$\begin{aligned}
\nabla \frac{f}{(f^TNf)^{\frac{1}{2}}} &= \frac{\nabla f}{(f^TNf)^{\frac{1}{2}}} - \left[\frac{1}{2}\,\frac{f_i\,p_j\,(f_lN_{lm}f_m)}{(f^TNf)^{\frac{3}{2}}}\right]_{i,j=1}^{n} \\
&= \frac{\nabla f}{(f^TNf)^{\frac{1}{2}}} - \left[\frac{1}{2}\,\frac{f_i\,N_{lm}\,((p_jf_l)\,f_m + f_l\,(p_jf_m))}{(f^TNf)^{\frac{3}{2}}}\right]_{i,j=1}^{n} \\
&= \frac{\nabla f}{(f^TNf)^{\frac{1}{2}}} - \frac{ff^TN\,\nabla f}{(f^TNf)^{\frac{3}{2}}}.
\end{aligned}$$

Notice, that the second derivative (4.5) exists in purely elastic material points as well as in purely plastic material points. It only does not exist in the elasto-plastic interface points where $\|\operatorname{dev} A\| = \beta$. For numerical computations we will use the value corresponding to the case $\|\operatorname{dev} A\| > \beta$ also in the critical interface case, where $\|\operatorname{dev} A\| = \beta$.

A Newton-like method is applied for the calculation of $\mathbf{u} \in \mathbf{R}^{d\cdot \mathrm{N}_{\mathcal{N}}}$ such that $De(\mathbf{u}) = 0$ and $\mathbf{u}$ satisfies the Dirichlet boundary condition:

$$\mathbf{u}_i = \mathbf{u}_{i-1} + \Delta\mathbf{u}_i \qquad (\forall i \in \mathbb{N}), \tag{4.7}$$

where $\Delta\mathbf{u}_i$ solves

$$-D^2e(\mathbf{u}_{i-1})\,\Delta\mathbf{u}_i = D\,e(\mathbf{u}_{i-1})\ .$$

The assembly of the stiffness matrix `EnergyDD` (it stands for $D^2e(u)$) and the right hand side `EnergyD` ($De(u)$) is implemented in the Matlab© as:

```
function [EnergyD,EnergyDD] = energy_derivatives(u, ...
p0Initial, nodes,elements,neumann,N,K,C,param)
SU = size(u,1);
EnergyD = zeros(SU,1); EnergyDD = sparse(SU,SU);
for j = 1:size(elements,1)
    vertices = nodes(elements(j,:),:);
    I = 2*elements(j,[1,1,2,2,3,3]) - [1,0,1,0,1,0];
    [B,area] = elem_B(vertices);
    eps = B*u(I);
    p0 = p0Initial(:,j);
    [p,pD_eps] = elem_p(j,eps,p0,N,K,C,param);
```

```
    ED(I) = ED(I) + area*B'*(C*eps - 2*param.mu*p);
    ED(I) = ED(I) - elem_volumeforce(vertices);
    EDD(I,I) = EDD(I,I) + area*B'*(C - 2*param.mu*pD_eps)*B;
end
for j = 1:size(neumann,1)
    vertices = nodes(neumann(j,:),:);
    I = 2*neumann(j,[1,1,2,2]) - [1,0,1,0];
    ED(I) = ED(I) - elem_surfaceforce(vertices);
end
```

The calculation of $p(\varepsilon(u))$ and $D_{\varepsilon(u)}\, p(\varepsilon(u))$ on the $j-th$ element T_j can be realized by the Matlab© function `elem_p`:

```
function [p,pD_eps] = elem_p(j,eps,p0,N,K,C,param)
p = p0;
pD_eps = zeros(3,3);
devAD_eps = K*C;
devA = devAD_eps*eps - 2*param.mu*p0;
norm_devA = sqrt(devA'*N*devA);
posFac = norm_devA - param.beta(j);
if (posFac > 0)
    p = devA*posFac/(param.delta*norm_devA) + p0;
    pD_eps = (devAD_eps - (param.beta(j)/norm_devA)* ...
             devAD_eps - (devA*((devA'*N)*devAD_eps))* ...
             norm_devA^2))/param.delta;
end
```

Notice, that $\mathbf{u}_i$ must satisfy (generally inhomogeneous) Dirichlet boundary conditions for all $i \in \mathbb{N}$. Therefore it is sufficient for the initial approximation $\mathbf{u}_0$ to solve the inhomogeneous Dirichlet conditions, and for $\Delta\mathbf{u}_i$ to solve the homogeneous Dirichlet conditions. For the termination of the Newton-like method we check, whether the relative error of the discrete approximation

$$\frac{|u_i - u_{i-1}|_\varepsilon}{|u_i|_\varepsilon + |u_{i-1}|_\varepsilon} \tag{4.8}$$

is smaller than a given prescribed bound $\epsilon \in \mathbb{R}^+$. Notice that the seminorm

$$|\cdot|_\varepsilon := (\int_\Omega ||\varepsilon(\cdot)||^2 \,\mathrm{d}x)^{1/2}$$

is more easily computable than an equivalent H_1 norm

$$||\cdot||_1 := (\int_\Omega (||\cdot||^2 + ||\nabla\cdot||^2)\,\mathrm{d}x)^{1/2}.$$

The quality of the solution in the next iteration step is measured by the relative error of the energy as

$$\frac{|e(u_i) - e(u_{i-1})|}{|e(u_i)| + |e(u_{i-1})|}. \tag{4.9}$$

The implementation of (4.8) reads:

```
function norm_delta_u = termination_criterion(u,u_old, ...
Delta_u,nodes,elements)
N_eps = [1,0,0; 0,1,0; 0,0,0.5];
norm_u_old_sq = 0; norm_u_sq = 0;
norm_du_sq = 0; norm_ED_sq = 0;
for j = 1:size(elements,1)
    vertices = nodes(elements(j,:),:);
    [B,area] = elem_B(vertices);
    eps_u_old = B*u_old(I); eps_u = B*u(I);
    eps_Delta_u = B*Delta_u(I);
    norm_u_old_sq = norm_u_old_sq + ...
                    area*(eps_u_old'*N_eps*eps_u_old);
    norm_u_sq = norm_u_sq + area*(eps_u'*N_eps*eps_u);
    norm_Delta_u_sq = norm_Delta_u_sq + ...
                     area*(eps_Delta_u'*N_eps*eps_Delta_u);
end
norm_Delta_u = sqrt(norm_Delta_u_sq);
norm_u = sqrt(norm_u_sq);
norm_u_old = sqrt(norm_u_old_sq);
norm_delta_u = norm_Delta_u / (norm_u_old + norm_u);
```

The implementation of the Newton-like method is realized via the Matlab© file `fem.m`.

```
d = [1; 1; 0];
K = eye(3) - d*d'*(1 + param.nu)/3;
N = [2,1,0;1,2,0;0,0,2];
C = param.lambda*[1,1,0;1,1,0;0,0,0] + ...
```

```
    param.mu*[2,0,0;0,2,0;0,0,1];
u = zeros(2*size(nodes,1),1); Delta_u = u; ED = u;
p0Initial = zeros(size(elements,1),3);
isPlasticElement = zeros(1,size(elements,1));
EDD = sparse(size(u,1),size(u,1));
[I,J] = separate_into_prescribed_and_free_nodes(...)
u = apply_dirichlet_boundary_conditions(...)
newton_epsilon = 1e-12; newton_iterations = 0;
norm_delta_u = newton_epsilon;
while (norm_delta_u >= newton_epsilon)
    [ED,EDD] = energy_derivatives(u,p0Initial,nodes, ...
               elements,neumann,N,K,C,param);
    ED(J) = ED(J) + EDD(J,:)*u(J);
    u_old = u;
    Delta_u(I) = EDD(I,I) \ ED(I);
    u(I) = u(I) - Delta_u(I);
    newton_iterations = newton_iterations + 1;
    norm_delta_u = termination_criterion(u_old, u, Delta_u);
end
post_processing
end
```

The quality of the discrete solution may be measured (e.g., see [CF00]) by the global error estimator η defined as

$$\eta = \frac{\sqrt{\sum_{T\in\mathcal{T}_h}\eta_T^2}}{\sqrt{\sum_{T\in\mathcal{T}_h}\int_T \sigma_h^* : \mathbb{C}^{-1}\sigma_h^*\,\mathrm{d}x}}\,, \tag{4.10}$$

where

$$\eta_T^2 = \int_T (\sigma_h - \sigma_h^*) : \mathbb{C}^{-1}\left(\sigma_h - \sigma_h^*\right)\,\mathrm{d}x\,,$$

and σ_h^* is a nodal Clement interpolation of the piecewise constant σ_h defined as

$$\sigma_h^*(v) = \frac{\sum_{\{k|v\in\overline{T_k}\}}|T_k|\sigma_h(T_k)}{\sum_{\{k|v\in\overline{T_k}\}}|T_k|}.$$

Utilizing obtained solution $\mathbf{u}$ (u_h respectively), the stress $\sigma(u_h)$ and its von Mises $\|\operatorname{dev}\sigma\|_F$ may be calculated per element. We are not only interested in the stress itself but also in its elastic and plastic parts and their nodal average value (see (4.10)). All this is realized in the Matlab© routine `post_processing`. Its implementation reads:

```
%% number of nodes / number of elements
nn = size(nodes,1); ne = size(elements,1);

%% von Mises and its elastic and plastic part: vM, vMe, vMp,
%% elastic and plastic part of the stress sigma: se, sp,
%% and their node-wise average: ase, asp.
vM = zeros(1,ne);   vMe = zeros(1,ne);  vMp = zeros(1,ne);
se = zeros(3,ne);   sp = zeros(3,ne);
ase = zeros(3,nn);  asp = zeros(3,nn);

areaOmega = zeros(1,nn);
yield = zeros(1,ne);
B = zeros(3,6);

for j = 1:ne
    aNodes = elements(j,:);
    vertices = nodes(aNodes,:);
    [B,area] = elem_B(vertices);
    areaOmega(aNodes) = areaOmega(aNodes) + area;
    I = 2 * elements(j,[1,1,2,2,3,3]) - [1,0,1,0,1,0];
    eps = B * u(I);

    se(:,j) = C * eps;     sp(:,j) = 2 * mu * p;
    dev_se = K * se(:,j);  dev_s = dev_se - sp(:,j);

    delta_p = p - p0;
    norm_delta_p = sqrt(delta_p' * N * delta_p);
    beta(j) = sigmaY * (1 + alpha(j) * H);
    vM(j) = sqrt(dev_s' * N * dev_s);
    vMe(j) = sqrt(dev_se' * N * dev_se);
    vMp(j) = sqrt(sp(:,j)' * N * sp(:,j));
    yield(j) = vM(j) - beta(j);

    ase(:,aNodes) = ase(:,aNodes) + area*se(:,j)*[1,1,1];
    asp(:,aNodes) = asp(:,aNodes) + area*sp(:,j)*[1,1,1];
end

ase = ase ./ ([1;1;1]*areaOmega);
asp = asp ./ ([1;1;1]*areaOmega);
error_estimation
```

The next task is to implement the calculation of the error estimator (4.10) in the Matlab© routine `error_estimation`, will not be presented here in detail.

4.4 Other Techniques Used

There are two additional numerical techniques implemented for the solution of the elastoplastic problem with perfectly plastic material ($H = 0$) in Example 4.

Nested Iteration Technique In order to obtain a reasonable initial approximation for the Newton-like method on the finer mesh, one can prolongate the solution u from the coarser mesh and take this value as the initial approximation u_0. This so called *nested iteration technique*, for a detailed info see [Hac85].

Damping Technique The idea of damping is to replace the upgrade of $\mathbf{u}_i$ defined in (4.7) by

$$\mathbf{u}_i = \mathbf{u}_{i-1} + \alpha_i \Delta \mathbf{u}_i$$

with a *damping* parameter $\alpha_i \leq 1$. The following strategy to determine α_i is based on the comparison of energies: α_i is originally set to 1 and halved until the energy functional is reduced, i.e., it holds

$$e(u_{i-1} + \alpha_i \Delta u_i) < e(u_{i-1}). \tag{4.11}$$

Chapter 5

Numerical Examples

The following tests were calculated on a computer with 2.4 GHz CPU, 2 Gb RAM using Matlab© version 7.0 on Linux OS. We define 'DOF' as the short form of *degrees of freedom*, and 'VPZ' to be the short form of *variation in plastic zones* which is calculated as follows: In the i-th iteration step the boolean vector $\mathbf{w}^i$ stores the information about which elements are plastic and which are not by defining its components

$$w_j^i := \begin{cases} 1 & \text{if } T_j \text{ is a plastic element,} \\ 0 & \text{else.} \end{cases}$$

Let the starting vector $\mathbf{w}^0 = 0$. Variation in plastic zones VPZ_{i-1}^i from the $(i-1)$-st to the i-th iteration step is defined by

$$\mathrm{VPZ}_{i-1}^i = \frac{100}{\mathrm{N}_{\mathcal{T}}} \sum_{j=1}^{n} |w_j^i - w_j^{i-1}|.$$

It all numerical examples, the termination bound $\epsilon = 1e - 12$ was used.

Example 1 (L-Shape)**.** *This example is taken from [ACFK02] and its geometry and the coarse grid triangulation are displayed in Figure 5.1. We assume non-homogeneous Dirichlet boundary conditions in polar coordinates* r, θ

$$\begin{aligned} u_r(r,\theta) =& \frac{1}{2\mu} r^\alpha \left[-(\alpha+1)\cos((\alpha+1)\,\theta) + (\mathrm{C}_2 - (\alpha+1))\mathrm{C}_1 \cos((\alpha-1)\,\theta) \right], \\ u_\theta(r,\theta) =& \frac{1}{2\mu} r^\alpha \left[(\alpha+1)\sin((\alpha+1)\,\theta) + (\mathrm{C}_2 + (\alpha-1))\mathrm{C}_1 \sin((\alpha-1)\,\theta) \right]. \end{aligned} \tag{5.1}$$

Level	1	2	...	6	7	8
DOF	10	66	...	20466	97282	391170
Relative Error:						
step 1	2.8383e-02	3.9827e-02	...	7.2243e-02	7.0236e-02	6.8321e-02
step 2	1.0467e-04	1.2352e-03	...	1.1004e-02	1.1063e-02	1.1022e-02
step 3	2.3781e-09	6.1409e-07	...	1.1453e-03	1.2746e-03	1.3552e-03
step 4	1.0944e-16	2.9589e-13	...	2.0826e-05	4.0743e-05	5.9611e-05
step 5			...	6.8005e-09	5.1957e-08	2.0693e-07
step 6			...	5.2211e-15	1.3866e-13	4.3361e-12
step 7			...			1.8774e-14
VPZ (%):						
step 0-1	16.67	10.42	...	10.59	10.61	10.62
step 1-2	0	2.083	...	2.873	2.816	2.752
step 2-3	0	0	...	0.2686	0.2218	0.1638
step 3-4	0	0	...	0.04069	0.02848	0.01882
step 4-5			...	0	0	0
step 5-6			...	0	0	0
step 6-7			...			0
Time (seconds)	2.00537	2.25042	...	142.29	590.106	2692.87
Error Estimator	0.401437	0.2482	...	0.0409114	0.0272622	0.0181553

Table 5.1: Convergence table in Example 1 **(Lshape)**. The table displays the relative error in displacements (4.8) and the variation of plastic zones (VPZ) for various uniformly refined meshes. The quality of the discrete solutions is measured by the global error estimator (4.10).

The critical exponent $\alpha \approx 0.544483737$ *is the solution of the equation*

$$\alpha \sin(2\omega) + sin(2\omega\alpha) = 0$$

with $\omega = \frac{3\pi}{4}$ *and* $\mathrm{C}_1 = -(\cos((\alpha+1)\omega))/\cos((\alpha-1)\omega), \mathrm{C}_2 = (2(\lambda+2\mu))/(\lambda+\mu)$*. It can be shown that the formulae (5.1) describe the solution of the perfect elastic problem with the same non-homogeneous Dirichlet boundary conditions also in the interior of the Lshape domain. Thus there is an strain-singularity in the reentrant corner, which can also be expected for the elasto-plastic case. The material parameters are defined as*

$$E = 1e5,\ \nu = 0.3,\ \sigma_Y = 2.2,\ H = 1.$$

Figure 5.2 shows the yield function (right) and the elastoplastic zones, where perfect elastic zones are colored green (light gray in case of a non-color print respectively), and elastoplastic zones are colored pink (dark grey respectively). The domain's displacement is multiplied by 3e3*. Table 5.1 reports on convergence behaviour of the Newton-like method for graduated uniform meshes.*

Example 2 (Wrench)**.** *This example simulates the deformation of a screw-wrench under pressure. Problem geometry is shown in Figure 5.3: A screw-wrench* sticks *on a screw (homogeneous Dirichlet boundary condition) and a*

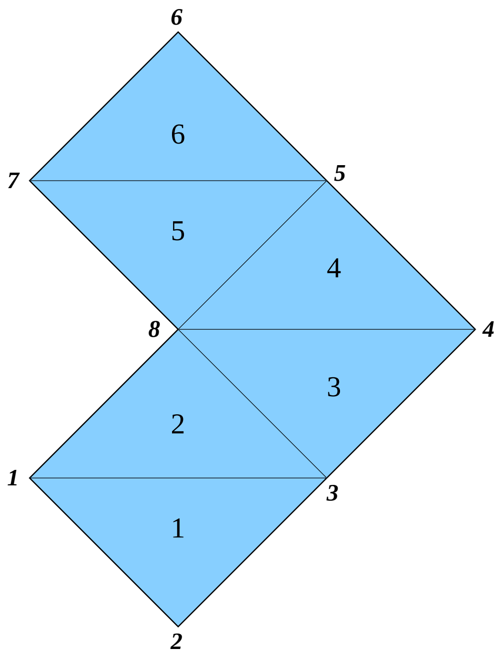

Figure 5.1: Problem geometry and the coarse triangulation of Example 1. The L-shape domain Ω is described by the polygon $(-1,-1)$, $(0,-2)$, $(2,0)$, $(0,2)$, $(-1,1)$, $(0,0)$.

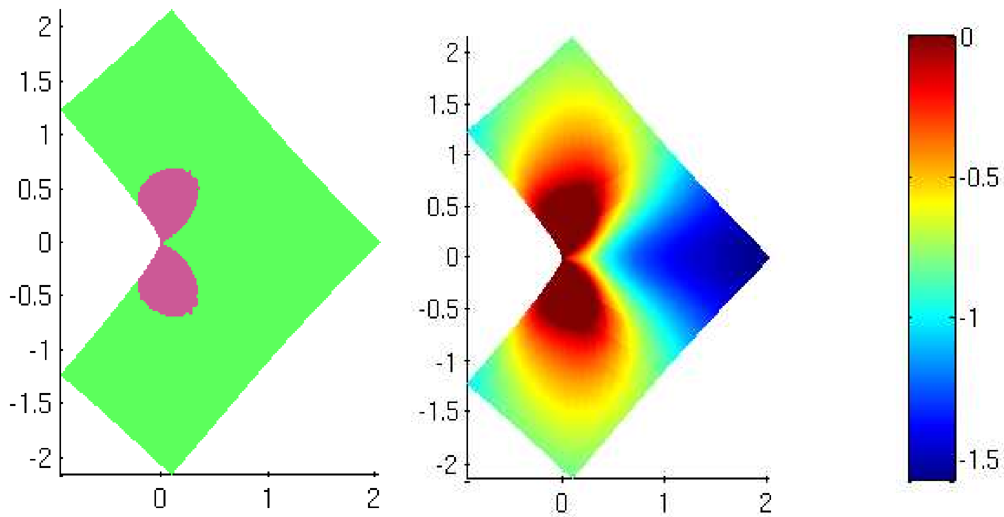

Figure 5.2: Plastic zones (left) and yield function (right) in Example 1.

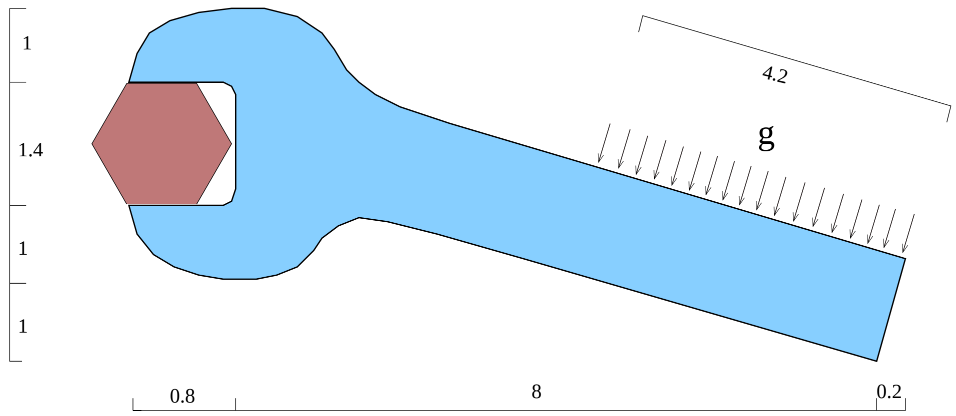

Figure 5.3: Problem geometry in Example 2.

surface load g is applied to a part of the wrench's handhold in interior normal direction (Neumann boundary condition). The material parameters are set

$$E = 2e8, \; \nu = 0.3, \; \sigma_Y = 2e6, \; H = 0.001$$

and the problem was calculated traction $g(x) = 6e4$. Figure 5.4 shows the yield function (right) and the elastoplastic zones, where perfect elastic zones are colored green (light gray in case of a non-color print respectively), and elastoplastic zones are colored pink (dark grey respectively). The displacement of the domain is multiplied by factor 10*. Table 5.2 reports on the convergence of the Newton-like method for graduated uniform meshes.*

Example 3 (Square)**.** *This is a self constructed example and serves for the comparison of problems with positive hardening parameter $H > 0$, and truly plastic ($H = 0$) problems. The example domain is a unit square $(x, y) \in [0, 1] \times [0, 1]$ which has zero-displacement prescribed on the part of the boundary where $x = 0$ and a surface load is applied on the opposite part of the boundary (see Figure 5.5). The material parameters are set*

$$E = 1 \; , \; \nu = 0.25 \; , \; \sigma_y = 0.75$$

and the surface load is of the intensity $g = 1$. We observe two different cases of hardening, where the hardening parameter is first set to $H = 1$, and then $H = 0$ (which means a perfectly plastic behaviour of the material, no hardening effect is applied). Figure 5.6 shows the graphical output in case of $H = 1$ and Figure 5.7 in the case of $H = 0$. Both figures show the yield function (right) and the elastoplastic zones, where perfect elastic zones

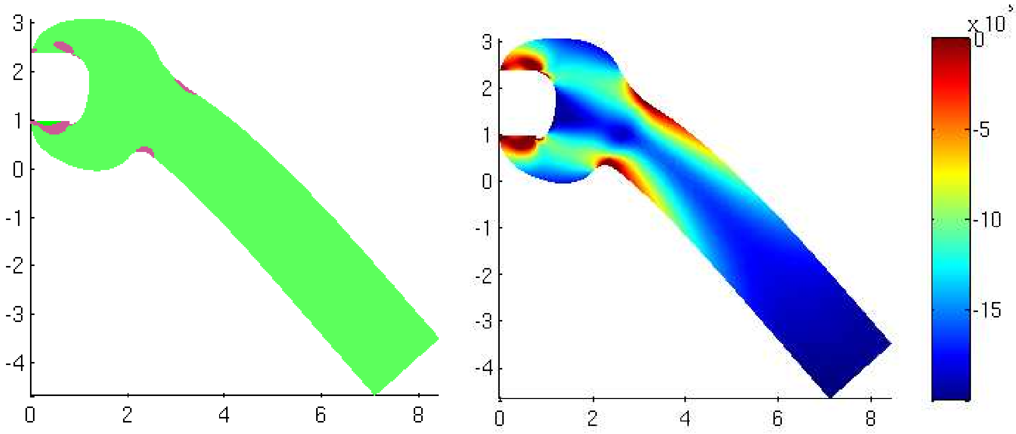

Figure 5.4: Plastic zones (left) and yield function (right) in Example 2.

Level	0	1	. . .	5	6	7
DOF	60	202	. . .	41662	165246	658174
Relative Error:						
step 1	2.3834e-14	3.6169e-03	. . .	1.3194e-01	1.4872e-01	1.5846e-01
step 2		2.3598e-06	. . .	5.6966e-02	6.9302e-02	7.9603e-02
step 3		1.5324e-11	. . .	7.5805e-03	1.3223e-02	2.9909e-02
step 4		4.5752e-15	. . .	4.0307e-04	2.4344e-03	3.5626e-03
step 5			. . .	5.9665e-06	2.1840e-04	1.2013e-04
step 6			. . .	2.9485e-10	1.5089e-05	1.0364e-05
step 7			. . .	7.8696e-14	3.8914e-09	1.1642e-09
step 8			. . .		1.5508e-13	2.9988e-13
VPZ (%):						
step 0-1	0	1.25	. . .	1.819	1.83	1.828
step 1-2		0	. . .	0.9741	1.168	1.27
step 2-3		0	. . .	0.3564	0.5591	0.7588
step 3-4		0	. . .	0.05127	0.1501	0.1418
step 4-5			. . .	0.002441	0.02563	0.02319
step 5-6			. . .	0	0.00183	0.004425
step 6-7			. . .	0	0	0
step 7-8			. . .		0	0
Time (seconds)	1.31385	2.58625	. . .	262.304	1177.64	4892
Error Estimator	0.780432	0.53131	. . .	0.0868307	0.0758023	0.0421956

Table 5.2: Convergence table in Example 2 **(wrench)**. The table displays the relative error in displacements (4.8) and the variation of plastic zones (VPZ) for various uniformly refined meshes. The quality of the discrete solutions is measured by the global error estimator (4.10).

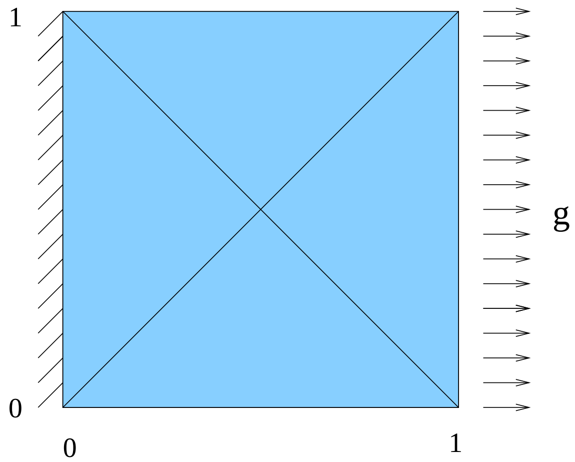

Figure 5.5: Problem geometry in Example 3.

are colored green (light gray in case of a non-color print respectively), and elastoplastic zones are colored pink (dark grey respectively). The domains' displacement is not magnified, the true deformation is shown in the pictures. Table 5.3 (representing the case $H = 1$*) and Table 5.4 (representing the case* $H = 0$*) report on the convergence of the Newton-like method for graduated uniform meshes.*

Example 4 (Plate with a Hole)**.** *This example is taken from [ea02] and serves as a benchmark problem in computational plasticity. The example domain is a thin plate represented by the square* $(-10, 10) \times (-10, 10)$ *with a circular hole of the radius* $r = 1$ *in the middle, as can be seen in Figure 5.8. A surface load* g *is applied on the plate's upper and lower edge. Due to symmetric geometry only the right upper quarter of the domain is discretized. Therefore it is necessary to incorporate homogeneous Dirichlet boundary conditions in the normal direction (gliding conditions) to both symmetric edges. The material parameters are set*

$$E = 206900,\ \nu = 0.29,\ \sigma_Y = \sqrt{\frac{2}{3}}\,450,\ H = 0.$$

It means our model is a perfect plasticity model. Figure 5.9 shows the yield function (right) and the elastoplastic zones, where perfect elastic zones are colored green (light gray in case of a non-color print respectively), and elastoplastic zones are colored pink (dark grey respectively). The domains' displacement is multiplied by 100*. Table 5.5 reports on the convergence of the*

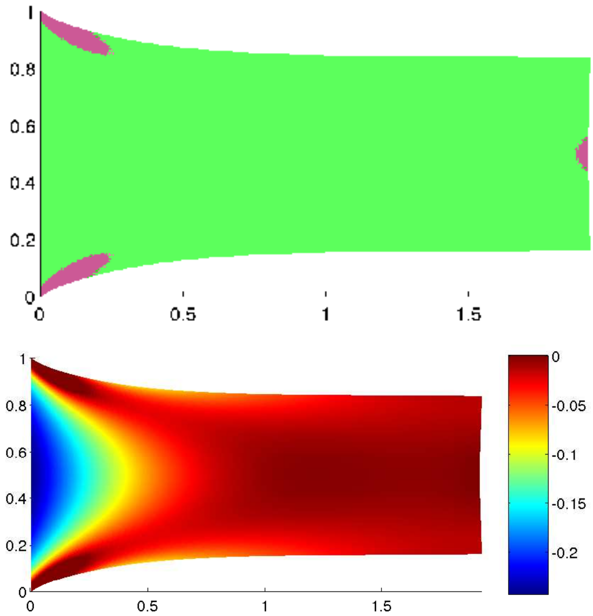

Figure 5.6: Plastic zones (left) and yield function (right) in Example 3 in case $H = 1$.

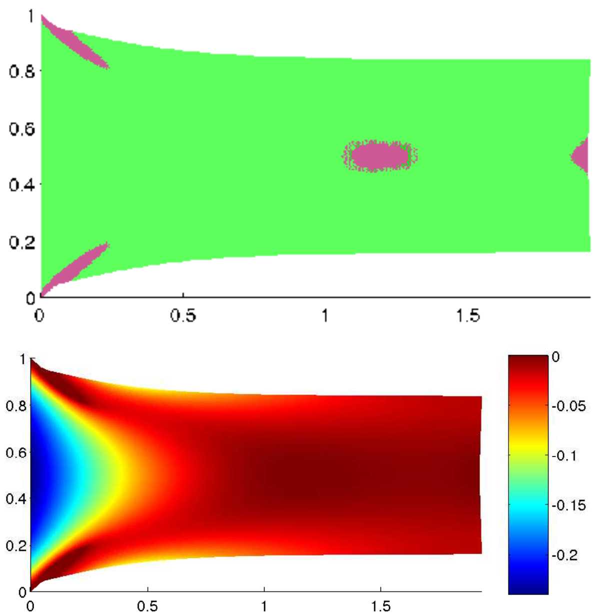

Figure 5.7: Plastic zones (left) and yield function (right) in Example 3 in case $H = 0$.

Level	0	1	...	5	6	7
DOF	6	20	...	4160	16512	65792
Relative Error:						
step 1	1.67948e-02	5.62960e-03	...	5.48869e-03	6.06131e-03	6.39332e-03
step 2	3.44605e-05	7.33811e-06	...	2.01132e-04	2.86164e-04	2.79363e-04
step 3	3.36819e-10	2.82448e-11	...	7.21780e-08	9.12035e-08	2.35338e-06
step 4	1.50017e-16	1.56205e-16	...	2.05151e-14	3.94780e-14	1.57881e-11
step 5			...			7.05586e-15
VPZ (%):						
step 0-1	25	37.5	...	2.02637	1.97754	1.9455
step 1-2	0	0	...	0.463867	0.445557	0.465393
step 2-3	0	0	...	0	0	0.0183105
step 3-4	0	0	...	0	0	0
step 4-5			...			0
Time (seconds)	2.2143	2.42969	...	18.1882	66.7801	330.939
Error Estimator	0.107404	0.0714261	...	0.0122737	0.00760944	0.00475053

Table 5.3: Convergence table in Example 3 **(Square)** in the case of $H = 1$. The table displays the relative error in displacements (4.8) and the variation of plastic zones (VPZ) for various uniformly refined meshes. The quality of the discrete solutions is measured by the global error estimator (4.10).

Level	0	1	...	5	6	7
DOF	6	20	...	4160	16512	65792
Relative Error:						
step 1	5.03227e-02	2.30661e-02	...	1.87329e-02	2.17813e-02	2.35984e-02
step 2	7.86281e-04	4.94048e-04	...	7.40276e-03	1.33097e-02	1.67965e-02
step 3	3.20219e-07	3.21271e-07	...	8.99501e-04	2.47052e-03	6.41590e-03
step 4	4.85554e-14	1.36983e-13	...	1.07093e-04	6.24283e-05	4.33666e-04
step 5			...	8.68903e-08	1.11550e-07	4.18118e-06
step 6			...	8.73918e-14	1.74937e-13	1.11410e-07
step 7			...			1.56830e-13
VPZ (%):						
step 0-1	25	37.5	...	2.02637	1.97754	1.9455
step 1-2	0	0	...	1.66016	1.17798	1.23138
step 2-3	0	0	...	1.46484	1.5625	1.42212
step 3-4	0	0	...	0.170898	0.512695	0.692749
step 4-5			...	0	0.0244141	0.0961304
step 5-6			...	0	0	0.00915527
step 6-7			...			0
Time (seconds)	2.45892	2.39072	...	22.9372	86.8105	427.568
Error Estimator	0.112262	0.071381	...	0.0135967	0.0095563	0.00695883

Table 5.4: Convergence table in Example 3 **(Square)** in the case of $H = 0$. The table displays the relative error in displacements (4.8) and the variation of plastic zones (VPZ) for various uniformly refined meshes. Comparing this table with Table 5.3 we observe, that the super-linearly convergence rate concerning the relative error is lost. At least, the Newton-like method *is* converging in this test example. This is not necessarily the case in examples where $H = 0$ (see Example 4). The quality of the discrete solutions is measured by the global error estimator (4.10).

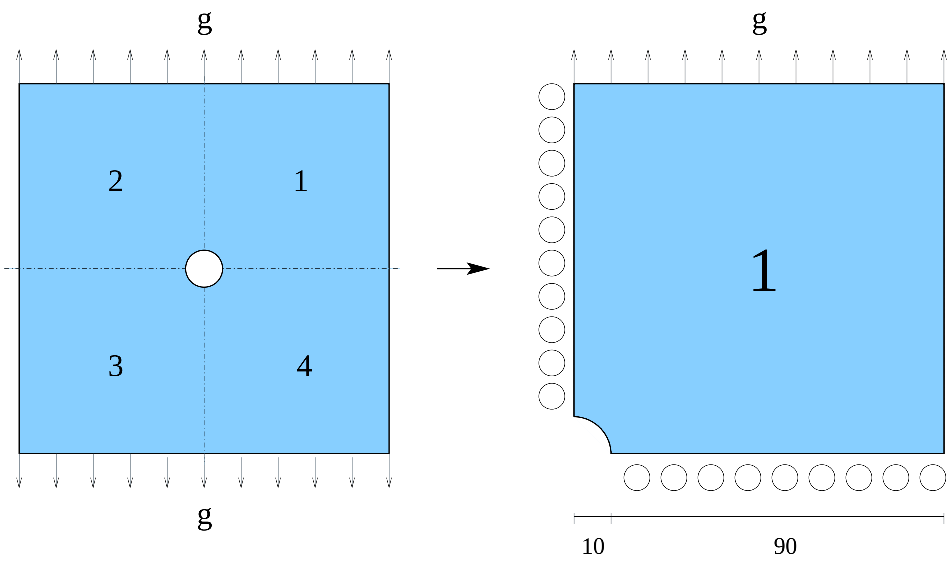

Figure 5.8: Problem geometry in Example 4.

Newton-like method for graduated uniform meshes. It turns out that the non-nested iteration technique which was successful in other previous example does not work here for finest mesh. Therefore, the nested iteration technique or the damping technique are used, see Table 5.6 for more details.

Level	0	1	...	3	4	5
DOF	245	940	...	14560	57920	231040
Non-nested iteration technique						
Relative Error:						
step 1	2.4308e-02	5.4158e-02	...	8.0495e-02	8.4982e-02	8.6934e-02
step 2	9.8924e-03	2.6174e-02	...	7.0273e-02	8.2874e-02	9.7932e-02
step 3	1.0180e-03	4.1482e-03	...	2.6452e-02	3.8208e-02	1.4122e-01
step 4	1.1566e-06	4.6425e-04	...	3.5268e-03	6.1751e-03	4.6951e-01
step 5	4.0331e-12	1.6937e-05	...	1.7461e-04	4.5520e-04	8.3690e-01
step 6	4.3289e-16	1.3371e-09	...	3.6869e-06	6.0711e-05	9.5657e-01
step 7		9.3330e-16	...	2.4166e-10	4.5021e-07	9.8160e-01
step 8			...	3.6081e-15	5.4823e-12	...
step 9			...		7.3296e-15	diverging
VPZ (%):						
step 0-1	2.667	4.778	...	5.299	5.345	5.356
step 1-2	3.11	5	...	7.104	7.252	7.498
step 2-3	0.4444	2.444	...	4.674	5.045	5.509
step 3-4	0	0.6667	...	1.639	2.08	0.5994
step 4-5	0	0.1111	...	0.3472	0.4948	1.815
step 5-6	0	0	...	0.02778	0.07465	0.3416
step 6-7		0	...	0	0.006944	0.1141
step 7-8			...	0	0	...
step 8-9			...		0	diverging
Time (seconds)	3.23081	8.16373	...	106.88	468.615	-
Nested iteration technique						
Relative Error:						
step 1	2.4308e-02	5.5612e-02	...	5.1909e-02	3.9135e-02	2.4310e-02
step 2	9.8924e-03	1.8466e-02	...	1.0428e-02	7.3208e-03	3.1321e-03
step 3	1.0180e-03	2.6082e-03	...	1.2247e-03	1.6236e-03	5.9788e-04
step 4	1.1566e-06	2.1786e-04	...	7.0150e-05	1.6808e-04	1.4709e-04
step 5	4.0330e-12	1.6854e-05	...	6.1389e-08	3.3952e-06	3.1330e-06
step 6	5.6042e-16	1.3203e-09	...	8.1421e-14	2.4807e-10	1.1140e-09
step 7		7.9697e-16	...		6.8650e-15	1.5225e-14
VPZ (%):						
step 0-1	2.667	6.333	...	14.7	15.24	15.28
step 1-2	3.11	3.889	...	2.257	1.307	0.6021
step 2-3	0.4444	2.111	...	0.8125	0.3594	0.1402
step 3-4	0	0.3333	...	0.1458	0.1181	0.03472
step 4-5	0	0.1111	...	0.006944	0.0191	0.007378
step 5-6	0	0	...	0	0	0
step 6-7		0	...		0	0
Time (seconds)	3.2685	11.1333	...	119.328	492.936	2119.71
Error Estimator	0.0519797	0.0456903	...	0.0244116	0.0153209	0.00881961

Table 5.5: Convergence table in Example 4 **(plate with a hole)**. The table displays the relative error in displacements (4.8) and the variation of plastic zones (VPZ) in iteration steps for various uniformly refined meshes. The quality of the discrete solutions is measured by the global error estimator (4.10).

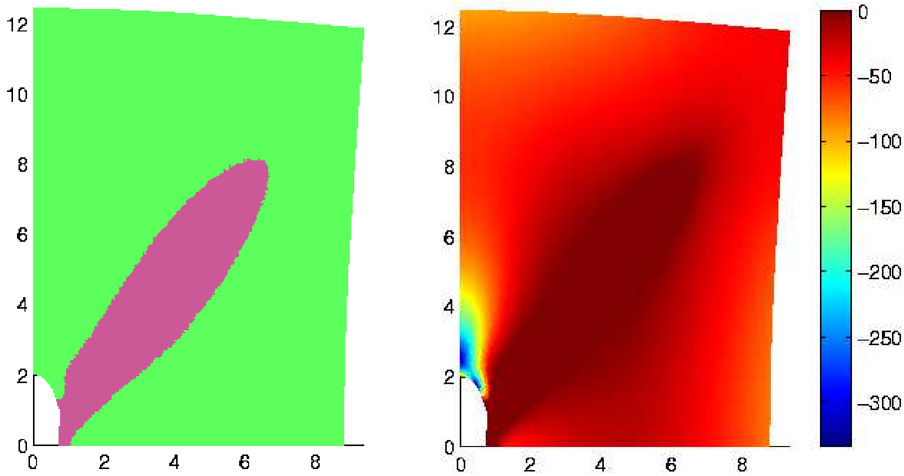

Figure 5.9: Plastic zones (left) and yield function (right) in Example 4.

Problem 'Plate with a Hole' at Level 5 (DOF=231040)					
	Standard Newton-like Method		Damped Newton-like Method		
	Error in $e(u)$	Error in u	Error in $e(u)$	Error in u	k
step 1	-3.1619e-01	8.6934e-02	-3.4320e-03	8.6934e-02	0
step 2	-5.1283e-02	9.7932e-02	-5.5442e-04	9.7932e-02	0
step 3	2.8336e-01	1.4122e-01	-6.2037e-04	1.4517e-01	2
step 4	2.1854e+00	4.6951e-01	-1.3852e-04	4.8643e-02	0
step 5	7.2304e+00	8.3690e-01	-1.9002e-04	7.9731e-02	2
step 6	2.1073e+01	9.5657e-01	-6.3455e-05	2.3192e-02	1
step 7	5.9547e+01	9.8160e-01	-2.0840e-05	1.1869e-02	1
step 8	1.3702e+02	9.8480e-01	-1.2660e-05	7.7685e-03	1
step 9	3.6256e+02	9.8221e-01	-6.1992e-06	2.3371e-03	0
step 10	9.0941e+02	9.8513e-01	-6.5443e-08	5.3965e-04	0
step 11	1.5903e+03	9.8493e-01	-9.1647e-09	2.9142e-04	0
step 12	3.1730e+03	9.7935e-01	-4.5144e-11	2.3221e-05	0
step 13	1.0887e+04	9.7633e-01	-1.3790e-15	1.3469e-07	0
step 14	...	...	-2.8347e-15	4.4192e-12	0
step 15	not converging		9.9597e-16	1.4070e-14	0

Table 5.6: Complementary convergence table in Example 4 **(plate with a hole)**. The standard Newton-like method with a zero initial approximation does not converge in Example 4 for refinement level 5 with 231040 degrees of freedom. Thus, the damping technique is applied. Both standard (non-damped with $\alpha = 1$) and damped Newton-like method ($\alpha_i = 2^{-k}$, where k denotes the number of damping steps) are compared: the relative errors in the displacement u_i and the relative errors in the energy $e(u_i)$ at the i-th iteration step are computed by (4.8) and (4.9). The right most column reports on how many damping steps k have been necessary to guarantee the energy reduction (4.11).

Chapter 6

Conclusions

The main contribution of this thesis was to show that the minimization functional $e(u)$ is Fréchet differentiable and that the derivative can be expressed analytically. Hence, the exact solution can be found by solving the nonlinear problem $De(u) = 0$ utilizing a solver of the field of smooth optimization. The second derivative is continuous in all points apart from the elastoplastic interface, i.e., the set which parts perfect elastic zones where $p = 0$ from elastoplastic zones where $p \neq 0$. The measure of the set of these interface points is known to be zero in the continuous case. Therefore, a Newton-like method is expected to converge in the discrete case also. We then discretized in space via h-FEM utilizing low-order ansatz functions. In all of the numerical examples we could observe that, in case the hardening parameter H does not equal zero, the Newton-like method indeed satisfies our expectations, i.e., it converges super-linearly and even quadratically in some cases.

This thesis does not contain any theoretical propositions about convergence and convergence rates or factors. Hence, all statements about convergence in this thesis must be understood as a guess which arose by observing computational results. However, those results give us the reason to expect that super-linearly (or even quadratically) convergence might be verified theoretically as well. Thus, one possible direction of extending the work from this thesis is the study of convergence analysis.

Hence the second derivative of the energy functional is discontinuous, the application of a semi-smooth Newton method or a Quasi-Newton method, such as Broyden method (BFGS method), is recommended. Another fruitful approach could be to apply hp-FEM instead of h-FEM or, at least, to increase the polynomial order of ansatz function when applying h-FEM. For this purpose, it is necessary to examine the order of smoothness of the exact solution first in order to justify such an approach.

All of the numerical examples of this thesis are two dimensional. Thus, a further approach to continue this work would be to implement the three dimensional case as well. It would also be interesting to re-implement the solver in other frameworks or program languages in order to compare with.

The application of Moreau-Yosida's theorem does not only allow for the construction of a new solver, but also opens up new aspects in the theoretical research of elastoplasticity. Hence, amongst all of the many possibilities of continuing this work, convergence analysis might be the most exciting one.

Appendix A
List of Used Notation

d	$\in \mathbb{N}$, space dimension
Ω	$\subset \mathbb{R}^d$, open domain
Γ	$= \partial\Omega$, domain boundary
Γ_D	$\subset \Gamma$, Dirichlet boundary (prescribed deformations)
Γ_N	$\subset \Gamma$, Neumann boundary (prescribed surface forces)
n	outer normal of Γ
σ	stress
ε	elastic strain
u	deformation
p	plastic strain
α	hardening parameter
f	body forces
u_D	prescribed deformations on Γ_D
g	prescribed surface forces on Γ_N
λ	$\in \mathbb{R}^+$, "Lamé modulus", Lamé constant
μ	$\in \mathbb{R}^+$, "sheer modulus", Lamé constant
E	$\in \mathbb{R}^+$, "Young's modulus"
ν	$\in \left[0, \frac{1}{2}\right]$, "Poisson ratio"
δ_{ij}	"Kronecker delta"
$\mathbb{C}$	$\in \mathbb{R}^{d\times d}_{d\times d}$ with $\mathbb{C}_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, elasticity tensor
H	$\in \mathbb{R}^+$, "modulus of hardening"
σ_y	$\in \mathbb{R}^+$, yield stress
φ	dissipation functional
ϕ	yield function
$\dot{f}$	$= \frac{\partial f}{\partial t}$, time derivative of a function f
∇f	$= \left(\frac{\partial f_i}{\partial x_j}\right)_{i,j}$, gradient of a (vector) function f
Δf	$= \sum_i \frac{\partial^2 f_i}{\partial^2 x_i}$, Laplace of a vector function f
Df	Fréchet Derivative of function f
$\lVert A\rVert_F$	$= \sqrt{\sum_{i,j} a_{ij}^2}$, Frobenius norm of a matrix A

Bibliography

[AC00] J. Alberty and C. Carstensen, *Numerical analysis of time-depending primal elastoplasticity with hardening*, SIAM J. Numer. Anal. **37** (2000), no. 4, 1271–1294.

[ACFK02] J. Alberty, C. Carstensen, S. A. Funken, and R. Klose, *Matlab implementation of the finite element method in elasticity*, Computing **69** (2002), no. 3, 239–263. MR 1 954 562

[ACZ99] J. Alberty, C. Carstensen, and D. Zarrabi, *Adaptive numerical analysis in primal elastoplasticity with hardening*, Comput. Methods Appl. Mech. Eng. **171** (1999), no. 3-4, 175–204.

[CF00] C. Carstensen and S. A. Funken, *Averaging technique for fe-a posteriori error control in elasticity: Part II: $\lambda-$ independent estimates.*, Tech. report, Christian-Albrechts-Universität zu Kiel, 2000, http://www.numerik.uni-kiel.de/reports/1999/99-14.html.

[ea02] E. Stein (et al.), *Error-controlled adaptive finite elements in solid mechanics*, John Wiley and Sons Ltd, 2002.

[Hac85] W. Hackbusch, *Multi-grid methods and applications*, Springer-Verlag Berlin, Heidelberg, 1985.

[HR95] W. Han and B. Reddy, *Computational plasticity: the variational basis and numerical analysis*, Computational Mechanics Advances 2 (1995), 283–400.

[HR99] W. Han and B.D. Reddy, *Plasticity: Mathematical theory and numerical analysis*, Springer-Verlag New York, 1999.

[Kos91] P. Kosmol, *Optimierung und Approximation*, Walter de Gruyter, 1991.

[Mor65] J.J. Moreau, *Proximité et dualité dans un espace hilbertien*, Bulletin de la Société Mathématique de France **93** (1965), 273–299.

[SH98] J.C. Simo and T.J.R. Hughes, *Computational inelasticity*, Springer-Verlag New York, 1998.

[Yos94] K. Yosida, *Functional Analysis*, Springer, 1994, Reprint of the 6th edition.

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Eidesstattliche Erklärung

Ich, Peter Gruber, erkläre an Eides statt, dass ich die vorliegende Diplomarbeit selbstständig und ohne Hilfe verfasst, andere als die angegebenen Quellen und Hilfsmittel nicht benutzt bzw. die als wörtlich oder sinngemäß entnommenen Stellen als solche kenntlich gemacht habe.

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