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Diploma Thesis

Optimal Control in Implant Shape Design

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Abstract

The goal of this thesis is in laying the ground for the implementation of an algorithm that can accurately determine the shape and position of an implant in the facial area. The behaviour of the soft tissue will be modeled using materials laws that are defined through polyconvex energy functions. It will be seen that the modeling as an optimal control problem with Neumann boundary control will be of advantage, especially with regard to the correct treatment of the contact surface between the implant and the surrounding soft tissue. In the nonlinear case the existence of solutions of the optimal control problem will be proven and a perspective on the problems to overcome in the context of well-posedness with respect to the control and the necessary optimality conditions will be given. Moreover the applicability of the linearized model, that bases upon Hooke's material law, will be discussed and the corresponding optimality conditions will be derived. These will be solved using a finite-element-discretization and the Newton method. For the choice of the Tichonoff regularization parameter the L-curve criterion will be used and the dependence of the optimal choice of this parameter, with respect to the stability and residual error, on the material constants will be examined.

Zusammenfassung

Ziel dieser Arbeit ist es die Grundlagen zur Implementation eines Algorithmuses, welcher die Position und Form eines Implantats im Bereich des Gesichtes exakt bestimmen kann, zu legen. Das Verhalten des Weichgewebes wird durch Materialgesetze, welche über polykonvexe Energiefunktionen definiert sind, modelliert. Zur Berechnung des Implantats erweist sich, insbesondere im Hinblick auf die korrekte Behandlung der Kontaktfläche zwischen Implantat und umliegendem Weichgewebe, die Modellierung als Optimalsteuerungsproblem mit Neumann-Randsteuerung als vorteilhaft. Im nichtlinearen Fall wird die Existenz von Lösungen des Optimalsteuerungsproblems bewiesen und ein Ausblick auf zu überwindende Schwierigkeiten im Hinblick auf die Wohlgestelltheit bzgl. der Steuerung sowie der notwendigen Optimalitätsbedingungen gegeben. Desweiteren wird die Anwendbarkeit eines linearisierten Modells, basierend auf Hooke's Materialgesetz, diskutiert und die zugehörigen Optimalitätsbedingungen werden hergeleitet. Diese werden mittels Finite-Elemente-Diskretisierung und dem Newton-Verfahren gelöst. Zur Wahl des Tichonoff-Regularisierungsparameters wird das L-Kurven-Kriterium herangezogen und die Abhängigkeit der optimalen Wahl dieses Parameters, bzgl. Stabilität und Größe des Residuums, von den Materialkonstanten untersucht.

Contents

Introduction

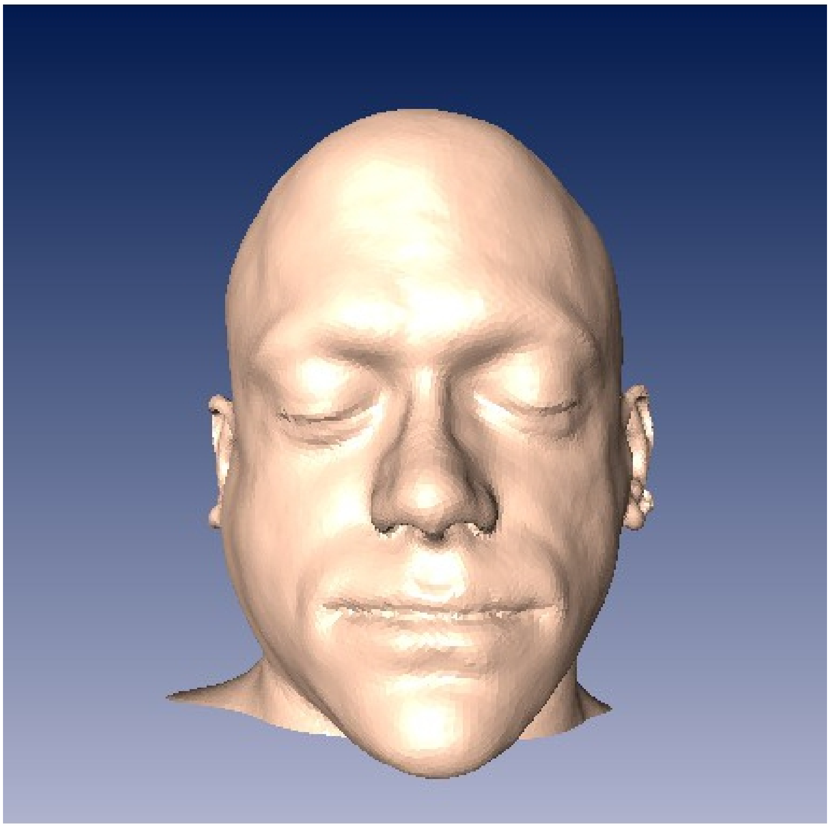

Figure 1: A model of a head on which an implant insertion should be performed

As in many parts of modern medicine the design of implants is today more dependent on the experience of medical scientists than on technical tools. In most cases the determination of an implant's shape is done by visually comparing CT (**c**omputer **t**omography or X-ray **c**omputed **t**omography) scans with implant models and choosing a model that seems to fit. This approach is very sensitive to the surgeon's skills and the geometry of the implant. Especially in the case of heavy fractures or natural deformations of the oral and maxillofacial bone structure (as in Figure 1) it is often difficult to accurately predict the shape of the patients face after the medical treatment. Consequently it would be of advantage if one could delegate the determination of an implant's shape from a given desired shape of the skin to a computer-assisted tool. This would allow to give reliable assistance regarding the training, preparation and verification of implant insertions. In order to provide such a tool it is necessary to develop appropriate mathematical models and numerical schemes for the calculation of the implant's shape.

As a first step in the derivation of such a model the behaviour of the soft tissue, surrounding an implant, must be described mathematically. In contrast to most "dead" soft tissues, that can be described by comparatively simple models, biological soft tissues are influenced by very complicated effects like the flow of blood and water or muscle contractions. The examination and description of these soft tissues is the main topic of the relatively new field of biomechanics, which refers to a great extend to elasticity theory. In this context it is necessary to determine a material law (also named constitutive equation) that describes the specific stress-strain relationship of a type of elastic material. In order to recognize the decisive role of material laws in the mathematical analysis and the quality of the model the next chapter is devoted to a short historical overview over the major progresses achieved in the description of biological soft tissues and the choices of material laws in the context of this thesis.

History of material laws

The history of material laws starts in 1660 with Hooke's material law, stated by Robert Hooke as a latin anagram. In 1678 he published the solution as "Ut tensio, sic vis" (engl.: "As the extension, so the force"). This material law is, due to its simplicity, still the most popular material law, and, unfortunately, many times used inadequately. It has been generalized by Jean Claude Saint-Venant in 1844 and Gustav Robert Kirchhoff in 1852 to the St.Venant-Kirchhoff material law. Both, Hooke's material law and the St.Venant-Kirchhoff material law assume a linear stress-strain relationship, but in contrast to the first, the second takes into account a geometric nonlinearity. Thus Hooke's material law is a geometric first-order approximation of the St. Venant-Kirchhoff material law. In the same period, namely in 1847, M. G. Wertheim showed, that the stress-strain relationship for human soft tissues is in general nonlinear and proposed the first material law incorporating a constitutive nonlinearity. The occurrence of both, the geometric and the constitutive, nonlinearities leads to very complicated models. Thus one of the major problems in elasticity theory is the determination of material laws that accurately model the behaviour of elastic materials and remain accessible to mathematical analysis.

Despite of being studied for a long time it took until the middle of the 20th century that, with the newly emerging field of biomechanics, major progresses in the search of material laws for soft tissues and their mathematical analysis could be achieved. This is on one hand due to the availability of the computer and the development of the finite element method, that allowed the verification of proposed material laws. On the other hand in World War II the research in elasticity theory as well as nonlinear field theory was of military interest and a lot of effort was spent in the progress of these fields during the war. Moreover both elastomers (rubber-like materials) and biological soft tissues exhibit a long-chain, cross-linked polymeric structure and in the first half of the 20th century the developments for both material types proceeded hand in hand ([Hu03]).

In 1972 Ray W. Ogden proposed material laws for isotropic, incompressible and compressible rubber-like materials in [Og72a, Og72b]. These material laws, generalizing the Mooney-Rivlin material law and the Neo-Hookean material law proposed by Ronald Rivlin in 1948, are capable to incorporate the change of the materials stiffness and nonuniqueness of solutions. Additionally they show an excellent agreement with experimental data for rubber-like materials (see a. o. [Og72a, Og72b]). This was followed in 1977 by John Ball's famous existence proofs in [Ba77] for polyconvex stored energy functions (see Def. 1.8). A generalization of the theorems that are important for this thesis is stated in the appendix as Theorem A.1. This theorem includes Mooney-Rivlin materials, incompressible Ogden materials and in the compressible case materials similar to Ogden materials (i.e. Ogden-type materials as used in [We07]). While Ogden's material law seems to fit perfectly for rubber-like materials, the fact that it does not incorporate anisotropic effects makes it not yet the material law of choice for human soft tissues (see a.o. [Ho03]).

Between 1967 and 1983 Fung developed a material law using the exponential function that can incorporate anisotropy and that still can be specified by relatively few material parameters (2 in the case isotropy, 4-9 for the different kinds of anisotropy). If the behaviour of a material can be described by this material law it is often called Fung-elastic. Experiments have shown that this constitutive equation is a good model for human soft tissue ([Fu93, Hu03]). There also exist a lot more material laws that do not play an important role in the modelling of biological soft tissues resp. are very new and more complicated and therefore will not be stated here. In [Hu03] and [Fu93] some of these can be found and references for more.

A very detailed discussion of biological soft tissues and their stress-strain relationships has been performed in [Fu93]. Fung observed that, in contrast to most other regions in the human body, the muscles in the face are reinforced with collagen fibres and thus exhibit an anisotropic, highly nonlinear behaviour. Additionally it could be seen that the stiffness of the material increases with muscle contraction. As experiments, published by Y.C. Fung in 1993 ([Fu93]), show the properties of the collagen fibres dominate the facial soft tissues behaviour for strain ratios bigger than 15%. For smaller strains the isotropic fat tissue, dermis, epidermis and the ground material, that can be described by linear material laws, mainly determine the stress-strain relationship. Therefore in this case the St.Venant-Kirchhoff law or, if the geometric nonlinearity can be neglected, Hooke's material law can be used in order to get linear models.

For larger strain ratios the facial soft tissue will be modeled as a quasi-incompressible Ogden-type material instead of a (possibly better) Fung-elastic material. First of all amongst the reasons for this choice is the fact that it can be shown that near stress-free states Ogden-type material laws are a second-order approximation of the linear St.Venant-Kirchhoff law ([Ci88, Thm. 4.10-2]) and that polyconvexity is closely related to the Legendre-Hadamard condition that assures the positivity of the bilinear form associated with the linearized problem ([Da08, Mo08]). Moreover the results will be compatible with the results in [We07] and thus fit into the setting of Theorem A.1. This will be crucial for the existence proof in chapter 4. The quasi-incompressibility assumption is due to the fact, that human soft tissue mainly consists of water and thus will be modeled as incompressible or quasi-incompressible dependent on the relative amount of water contained in the material. This assumption can be incorporated in compressible material laws using the material constants, which are in general the Lamé constants $\lambda > 0$ and $\mu > 0$ or equivalently the Poisson ratio $0 < \nu < \frac{1}{2}$ and Young's modulus $E > 0$. The Poisson ratio is a first-order approximation of the ratio between changes in length and diameter of cylindrical volumes of the material and is indirectly related to the material's compressibility. I. e. quasi-incompressible materials will be modeled using $\nu \geq 0.45$.

Note that in the following no differences between the dermis, epidermis, fat-tissue, muscles and other biological soft tissues that appear in the facial area will be considered. For an algorithm that is of practical use it must examined if it is sufficient to adjust the material constants in order to incorporate the existence of different types of soft tissues or if it is necessary to model more than one type of soft tissue.

The mathematical model

Having defined material laws, i.e. Hooke's law in the case that linearized models can be used and an Ogden-type material law otherwise, a model has to be determined that gives the implant's shape as output if a desired shape of the skin is given. This model should take into account possible difficulties in the numerical treatment. One of these difficulties that can be identified immediately is the occurrence of different materials, the solid implant and the elastic soft tissue, that share a boundary. This shared part of the boundary will in the following be denoted by Γ_3.

The first problem is the fact that the soft tissue can glide over the implant and thus points on the boundary of the soft tissue may change their relative position with respect to points on the boundary of the implant that can only be transformed by rigid body motions. In addition the elasticity of the material allows changes in the size of Γ_3 as seen in Figure 3. This again implies a different behaviour for points on the boundary of the implant and points on the boundary of the soft tissue.

Therefore it is difficult to accurately model Γ_3 and treat it numerically. Modelling the problem of the determination of the implant's shape as an obstacle problem or as shape optimization problem in general needs this shared boundary. The same holds for models that incorporate the implant's shape as Dirichlet boundary conditions on the soft tissue, as this would be the correct model if the implant would be glued to the soft tissue. Thus in order to avoid this problem it is desirable to choose a model, that does not need a discretization of the implant, and instead uses an indirect approach in order to take account of its influence.

An elegant way to do this is to model the implant by the force exerted on the soft tissue. First this allows to drop the discretization of the implant. Thus it is sufficient to only model the soft tissue and the forces exerted on it. Next this approach fits naturally in the models of continuum mechanics, in this case in elasticity theory, which are derived using equilibrium conditions for the appearing forces. Thus, considering the differential equations of elastostatics this force can be directly incorporated as Neumann boundary conditions.

Figure 2 gives a sketch of the incorporation of these forces on the boundary of the soft tissue. The corresponding deformed configuration is given in Figure 3. Here, the forces

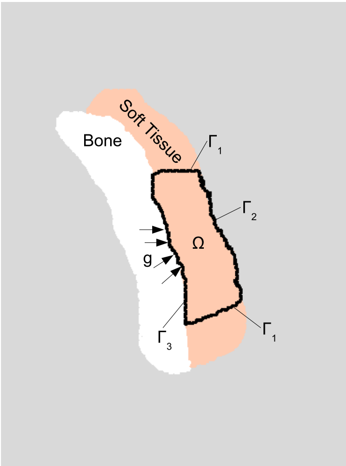

Figure 2: reference configuration

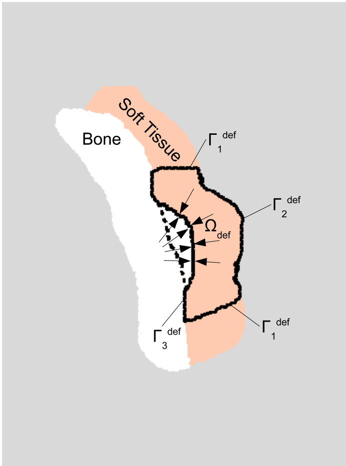

Figure 3: equilibrium state

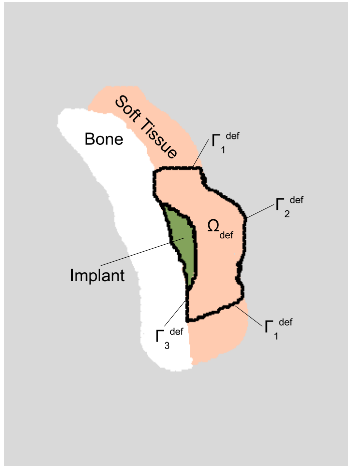

Figure 4: deformed configuration

in the soft tissue are in static equilibrium as the force exerted on the boundary is compensated through the force opposed by the soft tissue. The implant associated with this equilibrium state occupies the empty space between the bones and the soft tissue as sketched in Figure 4. The domain Ω marks the part of the soft tissue that changes its shape and position and will be the domain on which a model will be derived and treated numerically. As the impact of an implant insertion on most parts of a human's soft tissue are negligible it makes sense to consider just the part of the soft tissue where the implant has a noteworthy effect. Moreover the consideration of the whole human body, scanned at a reasonable resolution, would imply intolerably long calculation times. The virtual cutting out of Ω introduces an artificial boundary $\Gamma_1 \subset \partial\Omega$. As the reference configuration should be chosen such that the influence of the implant outside Ω, and thus also on Γ_1, is negligible, homogeneous Dirichlet boundary conditions will be imposed. As noted $\Gamma_3 \subset \partial\Omega$ denotes the part of the boundary where the implant acts and consequently inhomogeneous Neumann boundary conditions will be chosen. Finally the visible part of the boundary is denoted by $\Gamma_2 \subset \partial\Omega$ (the surface of the epidermis). Here no constraints on the boundary should be imposed. This corresponds to a zero force acting on Γ_2 and therefore homogeneous Neumann boundary conditions will be imposed.

Having defined a domain Ω and boundary conditions the relationship between an implant's force g and the deformations of the soft tissue in Ω can be established. The general form of this relationship in hyperelastic theory can be written as

$$u \in \text{argmin}_{\, v \in U_{ad}} I_g(v), \tag{1}$$

where u is the displacement as indicated in Figure 5, i.e. the force g moves $x \in \Omega$ to $x_{def} := \Phi(x) = x + u(x) \in \Omega_{def}$. U_{ad} is the set of admissible deformations and will be characterized in the next chapter. I_g is an energy functional, that measures the elastic energy associated with some $u \in U_{ad}$ and the Neumann boundary conditions g on Γ_3. This functional may have different forms depending on the given problem. While for convex functionals and convex U_{ad}, like in linearized elasticity, (1) is easy to solve, there exist cases that are relevant in practice that require more complex energy functions (see [We07, Fu93]).

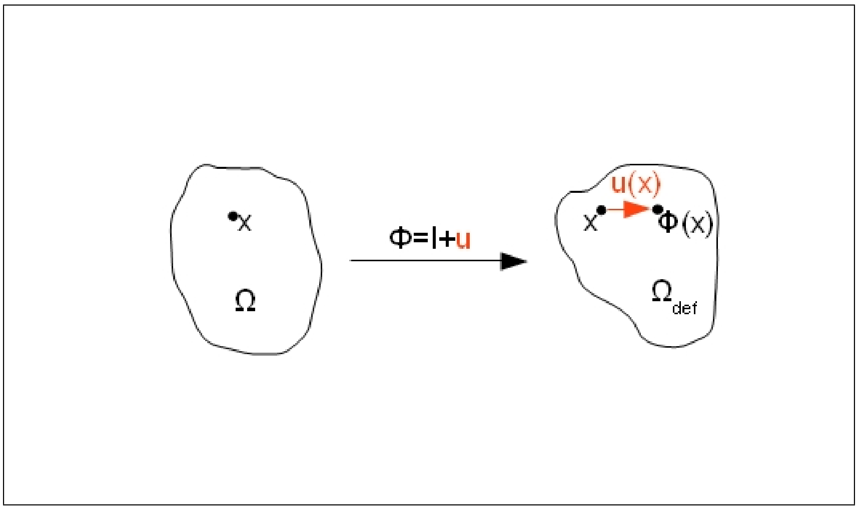

Figure 5: deformation Φ and displacement u

Leaves to incorporate the desired displacement u_{ref} on the visible part Γ_2 into the model. A priori it is, at least from the theoretical point of view, unlikely that for a chosen u_{ref} there exists an implant with corresponding boundary force g such that a solution u of (1) satisfies $u \equiv u_{ref}$ on Γ_2 (resp. a.e. on Γ_2 for weak solutions). Therefore this condition will be weakened to finding a boundary force g such that the solution u of (1) minimizes $\tilde{J}_1(u) = \|u - u_{ref}\|_{L^2(\Gamma_2;\mathbb{R}^3)}$ or equivalently $J_1(u) = \|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)}$ which is better to treat, as it is quadratic. Eventually the Tichonoff regularization parameter $\alpha > 0$ will be introduced to get the final energy functional

$$\min J(u,g) := \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)}$$

This leads to an optimal control problem as model, i.e.

$$\min J(u,g) := \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)} \tag{2}$$

s.t.

$$u \in \text{argmin}_{\,v \in U_{ad}} I_g(v) \tag{3}$$

and therefore the boundary force g is also called *control*. The main reason for the regularization parameter is that the boundedness of the boundary force g in $L^2(\Gamma_3;\mathbb{R}^3)$ must be assured. If this would not hold, the above system could become unbounded for unreachable displacements u_{ref}. In addition the presence of the regularization term allows better regularity results for the control. Finally, in linearized elasticity it permits, with the introduction of a Lagrange multiplier p, the elimination of the control from the necessary and sufficient first order conditions and write the optimality conditions as a coupled system of linear, elliptic differential equations (see chapter 2). Therefore the exerted force only appears formally in the derivation of the optimality conditions but never has to be used explicitly. The implant's shape and position are directly given through Γ_3, which is the shared boundary of the implant and the bones, and $\Phi(\Gamma_3) = (I+u)(\Gamma_3)$ as the shared boundary of the implant and the surrounding soft tissue.

In the following, after introducing some basic notation and properties from elasticity in chapter 1, the necessary and sufficient optimality for the above optimal control problem with constraints from linearized elasticity will be derived in chapter 2. In chapter 3 the optimality conditions will be adapted to a concrete example, solved numerically and the crucial dependence on the Tichonoff regularization parameter α will be analyzed. Finally in chapter 4 the existence of solutions of the nonlinear optimal control problem, where the material law is polyconvex and satisfies the assumptions of Theorem A.1, will be proven. As these material laws admit local nonuniqueness of solutions, the solution operator of the constraint (3) $S : g \mapsto u$ will in general not be continuous or even differentiable (for an examples of nonuniqueness see [Sp09], where [Ba02, Problem 8] is solved). Thus additional assumptions are necessary for the derivation of the necessary and sufficient optimality conditions (see section 4.3). This goes beyond the scope of this thesis and might be a topic of further research.

Note that plasticity, hysteresis effects and the age-dependency of the soft tissue are not considered in this thesis. Plasticity and hysteresis are only of interest if the soft tissue is exerted to forces and then released. The age-dependency is at least partly dependent on the stopping of the elastin production in puberty. Elastin has the "most linear" of all biosolid material laws and the linear perturbation associated with the ageing effect will be neglected. For practical use the age-dependency of the material parameters should also be examined.

1. Short Introduction to Elastostatics

In this chapter parts from elasticity theory that will be necessary later on and the strategy for deriving the corresponding differential equation will be presented. For sake of clarity this part is kept short, just explains the basic notation and material properties used in the context of this thesis. For a better overview the interested reader should consult [Ci88], [Ma83], [So46] and in the context of biological soft tissue [Fu93].

The consideration of static equilibriums states allows the use of the **stress principle of Euler and Cauchy** (Axiom 1.1) and its implication **Cauchy's theorem** (1.1) to formulate equilibrium conditions for the deformed body Ω_{def}. In chapter 1.3 the Piola transform will be introduced that allows to reformulate the equilibrium conditions in Ω and thus allows to avoid the difficulty of handling these conditions on the unknown domain Ω_{def}. Then in chapter 1.4 material laws will be discussed. Finally hyperelastic material laws will be introduced, a class of material laws for which the equilibrium conditions are equivalent to the **principle of virtual work** and thus naturally lead to a weak formulation.

Note that in the following only stationary states are considered, and the treatment in terms of manifolds is omitted for sake of shortness and clarity.

1.1. Kinematics

The domain occupied by a body in a certain (here: equilibrium) state is called the **reference configuration** Ω. If forces act on this body it deforms to a new configuration Ω_{def} as in Figure 2 & 3. This **deformation** is given through a mapping with the same name $\Phi : \Omega \ni x \mapsto \Phi(x) = x + u(x) \in \Omega_{\text{def}}$ (see Figure 5), where u is called **displacement** and is the unknown used in most cases for mathematical models. In order to be physically reasonable additional assumptions on Φ are necessary. The first assumption is motivated by the observation that self-penetration can not occur for elastic solids. Nevertheless it should possible to deform a material in such a way that it touches itself and consequently looses injectivity on the boundary. The determination of a physically reasonable condition that avoids self-penetration and in the same time admits the loss of injectivity on the boundary is a difficult matter. In elasticity theory this condition will be incorporated using the local orientation-preserving condition $\det(\nabla\Phi) = \det(I + \nabla u) > 0$ on Ω. This condition preserves the deformed body from local self-penetration and implies the local injectivity of Φ if $\Phi \in C^1$, but it can not avoid global self-penetration.

In addition some smoothness assumptions on Φ are necessary, as the Piola identity

$$\operatorname{div}\Big(\det(\nabla\Phi)\nabla\Phi^{-T}\Big) = \operatorname{div}\Big(\operatorname{cof}(\nabla\Phi)\Big) = 0,$$

which is necessary for the proof of Theorem 1.2, must make sense it will be required that $\Phi \in C^2(\Omega;\mathbb{R}^3)$. When having derived the differential equations of elasticity this regularity assumption can be weakened as the consideration of weak solutions then only requires $\Phi \in W^{1,p}(\Omega;\mathbb{R}^3)$ for some $p \geq 1$. Note that this generalization implies that the condition $\det(\nabla\Phi) > 0$ a.e. does not even admit local injectivity any more. An argument that nonetheless justifies this condition for hyperelastic materials will be given in section 1.5.

Considering the change in the length of line segments of deformations with respect to the euclidean norm introduces the first (geometric) nonlinearity that will appear in the differential equations of elasticity

$$\|\Phi(x+z)-\Phi(x)\|^2 = \|\nabla\Phi(x)z\|^2 + o(\|z\|^2) = z^*(\nabla\Phi(x))^*(\nabla\Phi(x))z + o(\|z\|^2)$$

Thus the change in the lengths of line segments is governed by the *(left) Cauchy-Green strain tensor* $C := (\nabla\Phi)^*(\nabla\Phi) = I + \nabla u^* + \nabla u + \nabla u^*\nabla u$. This motivates

Definition 1.1. *(Strain)*

The deviation of the Cauchy-Green strain tensor from the identity

$$E := \frac{1}{2}(C - I) = \frac{1}{2}\Big(\nabla u^* + \nabla u + \nabla u^*\nabla u\Big)$$

*is called **strain (tensor)**.*

*The linearization of the **strain tensor** for small displacements leads to the **symmetric gradient** $\nabla^s u := \frac{1}{2}\Big(\nabla u^* + \nabla u\Big)$.*

Remark 1.

- *Another argumentation leading to the Cauchy-Green strain tensor starts from the observation that a body's stress state is invariant with respect to rigid body motions. This approach can be found in* [Ze88, p. 169 f.]. *It starts with suitable assumptions on the strain tensor E and uses the polar decomposition.*
- *While the strain tensor vanishes for rigid body motions this is not the case for its linearization. The symmetric gradient is dependent on the chosen coordinate system (see Axiom* 1.2*).*
- *In the case that A is symmetric, i.e. $a_{ij} = a_{ji}$, holds for the inner product on matrix spaces $A : B = \mathrm{tr}(A^T B)$*

$$A : B = \mathrm{tr}(AB) = \sum_{i,j} a_{ji}b_{ij} = \frac{1}{2}\sum_{i,j} a_{ji}(b_{ij}+b_{ji}) = A : \Big(\frac{1}{2}(B+B^T)\Big)$$

  This implies for the symmetric gradient $\nabla^s u : \nabla v = \nabla^s u : \nabla^s v = \nabla u : \nabla^s v$ and therefore gives the symmetry of the bilinear form defined in the context of linearized elasticity (chapter 2, (14)*) .*

1.2. Equilibrium conditions

In mechanics it will be assumed, that all acting forces can be partitioned into volume and surface forces. The influence of these forces will be treated axiomatically, and in the context of static equilibria the main contributions have been made by Leonhard Euler and Augustin Louis Cauchy (see [Ci88]). Static equilibrium states are defined through

Axiom 1.1. *(Stress Principle of Euler and Cauchy)*
Consider a body occupying a deformed region $\bar{\Omega}_{\text{def}}$, subjected to a body force

$$f : \Omega_{\text{def}} \to \mathbb{R}^3$$

and a surface force

$$g : \Gamma_1^{\text{def}} \to \mathbb{R}^3,$$

where Γ_1^{def} is some measurable part of the boundary of Ω_{def}. Then there exists a vector field

$$t : \bar{\Omega}_{\text{def}} \times S \to \mathbb{R}^3 \qquad S := \{x \in \mathbb{R}^3 : |v| = 1\}$$

*called **Cauchy's stress vector** such that:*

1. *For any subdomain $A \subseteq \bar{\Omega}_{\text{def}}$ and at any point $x \in \Gamma_1^{\text{def}} \cap \partial A$ where the unit outer normal vector n exists, holds $t(x, n) = g(x)$.*
2. ***Axiom of force balance**: For any subdomain $A \subseteq \bar{\Omega}_{def}$ holds*
$$\int_A f(x)\ \mathrm{dx} + \int_{\partial A} t(x, n)\ \mathrm{ds} = 0 \tag{4}$$
3. ***Axiom of moment balance**: For any subdomain $A \subseteq \bar{\Omega}_{\text{def}}$ holds*
$$\int_A x \times f(x)\ \mathrm{dx} + \int_{\partial A} x \times t(x, n)\ \mathrm{ds} = 0 \tag{5}$$
where $\times$ denotes the vector/cross product.

An important consequence of this axiom is

Theorem 1.1. *(Cauchy's Theorem)*
Assume that $t(\cdot, n) \in C^1(\Omega_{\text{def}}; \mathbb{R}^3)$, $t(x, \cdot) \in C(S; \mathbb{R}^3)$ and $f \in C(\Omega_{\text{def}}; \mathbb{R}^3)$, with the definitions of Axiom 1.1. Then there exists a symmetric tensor field $T_{\text{def}} \in C^1(\Omega_{\text{def}}; \mathbb{S}^3)$ such that

$$t(x, n) = T_{\text{def}}(x)n \qquad \forall x \in \Omega_{\text{def}},\ n \in S \tag{6}$$

$$\operatorname{div}\Big(T_{\text{def}}(x)\Big) + f(x) = 0 \qquad \forall x \in \Omega_{\text{def}} \tag{7}$$

$$T_{\text{def}}(x) = T_{\text{def}}^T(x) \qquad \forall x \in \Omega_{\text{def}} \tag{8}$$

*The tensor T_{def} is called **Cauchy stress tensor**.*

Proof. See [Ci88, p. 63]. ■

Remark 2. *The main point is that one can express the stress vector with tensors. Then using Gauß' integral formula* (4) *can be written as*

$$\begin{aligned} \int_A f(x)\ \mathrm{dx} + \int_{\partial A} T_{\mathrm{def}}(x) n\ \mathrm{ds} &= 0 \\ \Leftrightarrow \int_A \Big[f(x) + \mathrm{div}\Big(T_{\mathrm{def}}(x) \Big) \Big]\ \mathrm{dx} &= 0 \end{aligned}$$

As this holds for every subdomain $A \subset \bar{\Omega}_{\mathrm{def}}$ this leads to the differential equation (7)*. The symmetry property* (8) *follows from* (5)*.*

The properties given in Cauchy's theorem are not sufficient for the determination of the displacement and the stress, when body and/or surface forces are given. This is clear, as (6) states that the stress can be written as tensor. The symmetry property (8) reduces the number of unknowns of T_{def} from nine to six. Now (7) gives three conditions for the determination of the six unknowns of the stress tensor and the three unknowns of the displacement. So more conditions are needed that describe the material specific relation between stresses and displacements resp. strains (material properties). These conditions are called *constitutive laws* and will be introduced in section 1.4.

Another difficulty is the formulation of the equilibrium equations on the deformed domain Ω_{def} which is not known á priori. So before turning to constitutive laws the Piola transform, that allows to transform the equilibrium conditions into conditions on the reference configuration Ω, will be introduced.

1.3. The Piola transform

Before stating the main properties of the Piola transform recall the definition of the cofactor matrix or equivalently the adjoint matrix:

Definition 1.2. *(cofactor matrix)*

Let $A = (a_{ij})_{i,j=1,\ldots n} \in \mathbb{R}^{n,n}$, $n > 0$ and denote by $A_{ij} \in \mathbb{R}^{n-1,n-1}$ the matrix, that appears when deleting the i-th row and j-th column from A. Then the scalars $(-1)^{i+j} \det(A_{ij})$ are called the ***cofactors*** *of A. The* ***cofactor matrix*** *is given through*

$$\mathrm{cof}(A) = \Big((-1)^{i+j} \det(A_{ij}) \Big)_{i,j=1,\ldots,n}$$

Remark 3.

- *Denoting the j-th column of a matrix B by B_j, the cofactors are related to the determinant via the Laplace's formula as*

$$\det(A) = \sum_{i=1}^{n} a_{ij} (-1)^{i+j} \det(A_{ij}) = A_j^T \mathrm{cof}(A)_j$$

- *Instead of the cofactor matrix it often makes sense to use the adjoint matrix that is given through the relation*

  $$\operatorname{adj}(A) = \operatorname{cof}(A)^T$$

  Then $\det(A) = \operatorname{adj}(A)_j A_j$*, and one can calculate the derivative of the determinant in a direction* δA *as*

  $$\det{}'(A)\delta A = \operatorname{cof}(A) : \delta A = \operatorname{tr}\Big(\operatorname{adj}(A)\delta A\Big)$$

- *The adjoint of the deformation, resp. displacement gradient can be interpreted as a local measure for changes in the surface's area.*

Now the following theorem gives the definition of the Piola transform and states the transformation rules for the divergence operator, normal components and surface elements

Theorem 1.2. *(Properties of the Piola Transform)*
Let $\Phi : \Omega \to \Omega_{\text{def}}$ *be the deformation associated with the pair* $(\Omega, \Omega_{\text{def}})$*. Then the* ***Piola transform*** $P_T : \bar{\Omega} \to \mathbb{M}^3$ *of the tensor* $T : \bar{\Omega}_{\text{def}} \to \mathbb{M}^3$ *is defined as*

$$\begin{aligned} P_T(x) &:= \det\Big(\nabla\Phi(x)\Big)T\Big(\Phi(x)\Big)\Big(\nabla\Phi(x)\Big)^{-T} \\ &= T\Big(\Phi(x)\Big)\operatorname{adj}\Big(\nabla\Phi(x)\Big)^T \end{aligned}$$

The following properties hold:

1. $\operatorname{div}\Big(P_T(x)\Big) = \Big(\det(\nabla\Phi)\Big)\operatorname{div}\Big(T\Big(\Phi(x)\Big)\Big) \qquad \forall x \in \Omega,$
2. $P_T(x)n \ \mathrm{ds} = T\Big(\Phi(x)\Big)n_{\text{def}} \ \mathrm{ds}_{\text{def}} \qquad \forall x \in \Omega$
   where ds_{def}, ds *are surface elements and* n_{def}, n *are the unit outer normals of* $\partial\Omega_{\text{def}}$ *resp.* $\partial\Omega$*.*
3. *The surface elements are related through*

   $$\det\Big(\nabla\Phi(x)\Big)\Big|\nabla\Phi(x)^{-T}n\Big| \ \mathrm{ds} = \Big|\operatorname{adj}\Big(\nabla\Phi(x)n\Big)^T\Big| \ \mathrm{ds} = \ \mathrm{ds}_{\text{def}}$$

Proof. See [Ci88, Thm. 1.7-1]. ■

Remark 4. *The Piola transform of the Cauchy stress tensor* T_{def}

$$\sigma(x) := \det\Big(\nabla\Phi(x)\Big)T_{\text{def}}\Big(\Phi(x)\Big)\Big(\nabla\Phi(x)\Big)^{-T} = T_{\text{def}}\Big(\Phi(x)\Big)\operatorname{adj}\Big(\nabla\Phi(x)\Big)^T$$

is called ***first Piola-Kirchhoff stress tensor*** *and is the stress tensor normally appearing in the differential equations of elasticity.*

In contrast to the Cauchy stress tensor the first Piola-Kirchhoff stress tensor is not symmetric in general, as $\operatorname{adj}\Big(\nabla\Phi(x)\Big)$ *does not admit this property. Recognizing that* $\operatorname{adj}(A) = \det(A)A^{-1}$ *for invertible matrices* A *one can symmetrize* σ *and gets the* ***second Piola-Kirchhoff stress tensor***

$$\Sigma(x) := \det\Big(\nabla\Phi(x)\Big)\Big(\nabla\Phi(x)\Big)^{-1} T_{\mathrm{def}}\Big(\Phi(x)\Big)\Big(\nabla\Phi(x)\Big)^{-T} = \Big(\nabla\Phi(x)\Big)^{-1}\sigma(x)$$

A discussion of the equations of elasticity in terms of the second Piola-Kirchhoff stress tensor is done in [Ci88] *and will not be considered here, as in this thesis hyperelastic materials are considered that naturally lead to a formulation in terms of the first Piola-Kirchhoff stress tensor.*

*Note that for small displacement gradients near stress free states (**natural states**, see Definition* 1.5*) the differences between the first and second Piola-Kirchhoff stress tensor and the Cauchy stress tensor only affect higher-order terms and thus may be neglected.*

1.4. Constitutive laws

Now having a tool for the formulation of the equilibrium conditions in the reference configuration we can turn to the missing conditions for the determination of displacements and stresses. These conditions not only possess a mathematical justification as given at the end of section 1.2. Also from a physical point of view it is clear that the underlying material has to be taken into account as to this point not even its general nature (solid, fluid or gas) has been considered. As noted, one of the main difficulties in nonlinear elasticity is the determination of suitable hypothesis on the constitutive law such that physical effects are modeled correctly and the model becomes accessible to mathematical analysis. For the definitions of the used sets of matrices see the notation section that follows the appendix.

Definition 1.3. *(Constitutive Law, Elastic Material)*

A material is called ***elastic*** *if for every stress tensor* S *there exists a mapping* $\hat{S}$ *such that*

$$S(x) = \hat{S}\Big(x, \nabla\Phi(x)\Big) \quad \textit{resp. for homogeneous materials } S(x) = \hat{S}\Big(\nabla\Phi(x)\Big) \tag{9}$$

for every deformation Φ *and all* $x \in \Omega$*. The mapping* $\hat{S}$ *is called* ***response function*** *and the relation* (9) *is the* ***constitutive law****.*

Remark 5. *One may define elastic materials in a more general way to include dependencies on velocities and memory effects. This is important for the study of elastic fluids. In this thesis these effects do not play any role and thus the above definition which also appears in most books about elasticity will be used.*

The following axiom allows to give further restrictions on the response functions of the stress tensors and from now on it will be assumed that this axiom is satisfied by all nonlinear material laws under consideration.

Axiom 1.2. *(Axiom of Material Frame Indifference/Objective Material)*

The Cauchy stress tensor $t(x,n) = T_{\text{def}}(x)n$ is independent of the choice of the coordinate system, i.e.

$$Qt(x,n) = t(Qx, Qn) \text{ for all } Q \in \mathbb{O}^3_+.$$

If this axiom holds the material is called ***objective****.*

Remark 6. *While the statement of the Axiom of Material Frame Indifference seems to be fulfilled naturally it may be violated by solutions of problems of linearized elasticity.*

The axiom of material frame indifference implies the following properties which will for simplicity only stated for homogeneous materials but hold in the same way in the heterogeneous case:

- *There exists a mapping $\tilde{\Sigma} : \mathbb{S}^3_> \to \mathbb{S}^3$ such that*

$$\hat{\Sigma}(F) = \tilde{\Sigma}(F^T F) \quad \forall F \in \mathbb{M}^3_+,$$

  i.e. the response function of the second Piola-Kirchhoff stress tensor depends only on the Cauchy-Green strain tensor.
  This also implies that

$$\hat{\Sigma}(F) = \hat{\Sigma}(QF) \quad \forall F \in \mathbb{M}^3_+, Q \in \mathbb{O}^3_+$$

- *For the first Piola-Kirchhoff stress tensor holds*

$$\sigma(F) = Q^T \sigma(QF) \quad \forall F \in \mathbb{M}^3_+, Q \in \mathbb{O}^3_+$$

- *For the response function of the Cauchy stress tensor holds*

$$\hat{T}_{\text{def}}(F) = Q^T \hat{T}_{\text{def}}(QF)Q \quad \forall F \in \mathbb{M}^3_+, Q \in \mathbb{O}^3_+$$

Next a material property will be stated that holds if the material expands in the same way in each direction.

Definition 1.4. *(Isotropy)*

A material and its response function $\hat{T}_{\text{def}}$ are called ***isotropic*** *at $x \in \bar{\Omega}$ if*

$$\hat{T}_{\text{def}}(x, FQ) = \hat{T}_{\text{def}}(x, F) \quad \forall F \in \mathbb{M}^3_+,\ \forall Q \in \mathbb{O}^3_+$$

This also implies that the response function of the Cauchy stress tensor depends only on the Cauchy-Green strain tensor. The material and its response function are called ***isotropic*** *if they are* ***isotropic*** *for every $x \in \bar{\Omega}$.*

A configuration is called ***isotropic*** *if for the deformation Φ leading to this configuration holds*

$$\hat{T}\Big(x, \nabla\Phi(x)Q\Big) = \hat{T}\Big(x, \nabla\Phi(x)\Big) \quad \forall Q \in \mathbb{O}^3_+$$

Despite of being a material property there exist isotropic states for every elastic material (except gases). These states are given in the following definition which corresponds to the assumption that there exists "unstressed states" (states in which all applied forces vanish).

Definition 1.5. *(Natural State)*

A reference configuration $\bar{\Omega}$ is called a ***natural state*** *if the* ***residual stress tensor***

$$T_R(x) := \hat{T}_{\text{def}}(x, I) \tag{10}$$

vanishes for all $x \in \bar{\Omega}$.

Remark 7. *Recalling the axiom of material frame indifference the relation* (10) *implies that any deformation that is a rigid body motion transforms natural states into natural states. Therefore, as the unit matrix commutes with every $Q \in \mathbb{M}^3$, natural states are always isotropic and in linearized elasticity near natural states isotropy is an adequate assumption. Unfortunately for many materials isotropy gets lost when the body experiences large deformations.*

In 1955 Ronald Rivlin and Jerald LaVerne Ericksen proved a useful and famous consequence of isotropy in the homogeneous case, that allows the expression of the Cauchy stress tensor in terms of the principal invariants of $(\nabla\Phi)^T\nabla\Phi$. This also lays the ground for the derivation of Hooke's law and thus justifies the use of this law if the corresponding assumptions are admissible. One of these assumptions is homogeneity and will be assumed to hold for the remainder of this section.

Theorem 1.3. *(Rivlin-Ericksen Theorem (1955))*

A response function for a Cauchy stress tensor $\hat{T}_{\text{def}} : \mathbb{M}^3_+ \to \mathbb{S}^3$ is isotropic and objective if and only if there exists a function $\bar{T} : \mathbb{S}^3_> \to \mathbb{S}^3$ such that $\hat{T}_{\text{def}}(F) = \bar{T}(F^T F)\,\forall F \in \mathbb{M}^3_+$ and

$$\bar{T}(B) = \beta_0(\iota_B)I + \beta_1(\iota_B)B + \beta_2(\iota_B)B^2 \quad \forall B \in \mathbb{S}^3_>$$

where $\beta_0, \beta_1, \beta_2$ are functions of the invariants $\iota_B = (\iota_1, \iota_2, \iota_3)$ of B. Recall that the invariants of a 3×3 matrix B with eigenvalues $\lambda_1, \lambda_2, \lambda_3$ are given through

$$\begin{aligned} \iota_1(B) &= \operatorname{tr}(B) = \lambda_1 + \lambda_2 + \lambda_3 \qquad \iota_2(B) = \operatorname{tr}\Big(\operatorname{adj}(B)\Big) = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \\ \iota_3(B) &= \det(B) = \lambda_1\lambda_2\lambda_3 \end{aligned}$$

Proof. See [Ba07, Thm. 1.8]. ∎

Corollary 1.4. *For an objective, isotropic material there exists a function $\bar{\Sigma} : \mathbb{S}^3_> \to \mathbb{S}^3$ such that $\hat{\Sigma}(\nabla\Phi) = \bar{\Sigma}(\nabla\Phi^T\nabla\Phi)$ and*

$$\bar{\Sigma}(C) = \gamma_1(\iota_C)I + \gamma_2(\iota_C)C + \gamma_3(\iota_C)C^2 \quad \forall C \in \mathbb{S}^3_>$$

The above results, restricting the response functions of the stress tensors to take very special forms only depending on the principal invariants, implies also a special form of the second Piola-Kirchhoff stress tensor:

Theorem 1.5. *Consider an objective, isotropic, elastic material and suppose that the functions γ_i, $i = 1, 2, 3$ of Corollary 1.4 are differentiable with respect to the invariants $\iota_i(E)$, $i = 1, 2, 3$. Then there exists $\pi, \lambda, \mu \in \mathbb{R}$, $i = 1, 2, 3$ such that*

$$\bar{\Sigma}(I + 2E) = -\pi I + \lambda \mathrm{tr}(E) + 2\mu E + o(E) \quad \forall (I + 2E) \in \mathbb{S}^3_>$$

Proof. See [Ci88, Thm. 3.7-1]. ■

Remark 8. *Only if the assumptions of above theorem are satisfied and $\pi = 0$ the constants λ, μ are called* ***Lamé constants****.*

The case $C = I \Leftrightarrow E = 0$ corresponds to stress free states when the reference configuration is a natural state. Therefore $\pi = 0$. Also, in this case, the first and second Piola-Kirchhoff stress tensors differ only in higher-order terms and therefore in linear elasticity one can use the one that seems to be more useful. For small displacement gradients this leads to

Definition 1.6. *(Hooke's Linear Material Law)*

The mapping

$$u \mapsto \sigma(u) := \lambda \mathrm{tr}(\nabla^s u) I + 2\mu \nabla^s u = \lambda_L \mathrm{div}(u) I + 2\mu \nabla^s u$$

is called ***Hooke's Law****. The* ***Lamé constants*** *λ, μ are assumed to be positive, which is justified by physical observations (see [Ci88, ch. 3.9]). Again σ is the first Piola-Kirchhoff stress tensor.*

Remark 9. *The material constant λ and μ are linked with the* ***Poisson ratio*** *ν and* ***Young's modulus*** *E through the formulas*

$$\nu = \frac{\lambda}{2(\lambda + \mu)} > 0 \qquad\qquad E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} > 0$$

respectively

$$\lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \qquad\qquad \mu = \frac{E}{2(1 + \nu)}$$

The ***Poisson ratio*** *ν is a first-order approximation of the ratio between changes in length and diameter of cylindrical volumes of the material. It is indirectly linked with the compressibility of a material, i.e. ν close to 0.5, which is an upper bound on this parameter, describe quasi-incompressible materials like human soft tissue.*

Young's modulus *E is a first order approximation of the ratio between stress and change in length in axial direction of cylindrical volumes of the material. Thus it is a measure for the force a material opposes to applied forces.*

1.5. Hyperelastic materials

An important class, which includes Ogden-type materials as considered in this thesis, is the class of hyperelastic materials. This subsection follows mainly the chapter about hyperelasticity in [Ci88, ch. 4.1] where proofs for the argumentation below can be found.

Definition 1.7. *(Hyperelasticity)*
An elastic material is ***hyperelastic*** *if there exists a function* $\hat{W}(x, F) : \bar{\Omega} \times \mathbb{M}^3_+ \to \mathbb{R}$, *which is for each* $x \in \bar{\Omega}$ *differentiable with respect to its second argument, such that*

$$\hat{\sigma}(x, F) = \frac{\partial \hat{W}}{\partial F}(x, F) \qquad \forall x \in \Omega,\, \forall F \in \mathbb{M}^3_+$$

where $\hat{\sigma}$ *is the response function of the first Piola-Kirchhoff stress tensor. The function* $\hat{W}$ *is called* ***stored energy function****.*

Remark 10.

- *The definition of hyperelasticity can be justified through a mechanical interpretation. It can be shown that an elastic material is hyperelastic if and only if "the work is non-negative for all closed processes"*([Ci88, p. 141]).
- *General stored energy functions must satisfy*
$$\det(F) \to 0^+ \Rightarrow \hat{W}(x, F) \to \infty \tag{11}$$
in order to be a good model for large deformations, as $\det\Big(\nabla\Phi(x))\Big) \to 0^+$ *implies* $\rho \to \infty$, *where* ρ *is the materials density. This condition means that in material that is heavily compressed very large stresses occur. This condition, on one side, assures that local self-penetration will not occur. Additionally it is related to the local nonuniqueness of solutions, as it conflicts with the desired estimates (boundedness, strict positivity of the second variation, monotonicity).*
- *The condition* (11)*, as well as the axiom of material frame indifference, imply that stored energy functions can not be convex* [Ci88, ch. 4.8]*. Also the strict convexity of the stored energy function would contradict examples for nonuniqueness of solutions.*

The "impossible convexity" of the stored energy function can be overcome with the assumption of polyconvexity, which admits condition (11) and was first introduced in the context of elasticity in [Ba77]:

Definition 1.8. *(Polyconvexity)*
A function $\hat{W} : \Omega \times \mathbb{F} \to \mathbb{R}$, *with* $\mathbb{F} \subset \mathbb{M}^3, \Omega \subset \mathbb{R}^3$, *is* ***polyconvex*** *if for each* $x \in \Omega$ *there exists a convex function*

$$\mathbb{W}(x, \cdot) : \mathbb{M}^3 \times \mathbb{M}^3 \times \mathbb{R}_+ \to \mathbb{R}$$

such that

$$\hat{W}(x, F) = \mathbb{W}\Big(x, F, \mathrm{adj}(F), \det(F)\Big) \qquad \forall F \in \mathbb{F}$$

Remark 11. *For general $\mathbb{F} \subset \mathbb{M}^n$ an analog definition holds taking into account all the subdeterminants of $F \in \mathbb{F}$.*

Now consider the differential equation (7) with a deformation $\Phi_0 = I + u_0$ and a conservative surface force g given on parts of the boundary $\Gamma_1 \cap \Gamma_2 = \emptyset$, $\bar{\Gamma}_1 \cup \bar{\Gamma}_2 = \partial\Omega$ and a conservative body force f. The conservativity assumption is justified in [Ci88, ch. 2.7]. It states that there exist functionals F, G, defined on the set of deformations $\mathcal{S} := \{\Phi \in C^1(\bar{\Omega}; \bar{\Omega}_{def} |\ \det(\nabla\Phi) > 0\,\text{a.e.}\}$, and taking the form

$$F(\Phi) = \int_\Omega F_P\Big(x, \Phi(x)\Big)\ \mathrm{dx} \qquad G(\Phi) = \int_{\Gamma_2} G_P\Big(x, \nabla\Phi(x)\Big)\ \mathrm{ds},$$

where the Gâteaux differentiable functions $F_P : \Omega \times \Omega_{\text{def}} \to \mathbb{R}$ and $G_P : \Gamma_2 \times \mathbb{M}^3_+ \to \mathbb{R}$ are called **potentials** of the applied body resp. surface force, such that for sufficiently smooth functions $\theta : \bar{\Omega} \to \mathbb{R}^3$ that vanish on Γ_1 holds:

$$\begin{aligned}\int_\Omega f\Big(x, \Phi(x)\Big)\theta(x)\ \mathrm{dx} &= F'(\Phi)\theta \\ \int_{\Gamma_2} g\Big(x, \nabla\Phi(x)\Big)\theta(x)\ \mathrm{ds} &= G'(\Phi)\theta\end{aligned}$$

This motivates from a mathematical point of view the definition of hyperelasticity above, as one has

$$\int_\Omega \hat{\sigma}\Big(x.\nabla\Phi(x)\Big) : \nabla\theta\ \mathrm{dx} = W'(\Phi)\theta \qquad W(\Phi) := \int_\Omega \hat{W}\Big(x, \nabla\Phi(x)\Big)\ \mathrm{dx}$$

where $\int_\Omega \hat{W}\Big(x, \nabla\Phi(x)\Big)\ \mathrm{dx}$ is called the **strain energy**. Therefore, in the above setting, the equilibrium conditions (6)-(8) together with the boundary conditions on Γ_1 and Γ_2 are equivalent to the **principle of virtual work** in the reference configuration:

$$W'(\Phi)\theta = F'(\Phi)\theta + G'(\Phi)\theta \tag{12}$$

for all sufficiently smooth functions $\theta : \bar{\Omega} \to \mathbb{R}^3$ that vanish on Γ_1. Setting $I(\Phi) = W(\Phi) - F(\Phi) - G(\Phi)$ equation (12) is equivalent to the statement that Φ is a critical point of I. Then recognizing that the functional I measures the energy associated with forces and induced stresses, a standard strategy for finding solutions of the equilibrium conditions in hyperelasticity is the minimization of this energy functional.

As a necessary assumption for the mathematical treatment of this minimization problem a minimizer $\bar{u}$ must fulfill $I(\bar{u}) < \infty$. If the corresponding stored energy function satisfies (11), this implies that $\det(I + \nabla\bar{u}) > 0$ a.e. in Ω. As noted in section 1.1 for $\bar{u} \in W^{1,p}(\Omega; \mathbb{R}^3)$ this can not any more interpreted as a local injectivity condition, but it prevents the material from local self-penetration as the energy associated to heavy compression is very big. In 1987 Philippe G. Ciarlet and Jindrich Nečas proposed the condition

$$\int_\Omega \det(\nabla\Phi)\ \mathrm{dx} \leq \mathrm{vol}\Big(\Phi(\Omega)\Big)$$

that allows to prove that Φ is injective a.e., in the sense that $\mathrm{card}\Big(\Phi^{-1}(x)\Big) = 1$ for almost all $x \in \Phi(\Omega)$. They also showed that in the case that the “free” part of the boundary, where homogeneous Neumann boundary conditions are imposed, is sufficiently smooth, then the tangential components of the normal stress vector vanish on this part of the boundary (in this thesis in general Γ_2). For a detailed discussion of injectivity properties the interested reader is referred to [Ba02] and the references given there.

While the existence of minimizers is clear from intuition for all “real” stored energy functions of hyperelastic materials, it is not trivial to give existence proofs for reasonable stored energy functions. The most important known is a generalization of Ball’s existence theorems for polyconvex energy functions (Theorem A.1), which also gives the existence proof needed in this thesis.

2. Linearized Elasticity and the Optimal Control Problem

In this chapter first the differential equations of linearized elasticity for Hooke's law will be given. Then in section 2.2 the necessary and sufficient optimality conditions for the corresponding optimal control problem for problems with and without constraints on the control will be derived. Using this theoretical results in chapter 3 the optimality conditions for the unrestricted problem will be solved numerically and the relationship between the material constants and the Tichonoff regularization parameter α will be analyzed.

2.1. The differential equations of linearized elasticity

The theory of linearized elasticity can be derived by linearizing both the constitutive equation, which relates the deformation gradient with the stress tensor, and the strain tensor $E(u) := \frac{1}{2}(\nabla u + \nabla u^* + \nabla u^* \nabla u)$ which reduces to the symmetric gradient $\nabla^s u := \frac{1}{2}(\nabla u + \nabla u^*)$. Alternatively one could derive the model of linearized elasticity directly, but some interesting connections between nonlinear and linear theory and connections to the constitutive equations do not occur "naturally" this way. One of these connections is the fact that if the stored energy function f is twice continuously differentiable at u_0 with respect to u then strict rank-1 convexity implies the strong Legendre-Hadamard condition (see [Da08, Mo08])

$$\frac{\partial^2 f(u_0)}{\partial(D_i u_m)\partial(D_j u_k)} d_i d_j v_k v_m > 0 \qquad \forall d, v \in \mathbb{R}^3 \setminus \{0\} \tag{13}$$

Recognizing that the following chain of implications holds (see [Da08, Mo08]):

$$\begin{aligned} \text{(strict) convexity} \quad &\Rightarrow \quad \text{(strict) polyconvexity} \\ \Rightarrow \text{(strict) quasi-convexity} \quad &\Rightarrow \quad \text{(strict) rank-1 convexity} \end{aligned}$$

this connection also holds for polyconvex functions, that are of interest in chapter 4. As the set

$$\mathcal{C} := \{v, d \in \mathbb{R}^3 : \quad |v| = |d| = 1\}$$

is compact one can define

$$c := \min_{v,d \in \mathcal{C}} \frac{\partial^2 f(u_0)}{\partial(D_i u_m)\partial(D_j u_k)} d_i d_j v_k v_m > 0$$

Therefore (13) is equivalent to

$$\frac{\partial^2 f(u_0)}{\partial(D_i u_m)\partial(D_j u_k)} d_i d_j v_k v_m > c|d|^2|v|^2 \qquad \forall d, v \in \mathbb{R}^3$$

This inequality can be used in order to derive the ellipticity condition for the Lemma of Lax and Milgram using the technique of freezing the coefficients. Thus the linearized equations of elasticity fit into the framework of linear elliptic equations and unique existence of solutions in $H^1(\Omega;\mathbb{R}^3)$ is given through the Lemma of Lax and Milgram.

In the context of elasticity the strong Legendre-Hadamard condition is often referred to as "stability condition". It is a local stability condition that allows to prove local uniqueness of solutions and the local stability of solutions using the implicit function theorem, if the solution operator is smooth enough, but does not give any global results (see [Sp09]). If one does not have a polyconvex stored energy function one can use conditions as in [Ci88, ch. 6.2, ch. 6.8] in order to get links between linearized elasticity and nonlinear elasticity. As stated above the linearization of the stored energy function near a natural state leads in many cases to Hooke's linear material law.

Thus in this case, the Euler equations of linearized elasticity take the form

$$\begin{aligned} -\mathrm{div}\Big(\lambda \mathrm{tr}(\nabla^s u)I + 2\mu\nabla^s u\Big) = -\mathrm{div}\Big(\sigma(u)\Big) &= K && \text{in } \Omega \\ u &= u_0 && \text{on } \Gamma_1 \\ \sigma(u)n &= g && \text{on } \Gamma_2 \end{aligned}$$

with $K \in H^{-1}(\Omega;\mathbb{R}^3)$, $u_0 \in H^{\frac{1}{2}}(\Gamma_1;\mathbb{R}^3)$, $g \in L^2(\Gamma_2;\mathbb{R}^3)$, $\Gamma = \Gamma_1 \cup \Gamma_2$, $\Gamma_1 \cap \Gamma_2 = \emptyset$. The corresponding weak formulation then is

$$\int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u\nabla^s v\Big)\ \mathrm{dx} = \int_\Omega Kv\ \mathrm{dx} + \int_{\Gamma_1} n\sigma(u_0)v\ \mathrm{ds} + \int_{\Gamma_2} gv\ \mathrm{dx}$$

for all $v \in H^1(\Omega;\mathbb{R}^3)$. The ellipticity of the bilinear form

$$b(u,v) := \int_\Omega \lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u\nabla^s v\ \mathrm{dx} \tag{14}$$

follows with Korn's second inequality (Theorem A.3). So the linearized problem for sufficiently smooth rank-1 convex and especially polyconvex stored energy functions and for stored energy functions of homogeneous, isotropic, elastic materials near a natural state fit into the framework of linear strongly elliptic systems. As already stated in Remark 6 solutions of these systems violate the axiom of material frame indifference which is the reason for speaking about "linearized elasticity" instead of "linear elasticity". This highlights that there exist cases in which solutions of the linearized systems may not be used as approximations for displacements in elasticity.

Another point that should be mentioned in the derivation of linearized elasticity is the assumption that ∇u is small in a strong sense. This allows to drop the orientation-preserving condition $\det(\nabla\Phi) > 0$ a.e. on Ω, which is necessary to get the convexity of the admissible set. An implication is clearly that for large displacement gradients self-interpenetration can occur when wrongly using linearized elasticity.

2.2. The optimal control problem for linearized elasticity

As Hooke's law is the material law that appears as linearization of Ogden-type materials, the optimal control problem will be considered exemplary for this case but as pointed out in the last chapter the same approach works for the case of strong rank-1 convexity and sufficient smoothness of the stored energy function. As noted, the requirement $\det(I + \nabla u) > 0$ will be dropped, as this condition leads to a non-convex admissible set $U := \{u \in W^{1,p}(\Omega; \mathbb{R}^3) | \det(I + \nabla u) > 0\}$ and consequently to a non-convex problem. Then the optimal problem stated in the introduction takes the form

$$\min\ J(u, g) := \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)} \tag{15}$$

s.t.

$$\int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u \nabla^s v\Big)\ \mathrm{dx} = \int_\Omega Kv\ \mathrm{dx} + \int_{\Gamma_3} gv\ \mathrm{dx} \quad \forall v \in H^1(\Omega; \mathbb{R}^3) \tag{16}$$

where $u_0 \equiv 0$ as usually in the context of linear differential equations and on Γ_2 homogeneous Neumann boundary conditions are prescribed.

As the cost functional is bounded from below and satisfies

$$\lim_{\|g\|_{L^2(\Gamma_3;\mathbb{R}^3)}\to\infty} J(u, g) = \lim_{\|u\|_{L^2(\Gamma_2;\mathbb{R}^3)}\to\infty} J(u, g) = \infty$$

it is possible to restrict the problem to $g \in \{g \in L^2(\Gamma_3; \mathbb{R}^3) | \|g\|_{L^2(\Gamma_3;\mathbb{R}^3)} \leq M\}$ for some sufficiently big constant M (i.e. if $K = 0$: $M = \frac{\|u_{ref}\|_{L^2(\Gamma_2;\mathbb{R}^3)}}{\sqrt{\alpha}}$). Therefore the existence of solutions follows directly with theorem A.9 and we can turn to the derivation of the the first order optimality conditions, following the formal Lagrange principle as in [Tr09]. Therefore first the definitions of the reduced energy functional and the variational inequality will be given.

Definition 2.1. *(reduced (cost) functional)*
Let $S :\ L^2(\Gamma_3; \mathbb{R}^3) \to H^1(\Omega; \mathbb{R}^3)$, $g \mapsto u$ be the control-to-state mapping, i.e. the solution operator $u = Sg$ of (16)*. Then the **reduced cost functional** is defined as*

$$f(g) := J\Big(S(g), g\Big) = \frac{1}{2}\|S(g) - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)} \tag{17}$$

The introduction of the solution operator of the differential equation allows to eliminate the constraints from the system (15) s.t. (16) and get the equivalent formulation

$$\min_{g\in L^2(\Gamma_3;\mathbb{R}^3)} f(g).$$

For this constraint-free formulation it is easy to derive first order optimality conditions if one has the differentiability of $\tilde{S} := \tau \circ S$, where $\tau :\ H^1(\Omega; \mathbb{R}^3) \to L^2(\Gamma_2; \mathbb{R}^3)$ is a trace operator. Both operators are linear and continuous. For the trace operator this follows from embedding theorems (see i.e. [Tr09, Thm. 7.2]), for $S: L^2(\Gamma_3;\mathbb{R}^3) \to H^1(\Omega;\mathbb{R}^3)$ this is given by the lemma of Lax and Milgram. Thus $\tilde{S}: L^2(\Gamma_3;\mathbb{R}^3) \to L^2(\Gamma_2;\mathbb{R}^3)$ is also linear and continuous and therefore also Fréchet-differentiable. Consequently the consideration of the solution operator with image in $L^2(\Gamma_2;\mathbb{R}^3)$ is sufficiently regular to allow the differentiation of $f: L^2(\Gamma_3;\mathbb{R}^3) \to \mathbb{R}$.

In order to consider also problems with constraints on g it will be assumed that $g \in G$, where G is the admissible subset for the control, i.e.

$$G = L^2(\Gamma_3;\mathbb{R}^3) \text{ resp. } G = \{g \in L^2(\Gamma_3;\mathbb{R}^3) : g_i(x) \geq 0 \text{ a.e. on } \Gamma_3, i = 1,2,3\}$$

.

Theorem 2.1. *(variational equality/inequality)*
If the control-to-state mapping with image in $L^2(\Gamma_2;\mathbb{R}^3)$ is differentiable, then if $\bar{g}$ is a local minimizer of (15) it satisfies

$$f'(\bar{g})(g-\bar{g}) = \int_{\Gamma_2} (\bar{u} - u_{ref})(u - \bar{u}) \text{ dx} + \alpha \int_{\Gamma_3} \bar{g}(g - \bar{g}) \text{ ds} \geq 0 \quad \forall g \in G \tag{18}$$

with $\bar{u} = S(\bar{g})$ and $u = S(g)$. For convex problems the converse is also true.

If no constraints on g are given, then the ***variational inequality*** *reduces to the* ***variational equality***

$$f'(\bar{g})(g-\bar{g}) = \int_{\Gamma_2} (\bar{u} - u_{ref})(u - \bar{u}) \text{ dx} + \alpha \int_{\Gamma_3} \bar{g}(g - \bar{g}) \text{ ds} = 0 \quad \forall g \in G \tag{19}$$

Proof. First it will be shown that $f'(\bar{g})h \geq 0$ for all $h \in G$. This follows directly from the optimality of $\bar{g}$ and the definition of f':

$$f'(\bar{g})h = \lim_{t\to 0} \frac{f(\bar{g}+th) - f(\bar{g})}{t}$$

For t sufficiently small the local optimality of $\bar{g}$ implies $f(\bar{g}+th) - f(\bar{g}) \geq 0$ and consequently $f'(\bar{g})h \geq 0$ for all $h \in L^2(\Gamma_3;\mathbb{R}^3)$. Replacing $h = g - \bar{g}$ this gives the desired inequality. If the admissible set G is open, then for sufficiently small t one also gets $\bar{g} - th \in G \Rightarrow f'(\bar{g})h \leq 0$. Thus $f'(\bar{g})(g-\bar{g}) = 0$ for all $g \in G$ in this case.

Now differentiating f at $\bar{g}$ in direction h gives

$$f'(\bar{g})h = \int_{\Gamma_2} (\bar{u} - u_{ref})\tilde{S}h \text{ ds} + \alpha \int_{\Gamma_3} \bar{g}h \text{ ds}$$

Replacing again $h = g - \bar{g} \Rightarrow Sh = u - \bar{u}$ gives the form of (18).

For convex functions the inverse statement follows directly from the fact that differentiable functions are convex if and only if the gradients are subgradients, i.e. if for all $g, \bar{g} \in G$ holds

$$f(g) \geq f(\bar{g}) + f'(\bar{g})(g-\bar{g}) \Leftrightarrow f(g) - f(\bar{g}) \geq f'(\bar{g})(g-\bar{g}) \geq 0 \qquad \blacksquare$$

Optimality conditions for problems without constraints on the control

Writing the variational equality as a linear equality in g it takes the form

$$f'(\bar{g})(g-\bar{g}) = \int_{\Gamma_3} \tilde{S}^*(\bar{u}-u_{ref})(g-\bar{g}) \ \mathrm{dx} + \alpha \int_{\Gamma_3} \bar{g}(g-\bar{g}) \ \mathrm{ds} = 0$$

where $\tilde{S}^*$ is the adjoint operator of $\tilde{S}$. Just as $\tilde{S}$, this operator is the solution operator for a differential equation. In order to determine the adjoint operator of $\tilde{S}$ the formal Lagrange principle will be used, i.e. first formally define the Lagrange function

$$\mathcal{L}(u,g,p) := J(u,g) - \int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(p) + 2\mu\nabla^s u \nabla^s p - Kp\Big) \ \mathrm{dx} + \int_{\Gamma_3} gp \ \mathrm{ds}$$

where p takes the role of a Lagrange multiplier. Supposing that the Lagrange function is well-defined, it can immediately be observed that (16) is given through $D_p\mathcal{L}(u,g,\bar{p})v = 0$. Defining the adjoint equation through $D_u\mathcal{L}(\bar{u},g,p)h = 0$ for all $h \in H^1(\Omega;\mathbb{R}^3)$, i.e. p solves

$$\int_\Omega \Big(\lambda \mathrm{div}(h)\mathrm{div}(p) + 2\mu\nabla^s h \nabla^s p\Big) \ \mathrm{dx} = \int_{\Gamma_2} h(\bar{u}-u_{ref}) \ \mathrm{ds} \qquad \forall h \in H^1(\Omega;\mathbb{R}^3) \tag{20}$$

one can determine the Lagrange multiplier. The existence of $p \in H^1(\Omega;\mathbb{R}^3)$ follows again with Korn's second inequality and the Lemma of Lax and Milgram and therefore the above definition of the Lagrange function $\mathcal{L}$ is well defined as continuously differentiable operator $\mathcal{L}: \ H^1(\Omega;\mathbb{R}^3) \times L^2(\Gamma_3;\mathbb{R}^3) \times H^1(\Omega;\mathbb{R}^3) \to \mathbb{R}$.

Now one has to prove that critical point of $\mathcal{L}$ also satisfies the variational inequality (18). Therefore first test (16), for different boundary controls g, $\bar{g}$, with p and (20) with $u-\bar{u}$, $u = S(g)$, $\bar{u} = S(\bar{g})$

$$\begin{aligned}
\int_\Omega \Big(\lambda \mathrm{div}(u-\bar{u})\mathrm{div}(p) + 2\mu\nabla^s(u-\bar{u})\nabla^s p\Big) \ \mathrm{dx} &= \int_{\Gamma_3} (g-\bar{g})p \ \mathrm{dx} \\
\int_\Omega \Big(\lambda \mathrm{div}(p)\mathrm{div}(u-\bar{u}) + 2\mu\nabla^s p\nabla^s(u-\bar{u})\Big) \ \mathrm{dx} &= \int_{\Gamma_2} (\bar{u}-u_{ref})(u-\bar{u}) \ \mathrm{ds}
\end{aligned}$$

As the left hand sides of the above equations coincide this implies

$$\int_{\Gamma_3} (g-\bar{g})p \ \mathrm{dx} = \int_{\Gamma_2} (\bar{u}-u_{ref})(u-\bar{u}) \ \mathrm{ds} \tag{21}$$

Thus one can replace the displacement in the variational equality

$$f'(\bar{g})(g-\bar{g}) = \int_{\Gamma_3} (g-\bar{g})p \ \mathrm{ds} + \alpha \int_{\Gamma_3} \bar{g}(g-\bar{g}) \ \mathrm{ds} = 0 \qquad \forall g \in L^2(\Gamma_3;\mathbb{R}^3)$$

The last necessary condition for critical points of $\mathcal{L}$, $D_g\mathcal{L}(u,\bar{g},p)h = 0$ gives with $h = g-\bar{g}$ the variational equality

$$\alpha \int_{\Gamma_3} \bar{g}(g-\bar{g}) \ \mathrm{ds} + \int_{\Gamma_3} p(g-\bar{g}) \ \mathrm{ds} = 0 \qquad \forall g \in L^2(\Gamma_3;\mathbb{R}^3)$$

and therefore it holds $\bar{g} = -\frac{1}{\alpha}p$ a.e. on Γ_3, where $\cdot|_{\Gamma_3}$ denotes the trace-operator $\Omega \to \Gamma_3$. Replacing the unknown control the necessary and, due to the strict convexity of J, sufficient first order optimality conditions are given in

Theorem 2.2. *The pair $(u, g) \in H^1(\Omega;\mathbb{R}^3) \times L^2(\Gamma_3;\mathbb{R}^3)$ is an optimal solution of* (15) *s.t.* (16) *if and only if $g = \frac{1}{\alpha}p$ a.e. on Γ_3 and the following system is satisfied:*

$$\int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u \nabla^s v\Big)\ \mathrm{dx} = \int_\Omega Kv\ \mathrm{dx} - \frac{1}{\alpha}\int_{\Gamma_3} pv\ \mathrm{dx} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3) \tag{22}$$

$$\int_\Omega \Big(\lambda \mathrm{div}(p)\mathrm{div}(v) + 2\mu\nabla^s p \nabla^s v\Big)\ \mathrm{dx} = \int_{\Gamma_2} (u - u_{ref})v\ \mathrm{ds} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3) \tag{23}$$

One can also observe that the linear and continuous solution operator $S_{ad} :\ L^2(\Gamma_2;\mathbb{R}^3) \to H^1(\Omega;\mathbb{R}^3)$ of the adjoint differential equation defines the adjoint operator and

$$\tilde{S}^* :\ L^2(\Gamma_2;\mathbb{R}^3) \simeq \Big(L^2(\Gamma_2;\mathbb{R}^3)\Big)^* \to \Big(L^2(\Gamma_3;\mathbb{R}^3)\Big)^* \simeq L^2(\Gamma_3;\mathbb{R}^3)$$

as $\tilde{S}^* = \tau_{\Gamma_3} \circ S_{ad}$, where, according to the representation theorem of Riesz, the dual spaces of the L^2-spaces have been identified with the spaces themselves and τ_{Γ_3} is a linear and continuous trace operator $H^1(\Omega;\mathbb{R}^3) \to L^2(\Gamma_3;\mathbb{R}^3)$. Setting w.l.o.g.

$$v = u - u_{ref},\ p = \tilde{S}^* v,\ h = g - \bar{g}$$

the above argumentation leading to (21) implies

$$(\tilde{S}^* v, h)_{L^2(\Gamma_3;\mathbb{R}^3)} = (p, g - \bar{g})_{L^2(\Gamma_3;\mathbb{R}^3)} = (u - u_{ref}, u - \bar{u})_{L^2(\Gamma_2;\mathbb{R}^3)} = (v, \tilde{S}h)_{L^2(\Gamma_2;\mathbb{R}^3)}$$

Optimality conditions for problems with constraints on the control

In implant shape design one may wish to impose an additional constraint on the control, i.e. $g_i(x) \geq 0$, $i = 1, 2, 3$ a.e. on Γ_3, as an implant can only exert pressure but no traction forces. Then the admissible set for the boundary control $L^2(\Gamma_3;\mathbb{R}^3)$ must be replaced by

$$G := \{g \in L^2(\Gamma_3;\mathbb{R}^3) :\ g_i(x) \geq 0 \,\text{a.e. on}\ \Gamma_3, i = 1, 2, 3\}$$

In this case one can not replace the control with the rescaled solution of the adjoint equation. Instead a point-wise equivalent formulation for the variational inequality

$$\alpha \int_{\Gamma_3} \bar{g}(g - \bar{g})\ \mathrm{ds} + \int_{\Gamma_3} p(g - \bar{g})\ \mathrm{ds} \geq 0 \qquad \forall g \in L^2(\Gamma_3;\mathbb{R}^3) \tag{24}$$

will be used that allows to state a minimum principle and derive a Karush-Kuhn-Tucker system (KKT system). The following lemma gives the point-wise equivalent to (24)

Lemma 2.3. *The following statements are equivalent:*

1. *The variational inequality* (24) *is fulfilled.*
2. *It holds*

$$\bar{g}_i(x) = \begin{cases} 0 & \text{if } \alpha\bar{g}_i(x) + p_i(x) > 0 \\ \geq 0 & \text{if } \alpha\bar{g}_i(x) + p_i(x) = 0 \end{cases} \qquad i = 1,2,3 \tag{25}$$

and $\alpha\bar{g}_i(x) + p_i(x) \geq 0$, $i = 1,2,3$ *a.e. on* Γ_3.

3. *The inequality*

$$\Big(\alpha\bar{g}_i(x) + p_i(x)\Big)\Big((v_i(x) - \bar{g}_i(x)\Big) \geq 0 \qquad \forall v \in G \tag{26}$$

and $\alpha\bar{g}_i(x) + p_i(x) \geq 0$, $i = 1,2,3$ *are fulfilled a.e. on* Γ_3.

Proof.

- Show 1. $\Rightarrow$ 2.:
First show that the case $\alpha\bar{g}_i(x) + p_i(x) < 0$ will not occur on a set of nonzero measure as this would violate the variational inequality. To see this take

$$F_i \subset \{x \in \Gamma_3 : \alpha\bar{g}_i(x) + p_i(x) < 0\}$$

and define

$$L^2(\Gamma_3;\mathbb{R}) \ni h_j(x) := \begin{cases} \bar{g}_j(x) + 1 & \text{if } x \in F_i \wedge j = i \\ \bar{g}_j(x) & \text{if } x \in \Gamma_3 \setminus F \end{cases} \qquad j = 1,2,3$$

Then

$$\int_{\Gamma_3} (\alpha\bar{g} + p)(h - \bar{g}) \text{ ds} = \int_{F_i} (\alpha\bar{g}_i + p_i) \text{ ds} < 0$$

Define

$$A^i_+ := \{x \in \Gamma_3 : \quad \alpha\bar{g}_i(x) + p_i(x) > 0\}, \; i = 1,2,3$$

and assume that 2. is not fulfilled, i.e. there exists a subset $E \in A^i_+$ for some i with $|E| > 0$ such that $\bar{g}_i > 0$ a.e. on E. Define

$$L^2(\Gamma_3;\mathbb{R}) \ni g_j(x) := \begin{cases} 0 & \text{if } x \in E \wedge j = i \\ \bar{g}_j(x) & \text{if } x \in \Gamma_3 \setminus E \end{cases} \qquad j = 1,2,3$$

Then follows

$$\int_{\Gamma_3} (\alpha\bar{g} + p)(g - \bar{g}) \text{ ds} = -\int_{E} (\alpha\bar{g}_i + p_i)\bar{g}_i \text{ ds} < 0$$

i.e. the variational inequality is violated.

- Show 2. $\Rightarrow$ 3.:
  For $x \in \Omega \setminus (\bigcup_i A_+^i)$ holds $\Big(\alpha \bar{g}_i(x) + p_i(x)\Big)\Big((v_i(x) - \bar{g}_i(x)\Big) = 0 \qquad \forall v \in G.$
  For $x \in A_+^i$ for some arbitrary $i \in \{1,2,3\}$ holds $\Big(\alpha \bar{g}_i(x)+p_i(x)\Big)\Big((v_i(x)-\bar{g}_i(x)\Big) = \Big(\alpha \bar{g}_i(x) + p_i(x)\Big)v_i(x) \geq 0 \qquad \forall v \in G.$
- Show 3. $\Rightarrow$ 1.:
  This follows directly by setting $v = g$ and integrating over Γ_3.

■

Remark 12. *Writing down the second statement of the above lemma as*

$$\Big(\alpha \bar{g}_i(x) + p_i(x)\Big)\bar{g}_i(x) \leq \Big(\alpha \bar{g}_i + p_i(x)\Big)v_i(x) \qquad \forall v \in G$$

leads to the weak minimum principle

$$\Big(\alpha \bar{g}_i(x) + p_i(x)\Big)\bar{g}_i(x) = \min_{v \in G} \Big(\alpha \bar{g}_i(x) + p_i(x)\Big)v_i(x)$$

and the minimum principle

$$\Big(\frac{\alpha}{2}\bar{g}_i(x) + p_i(x)\Big)\bar{g}_i(x) = \min_{v \in G} \Big(\alpha v_i(x) + p_i(x)\Big)v_i(x)$$

Using the point-wise equivalent formulations for the variational inequality one can derive the KKT-Theorem using the following

Theorem 2.4. *The variational inequality* (18) *is equivalent to the existence of a function* $\gamma \in L^2(\Gamma_3;\mathbb{R}^3)$, $\gamma_i(x) \geq 0$ *a.e. on* Γ_3 *for* $i = 1,2,3$ *such that*

$$\alpha \bar{g}(x) + p(x) - \gamma(x) = 0 \tag{27}$$

and

$$\sum_{i=1}^{3} \gamma_i(x)\bar{g}_i(x) = 0 \tag{28}$$

and $\alpha \bar{g}_i(x) + p_i(x) \geq 0$, $i = 1,2,3$ *a.e. on* Γ_3*, where* p *is the solution of the adjoint equation* (20).

Proof.

- First it will be shown that the variational inequality leads to the above conditions. First define

$$\gamma \;:=\; (\alpha \bar{g} + p)_+$$

where for $s \in \mathbb{R}$, s_+ is defined through $s_+ := \frac{1}{2}(|s| + s)$ and in the same way point-wise for $s \in \mathbb{R}^n$. Then clearly holds $\alpha\bar{g} + p = \gamma$ and γ is non-negative by definition. (25) in the above lemma gives the relation

$$\gamma_i(x) \neq 0 \Rightarrow \bar{g}_i(x) = 0 \qquad \text{a.e. in } \Gamma_3$$

which gives (28). The inequality $\alpha\bar{g}_i(x) + p_i(x) \geq 0$, $i = 1,2,3$ a.e. in Γ_3 has already been shown in Lemma 2.3.

- Now we show that the above conditions (27) and (28) imply (24). Consider the set $\mathcal{N}_i = \{x \in \Gamma_3 : \bar{g}_i(x) = 0\}$. Then for $g \in G$ holds $g_i - \bar{g}_i = g_i \geq 0$ a.e. in $\mathcal{N}_i$. For $x \in \Gamma_3 \setminus \mathcal{N}_i$ follows with (28) that $\alpha\bar{g}_i + p_i = 0$ a.e. and as $\alpha\bar{g}_i(x) + p_i(x) \geq 0$, $i = 1,2,3$ a.e. (26) is satisfied on Γ_3.

■

Corollary 2.5. *The KKT System*

Instead of the optimality system (22) *and* (23) *one gets the Karush-Kuhn-Tucker system*

$$\int_\Omega \lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u\nabla^s v \, \mathrm{dx} = \int_\Omega Kv \, \mathrm{dx} + \int_{\Gamma_3} gv \, \mathrm{dx} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3) \quad (29)$$

$$\int_\Omega \lambda \mathrm{div}(p)\mathrm{div}(v) + 2\mu\nabla^s p\nabla^s v \, \mathrm{dx} = \int_{\Gamma_2} (u - u_{ref})v \, \mathrm{ds} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3) \quad (30)$$

$$\alpha\bar{g}(x) + p(x) - \gamma(x) = 0 \qquad \textit{a.e. on } \Gamma_3,\ \gamma \in G \quad (31)$$

$$\sum_{i=1}^{3} \gamma_i(x) g_i(x) = 0 \qquad \textit{a.e. on } \Gamma_3 \quad (32)$$

$$\alpha g_i(x) + p_i(x) \geq 0 \qquad \textit{a.e. on } \Gamma_3,\ i = 1,2,3 \quad (33)$$

Remark 13. *Like in the case without constraints one can eliminate the control g as optimality implies* (*see* [Tr09, Theorem 2.28])

$$\bar{g}_i(x) = \mathbb{P}_{[0,\infty)}\Big(-\frac{1}{\alpha}p_i(x)\Big) \quad i = 1,2,3, \ \textit{a.e. on } \Gamma_3 \qquad (34)$$

where $\mathbb{P}_{[0,\infty)}$ is the projection operator $\mathbb{R} \to [0,\infty)$, i.e. $\mathbb{P}_{[0,\infty)}(x) = \max(0,x)$. Thus one can replace (31)-(33) *with* (34). *The projection operator is not differentiable in $x = 0$ but everywhere Newton-differentiable* (*see* [Tr09]). *In addition it is weakly differentiable and can be incorporated in the system* (22) & (23) *and thus also the KKT-conditions* (29)-(33) *can be solved directly by solving a nonlinear system of PDEs.*

Corollary 2.6. *Using the projection operator $\mathbb{P}_{[0,\infty)}$ the KKT-conditions* (29)-(33) *are equivalent to the system*

$$\int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u\nabla^s v\Big) \, \mathrm{dx} = \int_\Omega Kv \, \mathrm{dx} + \int_{\Gamma_3} \mathbb{P}_{[0,\infty)}\Big(-\frac{1}{\alpha}p\Big)v \, \mathrm{dx} \qquad (35)$$

$$\int_\Omega \Big(\lambda \mathrm{div}(p)\mathrm{div}(w) + 2\mu\nabla^s p\nabla^s w\Big) \, \mathrm{dx} = \int_{\Gamma_2} (u - u_{ref})w \, \mathrm{ds} \qquad (36)$$

for all $v, w \in H^1(\Omega;\mathbb{R}^3)$.

3. Optimal Control in Implant Shape Design

In this chapter the optimality system derived in section 2.2 will be solved numerically for the problem stated in the introduction. Therefore the material-dependent parameters must be chosen accurately and it is necessary to determine the cases that allow the application of linear models. Then a numerical strategy for the solution of the optimal control problem is chosen and implemented. It will be seen that the problem is difficult even for the easy case of a linear system of elliptic differential equations and it is necessary to have good solvers for the calculation of solutions of the arising systems of equations. Finally some solutions for the considered example problem will be presented and the dependence of the Tichonoff regularization parameter α on the material parameters will be examined.

3.1. Physical problem setting

In chapter 1 it has been shown that for homogeneous, isotropic, elastic materials near natural states linearized elasticity is an adequate assumption. More precisely experiments performed and published by Y.C. Fung in ([Fu93]) show that linear material laws are an adequate model as long as the strain ratio, i.e. the relative strain, is smaller than 15%. In addition, for small displacements in homogeneous materials it is a reasonable assumption that also the displacement gradients ∇u are small. Then considering the strong C^2-setting used in the derivation of elasticity theory, this implies that $\det(I + \nabla u) \gg 0$ on Ω. Thus the assumption of small displacement gradients allows to drop the condition $\det(I + \nabla u) > 0$. This is advantageously as the orientation-preserving condition opposes the desired convexity of the set of admissible pairs (u, g). For unconstrained $g \in L^2(\Gamma_3; \mathbb{R}^3)$ the linearity of the solution operator of the differential equations of linearized elasticity implies that the set of admissible pairs is a linear subspace of $H^1(\Omega; \mathbb{R}^3) \times L^2(\Gamma_3; \mathbb{R}^3)$. In the case that positivity constraints on g are imposed, the set of admissible pairs is no longer a linear subspace but still remains convex. Therefore in both cases the strict convexity of the quadratic cost functional

$$J(u, g) = \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|_{L^2(\Gamma_3;\mathbb{R}^3)}$$

implies that the necessary optimality conditions are sufficient.

Recall that in the context of implant shape design Ω denotes a part of the facial soft tissue and its boundary is composed of three parts, namely Γ_1, the artificial boundary that appears when cutting out a region of interest out of scanned data, Γ_2, the visible part, and Γ_3, the part of the boundary where the implant should be. For the computations performed Figure 6 shows the part of the face that will be considered as reference configuration. Figure 7 and Figure 8 show the surface Γ_2 and the desired deformation u_{ref}. This deformation has been calculated using linearized elasticity with Lamé constants $\lambda = 3.1 * 10^8$ and $\mu = 3.45 * 10^7$ and omitting the body forces K. These are mainly the gravitational forces that are dependent on the orientation of the reference configuration. The calculation of the implants effect should be independent of orientation dependent effects and therefore the assumption $K = 0$ is reasonable. As one can see the given deformation u_{ref} is not nice, but it makes the visual verification of the results easier.

According to theorem 2.2 the optimality system for the problem of optimal implant shape design in linearized elasticity takes the form

$$\int_\Omega \Big(\lambda \mathrm{div}(u)\mathrm{div}(v) + 2\mu\nabla^s u \nabla^s v\Big)\, \mathrm{dx} = -\frac{1}{\alpha}\int_{\Gamma_3} pv \, \mathrm{dx} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3) \tag{37}$$

$$\int_\Omega \Big(\lambda \mathrm{div}(p)\mathrm{div}(v) + 2\mu\nabla^s p \nabla^s v\Big)\, \mathrm{dx} = \int_{\Gamma_2} (u - u_{ref})v \, \mathrm{ds} \quad \forall v \in H^1(\Omega;\mathbb{R}^3) \tag{38}$$

The projection operator of Remark 13 can be implemented, but has no effect as in the considered problem any control will be positive and thus it is not used in the following as with or without this operator the Newton method converges after one step to the same result. For the Lamé constants as well as the regularization parameter α different choices will be considered and the dependence of the regularization parameter on the Lamé constants will be analyzed.

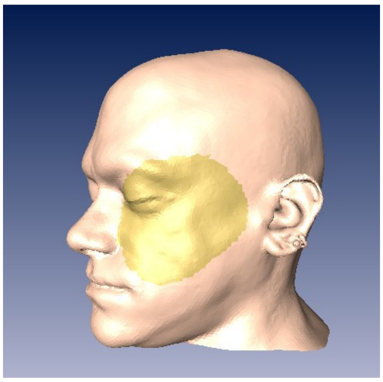

Figure 6: considered geometry

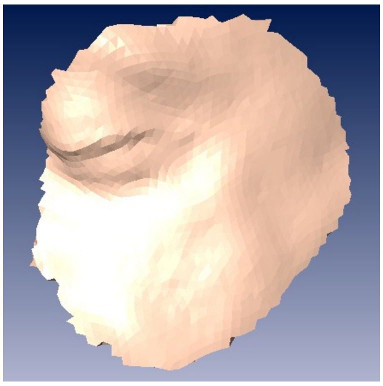

Figure 7: reference configuration

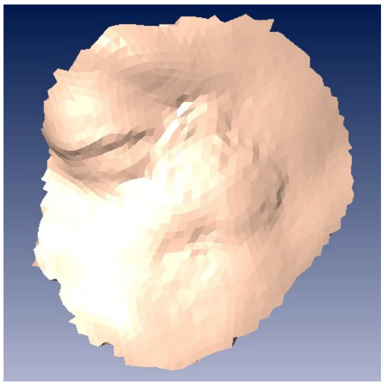

Figure 8: deformed configuration u_{ref}

3.2. Implementation

For the implementation of a solution of the optimality system (37)&(38) a scan of the human head (Figure 6) has been provided by Dr. Stefan Zachow, including a tetrahedral grid. Using ZIBAmira, a visualization and manipulation tool for bio-medical data, the reference configuration has been defined and a subgrid has been extracted. In order to define boundary conditions a surface grid has been extracted from the subgrid. On this geometry the system (37)&(38) has been discretized using the finite element library Kaskade7, that is based on the DUNE toolbox. The grid manager UGGrid from the

UG toolbox (UG = unstructured grid) has been chosen as it can easily handle the three-dimensional grids used (10.924 nodes, 41.973 triangles) and for future calculations supports local refinements. As for three-dimensional grids the stiffness matrix for higher order Ansatz spaces becomes complicated linear Ansatz spaces will be used for u and p. The resulting system has been solved performing one Newton-step. As solver for the appearing system of equations PARDISO, a solver for large sparse linear systems of equations, has been used. Other direct and iterative solvers (with preconditioning) failed due to the bad conditioning of the system. Probably special preconditioners optimized for the the differential equations of linearized elasticity, as proposed in [Au06], would help.

The incorporation of mixed boundary conditions is not yet supported by the current version of Kaskade7, as it has only recently been incorporated into the actual version of DUNE, and therefore these conditions are incorporated using a scalar field defined on Ω and taking as values indices associated with the boundary conditions. For points that lie on the intersection $\Lambda = (\Gamma_1 \cap \Gamma_2) \cup (\Gamma_1 \cap \Gamma_3)$ of parts of the boundary with different boundary conditions the choice is not unique. In the following these points get the index of the corresponding Neumann boundary conditions. This is possible as Ω is chosen big enough such that the effect of the implant on the soft tissue near Λ is negligible. Then the Dirichlet boundary conditions are approximately satisfied on Λ automatically. A nice feature of this approach is the fact that the boundary conditions will be implicitly adjusted if adaptivity is implemented.

3.3. Numerical results

While the Lamé constants are determined by the material under consideration and the desired displacement on Γ_2 is known, it leaves to assign a value to the Tichonoff regularization parameter $\alpha > 0$. For the theory the existence of α is advantageous as it assures the boundedness of the control. Additionally for $\alpha > 0$ there exist better regularity results for the control than could be expected from the known regularity results for solutions of the differential equations itself (see [Tr09]) and it is possible to eliminate the control from the optimality system. For the numerical treatment the presence of the regularization parameter causes problems. As α must be chosen very small in order to get numerical solutions u such that the residuum $\|u - u_{ref}\|_{L^2(\Omega;\mathbb{R}^3)}$ is small this can lead to ill-conditioned Hessian matrices when solving the optimality system (37)&(38). Thus it may be necessary to use methods that try to prevent ill-conditioning of the Hessian as in [No99, Ch. 17].

The danger of ill-conditioning is a serious issue in the context of optimal control with constraints from elasticity theory. Recalling that Young's modulus E measures the force opposed by the soft tissue to deformations it is reasonable to assume that g should be at least in $O(E)$ and thus $\alpha \ll E^{-2} * \|u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)}$ in order to compensate the appearance of $\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)}$ in the cost functional $J(u, g)$. The dependence on Young's modulus E is strongly supported by numerical experiments as, exemplary for $\nu = 0.45$, in Figure 9. This dependence has been analyzed for $E = 10^5, \ldots, 10^{10}$ and $\nu = 0.20, \ldots, 0.46$ with similar results. For the dependence on the Poisson ratio ν it was observed that bigger values of ν allow slightly smaller regularization parameters, but the influence was negligible in all the considered problems.

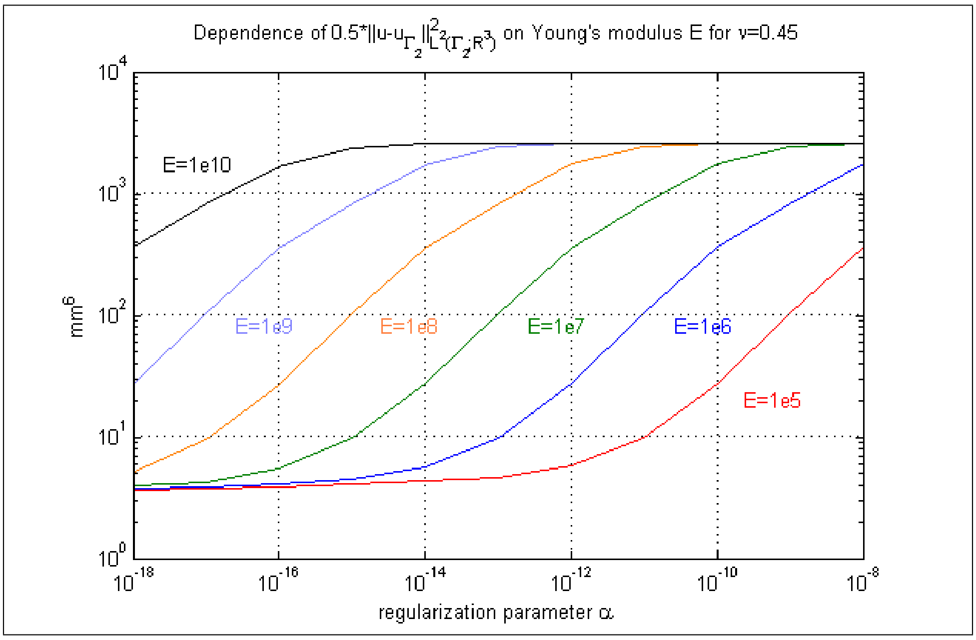

Figure 9: Dependence on Young's modulus

A robust way to find good values for α, that tries to avoid ill-conditioning, considers the L-curve, a plot of $\|g\|_{L^2(\Gamma_3;\mathbb{R}^3)}$ against the residuum

$$\|u - u_{ref}\|_{L^2(\Gamma_2;\mathbb{R}^3)} = \|Sg - u_{ref}\|_{L^2(\Gamma_2;\mathbb{R}^3)}$$

The flat part of this curve is the part where the residual error dominates the behaviour of $J(u, g)$ in contrast to the steep part, where the norm of the control is dominant and only small progress in the residuum can be observed. Consequently the biggest values of α that admit small residuums are in the parts of high curvature in the L-curve. According to [Ha93] the best choice is the point of highest curvature as the point with best trade-off between error and stability.

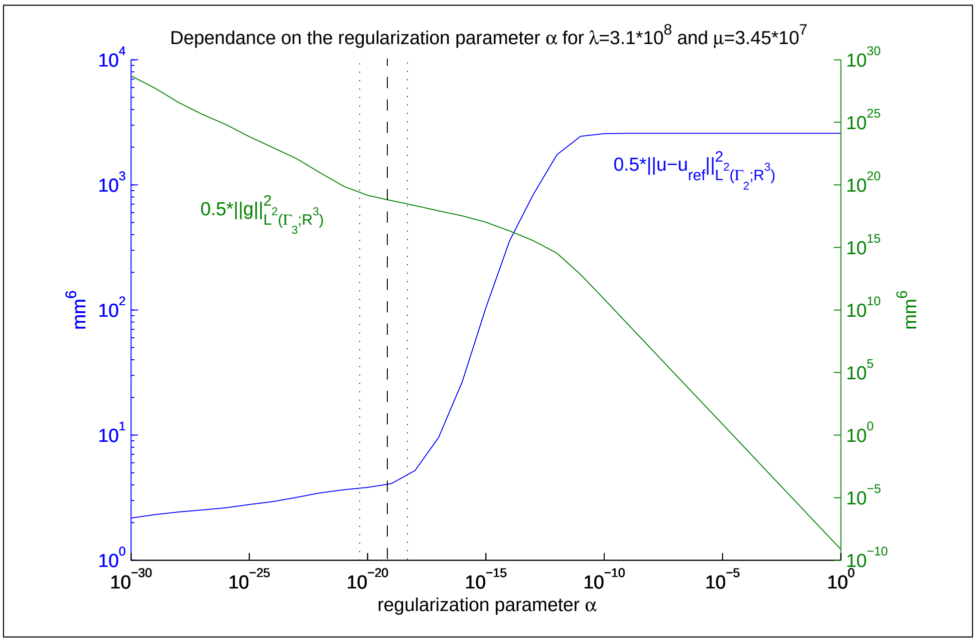

Figure 10: Dependence on α for $E = 2.50 * 10^5$ and $\nu = 0.45$

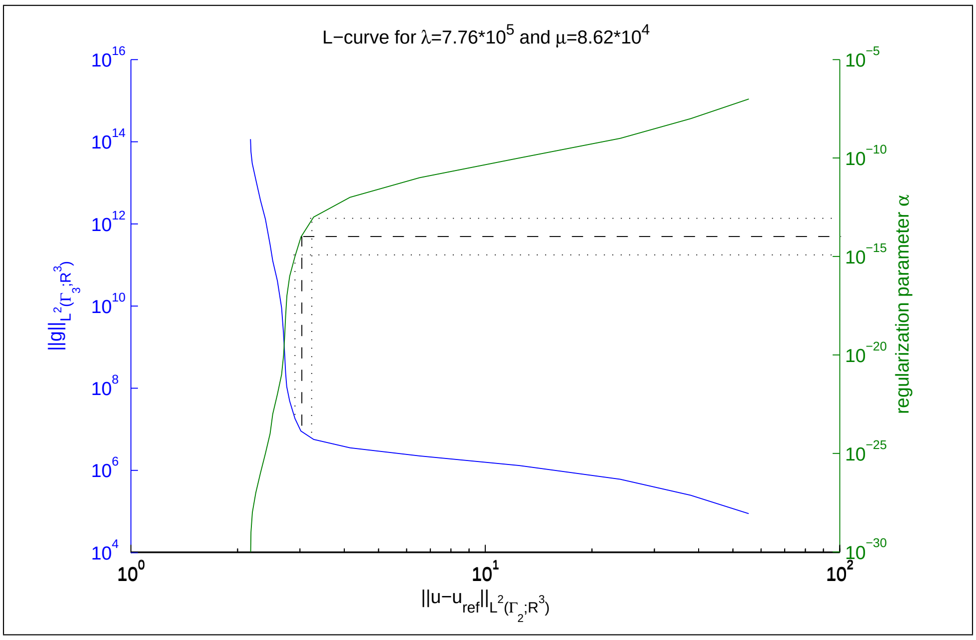

Figure 11: L-curve for $E = 2.50 * 10^5$ and $\nu = 0.45$

In Figures 10 & 12 the dependence of the control and $\frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)}$ on the Tichonoff parameter α are given, for the Lamé constants used in [We07] and in the calculation of u_{ref}. The L-curves, together with the corresponding regularization parameters, are given in Figures 11 & 13. The dotted lines indicate the area of high curvature in the L-curve and the dashed line the point of highest curvature. This coincides with the interval in Figures 10 & 12 where the residual error is small and the system stays stable. For smaller values of the regularization parameter these Figures indicate a stable behaviour, but the visual verification shows that the solutions are senseless for almost all points that do not lie on Γ_3.

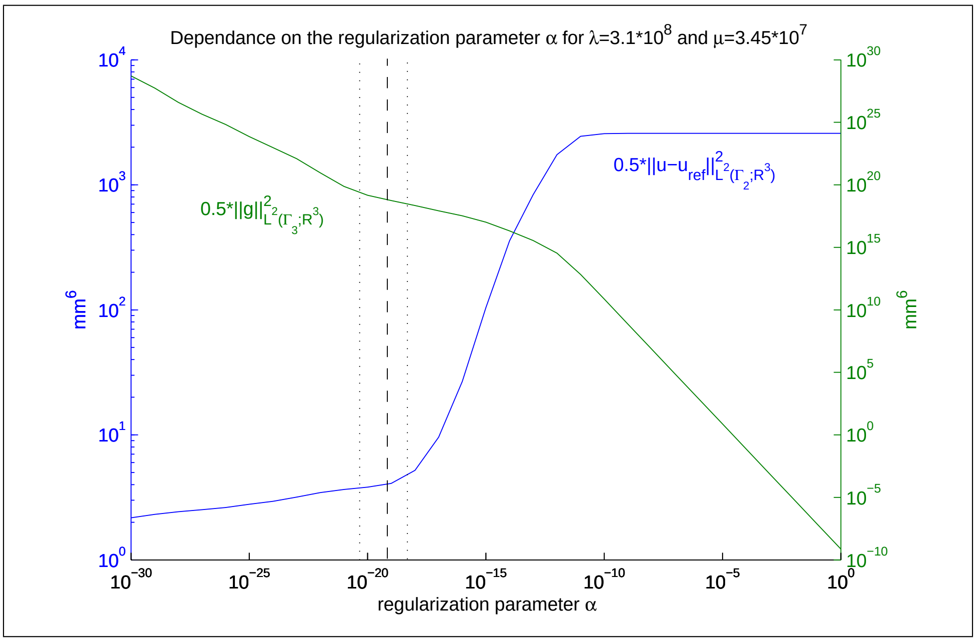

Figure 12: Dependence on α for $E = 10^8$ and $\nu = 0.45$

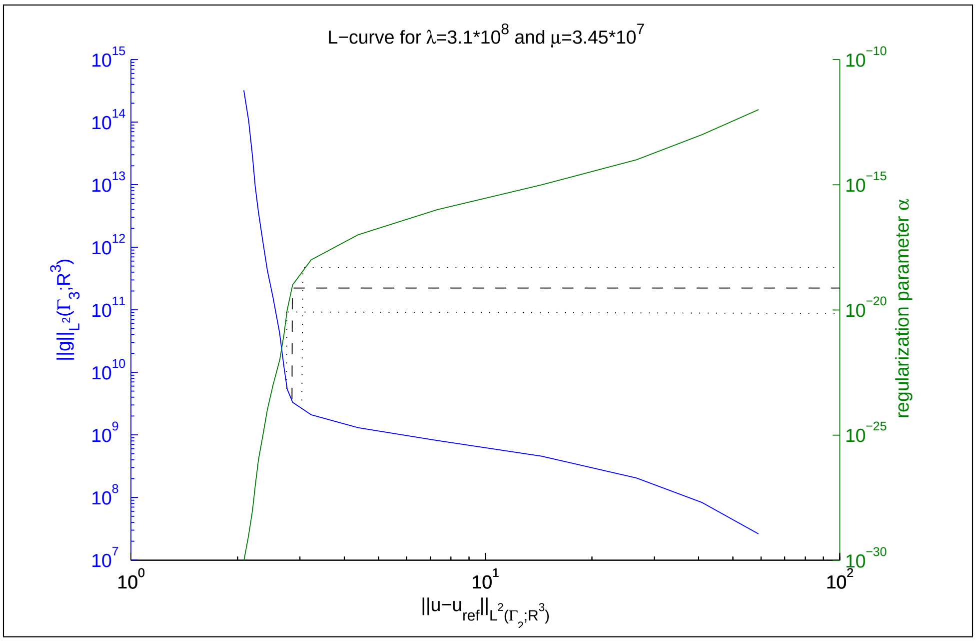

Figure 13: L-curve for $E = 10^8$ and $\nu = 0.45$

It was observed that the value of the Tichonoff parameter α that corresponds to the point of highest curvature in the L-curve is approximately given as

$$\alpha_{opt} \approx 0.7 * 10^{-3} * E^{-2} \tag{39}$$

This choice of α is already sufficiently small to cause the failure of many solvers when solving the system of equations arising from the FEM-discretization. As the influence of the regularization parameter on the cost functional $J(u, g)$ also depends on the geometry of the considered region of the soft tissue Ω it seems to be possible that there exist realistic cases such that all choices of α that imply a small residual error lead to ill-conditioned problems. In the context of implant shape design in the facial area this also can not be excluded, but the relatively thin soft tissue in the face and the observation, that for realistic implants the ratio $\frac{\Gamma_2}{\Gamma_3}$ will not become too small, feeds the hope that this problem will not occur.

Another problem implied by the existence of small Tichonoff regularization parameters occurs if the part of the boundary Γ_3, where the implant acts, is chosen too big. Then it can happen, that at parts of Γ_3, where the implant should not act, artefacts of the control occur. This effect is a common feature of optimal control problems, as for α small enough the influence of the term $\frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)}$ is negligible or can even be numerically equal to zero. It seems unlikely that this can be avoided by other means than a careful determination of the reference configuration.

Finally the solutions for $\alpha = 10^{-15}$, 10^{-19} and Lamé constants $\lambda = 3.1 * 10^8$ and $\mu = 3.45 * 10^7$, i.e. $E = 1.0 * 10^8$ and $\nu = 0.45$, will be given and compared to the desired shape of the reference configuration. While the solution for $\alpha = 10^{-15}$ is close to the reference configuration, the solution for $\alpha = 10^{-19}$ not distinguishable from the prescribed deformation. The implant used for the calculation of the reference solution is given in Figure 19 and the calculated implant in Figure 20. The buckling that can be observed in the calculated implant is again a concequence of the small choice of the Tichonoff-regularization parameter. It allows perturbations of the control that are sufficiently small in $L^2(\Gamma_3;\mathbb{R}^3)$ to vanish numerically in the cost functional. The impact of this perturbation can exemplary be seen in the comparison of the given and the calculated implant in Figure 18. These solutions of the optimal control problem and the corresponding implant shapes again show how important an appropriate choice of α is for a proper implant design. Moreover they support that special care has to be taken to get a better conditioning of the systems of equations that have to be solved.

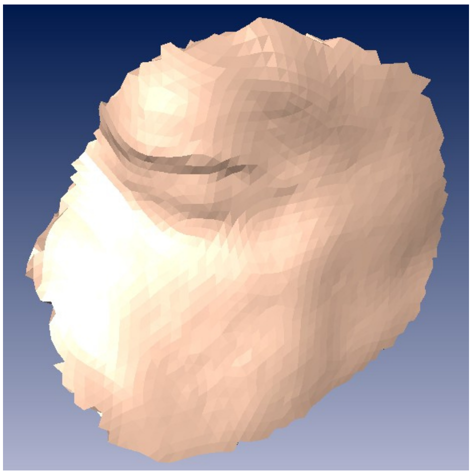

Figure 14: reference configuration

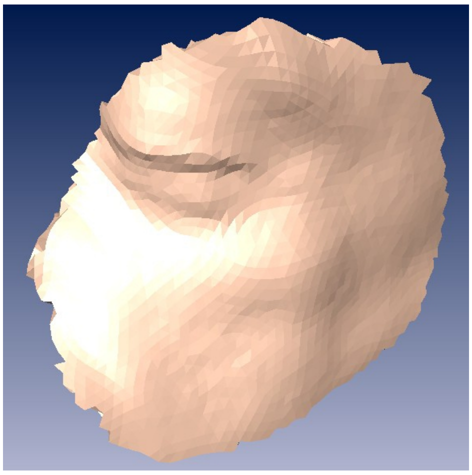

Figure 15: $\alpha = 10^{-15}$

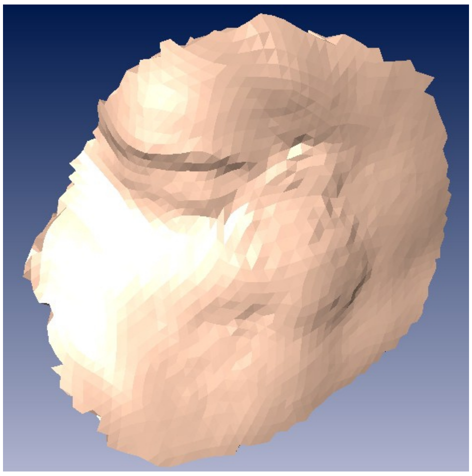

Figure 16: $\alpha = 10^{-19}$

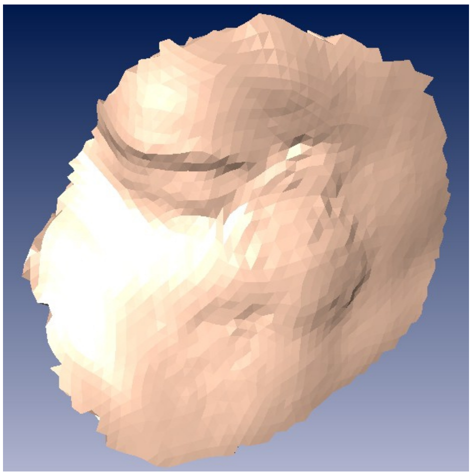

Figure 17: reference solution

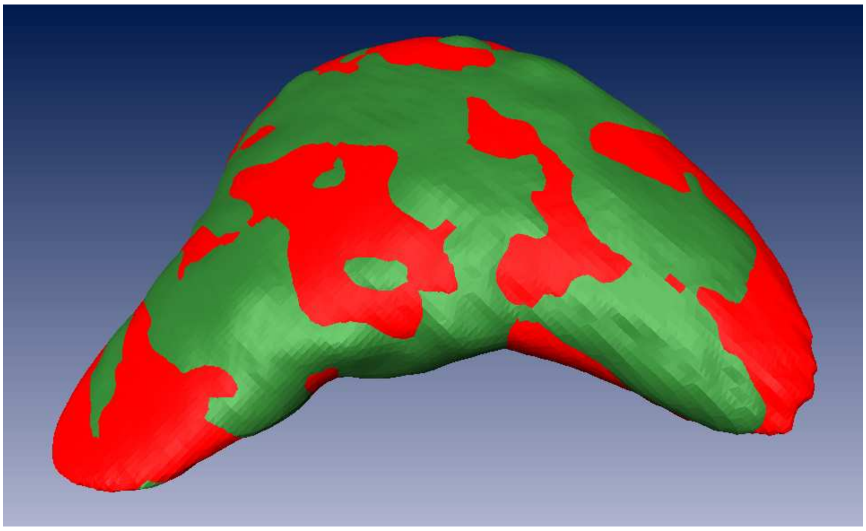

Figure 18: *red*: reference implant
green: calculated implant for $\alpha = 10^{-19}$

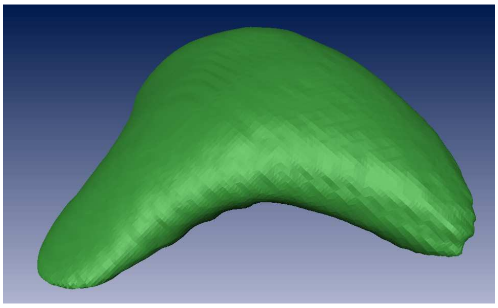

Figure 19: reference implant

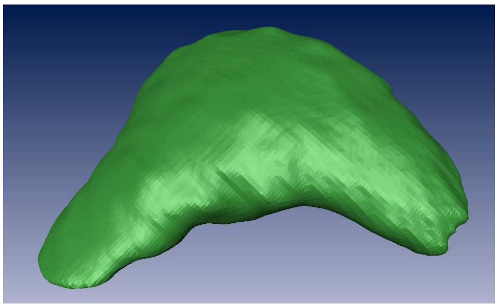

Figure 20: calculated implant

4. Towards Optimal Control in Nonlinear Elasticity

The consideration of models that incorporate both nonlinearities, the geometric and the constitutive, becomes quite involved. In general, material laws that are sufficiently general do not admit local uniqueness of the solutions and thus are difficult to treat. In the next section the necessity of these models will be discussed. Then, in order to perform a first step towards the analytical solution of the nonlinear approach of implant shape design, in section 4.2 the existence of solutions of the optimal control problem with constraints satisfying the assumptions of theorem A.1 will be proven. Finally in section 4.3 some of the problems in the derivation of necessary and sufficient optimality conditions, amongst others a concequence of insufficient regularity of the elastic energy functional, will be stated and shortly discussed.

4.1. Necessity of geometric and constitutive nonlinearity

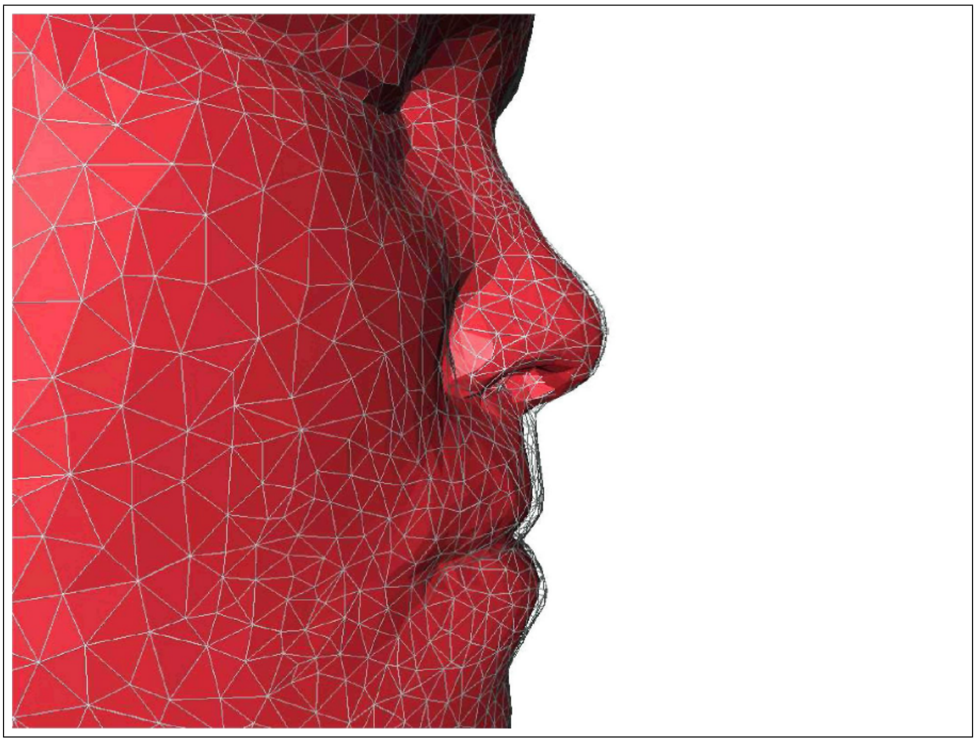

Figure 21: Displacement of soft tissue due to bone movement
Opaque surface: with geometric nonlinearity. *Mesh lines*: linearized elasticity

Figure 21, which is taken from [We07], supports that the accurate calculation of displacements due to implant insertions (resp. bone movements) requires nonlinear elasticity theory. One reason, that is shown in the above figure, is that the appearing displacement gradients are not small enough. Then the product $(\nabla\Phi)^T\nabla\Phi$ can not be linearized and the geometric nonlinearity has to be taken into account.

The other reason is the fact that linear material laws may not be adequate, as the collagen fibres distributed in human soft tissue endow the material with directional properties. For soft tissue like the ones appearing in ligament or tendon there is one distribution of the collagen fibres and thus, in a macroscopic sense, one preferred direction of deformation. Other soft tissues like in artery walls contain two different distributions of collagen fibres that impose two preferred directions of deformation. In these directions the material can be deformed easily in contrast to directions that are orthogonal to the preferred direction(s), where deformations require much more energy. It could be observed that in the epidermis and dermis the soft tissue's behaviour is isotropic and thus has no preferred directions of deformations. The same holds for most muscles, that mainly consist of actin proteins and also posses a linear stress-strain relationship. In the facial area this is not the case, as the muscles are fibre-reinforced and thus exhibit a transversely isotropic behaviour, i.e. there exists one preferred direction. Besides asking for complicated material laws the direction of the collagen fibres may change during a deformation and thus the anisotropic behaviour may also change.

The visco-elastic behaviour of these collagen fibres implies a highly nonlinear stress-strain relationship. As reported in [Fu93] for strain ratios above 15% the soft tissue's stress-strain relationship becomes exponential-like. In addition to this nonlinear behaviour introduced by the anisotropy of soft tissue the stiffness of the material changes in a nonlinear way. For deformations in the directions of the collagen fibres the stiffness increases with muscle contraction while it remains constant for directions orthogonal to the fibre direction (see [Ch03]). This increase in the materials stiffness is small if the fibres length is small compared to its maximal length (the length the fibre can attain without breaking), if the fibres length is close to the point where the fibres breaks up in two parts a big increase in the material stiffness can be observed, i.e. the stress increases much faster than the strain. Thus the consideration of the anisotropic behaviour and the increase in the materials stiffness require nonlinear material laws.

This is often done using Ogden-type material laws for "rubber-like" materials as in [We07]. These material laws possess the advantage that near a natural state they are second-order approximations to the linear St.Venant-Kirchhoff material law. While experiments as in [We07, Ch04] show good results for this type of functions it has been pointed out in [Ho03, Hu03] that this class of functions is still not good enough. The main reasons are the compressibility and isotropy of "rubber-like" materials in contrast to human soft tissue, that mainly consists of water and therefore must be modeled as a quasi-incompressible material and at least partly shows anisotropic behaviour. The compressibility implies $\det(\nabla\Phi) = 1$ a.e. on Ω. As for the condition $\det(\nabla\Phi) > 0$ this condition implies that U_{ad} is not convex and nonlinearities of third order are introduced. Additionally the set of functions that violate these assumptions lies dense in U_{ad} for $U_{ad} \subset W^{1,p}(\Omega;\mathbb{R}^3)$ and $1 \leq p < \infty$ and therefore the constraints on the determinant will often be dropped in numerical computations in the hope that they will at least approximately fulfilled naturally. This is not unreasonable for the assumption $\det(\nabla\Phi) = 1$ a.e.

on Ω as compressibility will implicitly be modeled by the choice of material parameters. So values of the Poisson ratio ν close to 0.5 model quasi-incompressible materials as, i.e. facial soft tissue. For the orientation preserving conditions this is not so easy. It has to be assured that the desired deformation u_{ref} is defined in a way such that the numerical solution u of the optimal control problem satisfies $\det(I + \nabla u) > 0$ a.e. on Ω without imposing this condition. This is difficult but from a practical point of view it may be reasonable assumption.

Also the theoretical treatment of adequate energy functions becomes more involved. As noted in Remark 10 stored energy function can not be convex and the non-uniqueness of solutions, that has been observed in experiments, must be modeled accurately. The derivation of material laws that consider the experimental observations and still remain accessible to the mathematical analysis is a difficult problem in elasticity theory. Currently the most general existence results base on the results of John Ball in 1977 and the one fitting to the boundary conditions of implant shape design is a generalized version of these results and stated in the Appendix as Theorem A.1. Ogden-type materials are one class of functions that satisfy the hypothesis of this theorem and it is possible to prove the existence of solutions for the optimal control problem

$$\min J(u,g) = \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\Gamma_2;\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)} \tag{40}$$

s.t.

$$u \in \text{argmin }_{u \in U_{ad}} I_g(u), \tag{41}$$

where I_g is an energy functional associated with a polyconvex stored energy function, i.e.

$$I_g(u) = \int_\Omega W(u)\ \mathrm{dx} - \int_{\Gamma_3} gu\ \mathrm{ds},$$

where W is polyconvex. Another, more general, class of functions that could be considered are quasi-convex functions. Proofs for the existence of solutions of the minimization problems $u \in \text{argmin }_{u \in U_{ad}} I_g(u)$ where W is only quasi-convex need in general growth constraints that conflict with the condition $W(u) \to \infty$ for $\det(I + \nabla u) \to 0$. Therefore the existence of energy minimizers for elastostatics for quasi-convex stored energy functions is still an unsolved problem (see [Ba02, Problem 1]). The same holds for the problem of verification of poly- and quasi-convexity for anisotropic stored energy functions ([Ba02, Problem 2]).

The next chapter is devoted to the proof of the existence of solutions of the optimal control problem for polyconvex stored energy functions.

4.2. Existence of solutions

In this chapter the following theorem which states that there exist solutions to the optimal control under consideration will be proven. Therefore the following two lemmas will be needed:

Lemma 4.1. *Let*

$$U := \{u \in W^{1,p}(\Omega;\mathbb{R}^3) : \operatorname{adj}(\nabla u) \in L^q(\Omega;\mathbb{R}^{3,3}),\ \det(\nabla u) \in L^r(\Omega;\mathbb{R}),\\ r > 1,\ q \geq \frac{p}{p-1},\ u = u_0 \text{ a.e. on } \Gamma_1\}$$

with $u_0 \in W^{\frac{p-1}{p},p}(\Gamma_1;\mathbb{R}^3)$, $\Gamma_1 \subseteq \Gamma$, $|\Gamma_1| > 0$ *and let*

$$W : U \to \mathbb{R},\ u \mapsto \int_\Omega f\Big(\nabla u(x)\Big)\ \mathrm{dx}$$

with f *satisfying the coerciveness inequality of Theorem* A.1, *i.e. there exist constants* $\gamma > 0$, $\beta \in \mathbb{R}$, $p \geq 2$, $q \geq \frac{p}{p-1}$, $r > 1$ *such that*

$$W(u) \geq \gamma(\|\nabla u\|^p_{L^p(\Omega;\mathbb{R}^{3,3})} + \|\operatorname{adj}(\nabla u)\|^q_{L^q(\Omega;\mathbb{R}^{3,3})} + \|\det(\nabla u)\|^r_{L^r(\Omega;\mathbb{R})}) + \beta$$

Then $I_g(u) := W(u) - \int_{\Gamma_3} gu\ \mathrm{ds}$ *with* $g \in L^{p'}(\Gamma_3)$, $\frac{1}{p} + \frac{1}{p'} = 1$, $|\Gamma_3| > 0$, $\Gamma_1 \cap \Gamma_3 = \emptyset\, \Gamma_3 \subseteq \Gamma$ *also satisfies a coerciveness inequality, i.e. there exist constants* $\tilde{\gamma} > 0$, $\tilde{\beta} \in \mathbb{R}$ *such that*

$$I_g(u) \geq \tilde{\gamma}(\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^{3,3})} + \|\operatorname{adj}(\nabla u)\|^q_{L^q(\Omega;\mathbb{R}^{3,3})} + \|\det(\nabla u)\|^r_{L^r(\Omega;\mathbb{R})}) + \tilde{\beta} \tag{42}$$

Proof. Note that in the following the parts of the coerciveness inequality that contain $\operatorname{adj}(\nabla u)$ and $\det(\nabla u)$ will be omitted as they are not touched by the boundary integral and the following estimates will show that $\tilde{\alpha} < \alpha$.

Using the coerciveness and Hölder's inequality in the second line and the generalized Poincaré's inequality (Theorem A.7) in the third line one gets the following estimate

$$\begin{aligned}
I_g(u) &:= W(u) - \int_{\Gamma_3} gu\ \mathrm{ds}\\
&\geq \gamma\|\nabla u\|^p_{L^p(\Omega;\mathbb{R}^{3,3})} + \beta\|g\|_{L^{p'}(\Gamma_3;\mathbb{R}^3)}\|u\|_{L^p(\Gamma_3;\mathbb{R}^3)}\\
&\geq \min(\frac{\gamma}{2}, \frac{\gamma}{2c_{gP}})\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} - \frac{\gamma}{2}\left|\int_{\Gamma_1} u_0\ \mathrm{ds}\right|^p + \beta - \|g\|_{L^{p'}(\Gamma_3;\mathbb{R}^3)}\|u\|_{L^p(\Gamma_3;\mathbb{R}^3)}\\
&\geq c_1\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} + c_2 - \|g\|_{L^{p'}(\Gamma_3;\mathbb{R}^3)}\|u\|_{L^p(\Gamma_3;\mathbb{R}^3)}
\end{aligned}$$

with $c_1 := \min(\frac{\gamma}{2}, \frac{\gamma}{2c_{gP}})$ and $c_2 := \beta - \frac{\gamma}{2}\left|\int_{\Gamma_1} u_0\ \mathrm{ds}\right|^p$.

Now consider the set

$$U_g := \{u \in W^{1,p}(\Omega;\mathbb{R}^3) : \quad \|u\|^{p-1}_{W^{1,p}(\Omega;\mathbb{R}^3)} \leq \frac{2}{c_1}\|g\|_{L^{p'}(\Gamma_3;\mathbb{R}^3)}\}$$

As $\|u\|_{L^p(\Omega;\mathbb{R}^3)} \leq \|u\|_{W^{1,p}(\Omega;\mathbb{R}^3)}$, for all $u \in U_g$ holds

$$c_1\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} + c_2 - \|g\|_{L^{p'}(\Omega;\mathbb{R}^3)}\|u\|_{L^p(\Omega;\mathbb{R}^3)} \geq c_1\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} + \tilde{\beta} \tag{43}$$

with $\tilde{\beta} = c_2 - \left(\frac{c_1}{2}\right)^{\frac{1}{p-1}} \|g\|^{p'}_{L^{p'}(\Omega;\mathbb{R}^3)}$. Next assume $u \notin U_g$. This is equivalent to

$$c_1\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} - \|g\|_{L^{p'}(\Omega;\mathbb{R}^3)}\|u\|_{L^p(\Omega;\mathbb{R}^3)} \geq \frac{c_1}{2}\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)}$$

and thus

$$c_1\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} + c_2 - \|g\|_{L^{p'}(\Omega;\mathbb{R}^3)}\|u\|_{L^p(\Omega;\mathbb{R}^3)} \quad \geq \quad \frac{c_1}{2}\|u\|^p_{W^{1,p}(\Omega;\mathbb{R}^3)} + c_2 \tag{44}$$

Setting $\tilde{\gamma} = \frac{c_1}{2}$ the inequalities (43) and (44) yield (42).

■

Lemma 4.2. *Let* $\hat{W}$ *be the stored energy function of Theorem* A.1 *and set* $I_g(u) = \int_\Omega \hat{W}(x, \nabla u(x))\ \mathrm{dx} - \int_{\Gamma_3} gu\ \mathrm{ds}$ *with* g, Γ_3 *as in Lemma* 4.1. *Then* I_g *is weakly sequentially lower semicontinuous.*

Proof. This proof is part of the proof of Theorem A.1 in [Ci88].

Firstly as $\{I(u_k)\}_{k\in\mathbb{N}}$ is w.l.o.g. bounded, Lemma 4.1 gives the boundedness of

$$\Big\{u_k, \mathrm{adj}(\nabla u_k), \det(\nabla u_k)\Big\}_{k\in\mathbb{N}} \text{ in } W^{1,p}(\Omega;\mathbb{R}^3) \times L^q(\Omega;\mathbb{R}^{3,3}) \times L^r(\Omega;\mathbb{R})$$

Hence with Theorem A.6 there exists a weakly convergent subsequence with weak limit $\Big(\bar{u}, \mathrm{adj}(\nabla\bar{u}), \det(\nabla\bar{u})\Big)$ and

$$\int_\Omega \hat{W}(x, \nabla u_k(x))\ \mathrm{dx} \leq \int_\Omega \hat{W}(x, \nabla u_l(x))\ \mathrm{ds},\ \forall k \geq l$$

With Theorem A.4 (Mazur) there exists a function $N : \mathbb{N} \to \mathbb{N}$ and a sequence of sets of real numbers $\{\alpha(n)_k\}_{k=n}^{N(n)}$ such that $\alpha(n)_k \geq 0$, $\forall k$ and $\sum_{k=n}^{N(n)} \alpha(n)_k = 1$ such that the sequence

$$v_n := \sum_{k=n}^{N(n)} \alpha(n)_k \Big(\nabla u_k, \mathrm{adj}(\nabla u_k), \det(\nabla u_k)\Big)$$

converges strongly to $\Big(\nabla\bar{u}, \mathrm{adj}(\nabla\bar{u}), \det(\nabla\bar{u})\Big)$ in $L^p(\Omega;\mathbb{R}^{3,3}) \times L^q(\Omega;\mathbb{R}^{3,3}) \times L^r(\Omega;\mathbb{R})$. From the polyconvexity assumption of Theorem A.1 follows that $\mathbb{W}(x,\cdot)$ is continuous for almost all $x \in \Omega$. Using the same argument as at the end of the proof of Theorem 4.3, which is taken from the proof of Theorem A.1 in [Ci88] it can be shown that $\det(\nabla\bar{u}) > 0$ holds a. e. on Ω. Thus for almost all $x \in \Omega$ holds

$$\begin{aligned}
\hat{W}(x, \nabla\bar{u}(x)) \quad &= \quad \mathbb{W}\bigg(x, \Big(\nabla\bar{u}(x), \mathrm{adj}(\nabla\bar{u}), \det(\nabla\bar{u})\Big)\bigg) \\
&= \quad \lim_{n\to\infty} \mathbb{W}\bigg(x, \sum_{k=n}^{N(n)} \alpha(n)_k \Big(\nabla u_k, \mathrm{adj}(\nabla u_k), \det(\nabla u_k)\Big)\bigg)
\end{aligned}$$

Using this relation, Fatou's lemma and the convexity of $\mathbb{W}$ one can show that $\int_\Omega \hat{W}(x, \nabla\bar{u}(x))\ \mathrm{dx} \leq \liminf_{k\to\infty} \int_\Omega \hat{W}(x, \nabla u_k(x))\ \mathrm{dx}$:

$$\begin{aligned}
\int_\Omega \hat{W}(x, \nabla\bar{u}(x))\ \mathrm{dx} &= \int_\Omega \liminf_{n\to\infty} \mathbb{W}\Big(x, \sum_{k=n}^{N(n)} \alpha(n)_k \Big(\nabla u_k, \operatorname{adj}(\nabla u_k), \det(\nabla u_k)\Big)\Big)\ \mathrm{dx} \\
&\leq \liminf_{n\to\infty} \int_\Omega \mathbb{W}\Big(x, \sum_{k=n}^{N(n)} \alpha(n)_k \Big(\nabla u_k, \operatorname{adj}(\nabla u_k), \det(\nabla u_k)\Big)\Big)\ \mathrm{dx} \\
&\leq \liminf_{n\to\infty} \sum_{k=n}^{N(n)} \alpha(n)_k \int_\Omega \hat{W}(x, \nabla u_k)\ \mathrm{dx} \\
&\leq \liminf_{n\to\infty} \int_\Omega \hat{W}(x, \nabla u_n)\ \mathrm{dx}
\end{aligned}$$

$\int_{\Gamma_3} g\bar{u}\ \mathrm{ds} = \lim_{n\to\infty} \int_{\Gamma_3} g u_n\ \mathrm{ds}$ holds by definition of the weak convergence and thus $I_g(\bar{u}) \leq \liminf_{k\to\infty} I(u_k)$.

■

Before turning to the main result of this chapter recall the definition of the admissible set of displacements

$$\begin{aligned}
U :=&\{u \in W^{1,p}(\Omega;\mathbb{R}^3) : \operatorname{adj}(\nabla u) \in L^q(\Omega;\mathbb{R}^{3,3}),\ \det(\nabla u) \in L^r(\Omega;\mathbb{R}), \\
&\det(\nabla u) > 0 \text{ a.e. in } \Omega,\ u = u_0 \text{ a.e. on } \Gamma_1\}
\end{aligned}$$

Theorem 4.3. *Let* $g \in G := L^2(\Gamma_3;\mathbb{R}^3)$, $u|_{\Gamma_1} = u_0 \in W^{\frac{p-1}{p},p}(\Gamma_1;\mathbb{R}^3)$, $u_{ref} \in L^2(\mathbb{S};\mathbb{R}^3)$, *where* $\mathbb{S} = \Omega$ *or* $\mathbb{S} = \Gamma_2 \subseteq \Gamma$, *and let* $\hat{W} : \Omega \times U \to \mathbb{R}$ *satisfy the assumptions of theorem* A.1 *and set* $I_g(u) := \hat{W}(u) - \int_{\Gamma_3} gu\ \mathrm{ds}$. *Then there exists at least one pair* $(\bar{u}, \bar{g}) \in U \times G$ *that is an optimal solution of the optimal control problem*

$$\min\ J(u, g) := \frac{1}{2}\|u - u_{ref}\|^2_{L^2(\mathbb{S};\mathbb{R}^3)} + \frac{\alpha}{2}\|g\|^2_{L^2(\Gamma_3;\mathbb{R}^3)} \tag{45}$$

s.t.

$$u \in \operatorname{argmin}_{v\in U} I_g(v) \tag{46}$$

Proof. For sake of clarity the proof will be shown for $\mathbb{S} = \Omega$. It works in an analogous way for $\mathbb{S} = \Gamma_2$ using the trace-operator.

First it will be shown that there exists a weakly convergent subsequence $(u_k, g_k)_{k\in\mathbb{N}}$ converging to a minimizer of the optimal control problem. Then the sequentially weakly lower semi-continuity of the energy and the cost functional will be used to show the minimizing property for the weak limit of this subsequence. Finally, using Mazur's theorem and the polyconvexity, it will be shown that the weak limit of $(u_k, g_k)_{k\in\mathbb{N}}$ is again in $U_{ad} \times G$, i.e. that the weak limit of the sequence of displacements $\tilde{u}$ satisfies $\det(I + \nabla\tilde{u}) > 0$ a.e. on Ω.

1. *Existence of a weakly convergent subsequence*:
The energy functional $J(u,g)$ is bounded from below and thus there exists a minimizing sequence $(u_k, g_k)_{k\in\mathbb{N}}$ with $g_k \in G$ and $u_k \in U$ with u_k being a minimizer of $I_{g_k}(u)$, i.e. u_k is the displacement associated with g_k (Theorem A.1). The sequence $\{g_k\}_{k\in\mathbb{N}}$ contains a subsequence bounded in G by some constant C_g and as G is reflexive there exists a weakly convergent subsequence which will again be denoted as $\{g_k\}_{k\in\mathbb{N}}$ with weak limit $\bar{g} \in G$.
First, we have to show that the sequence $\{I_{g_k}(u_k)\}_{k\in\mathbb{N}}$ is also bounded. Setting $\|\cdot\|_U := \|\cdot\|_{W^{1,p}(\Omega;\mathbb{R}^3)}$, $\|\cdot\|_G := \|\cdot\|_{L^2(\Gamma_3;\mathbb{R}^3)}$ and using Hölder's inequality and the continuity of the trace operator one gets an estimate for the sensitivity of the elastic energy functional with respect to changes in the Neumann boundary conditions
$$I_{g_k}(u) - I_{g_l}(u) = \int_{\Gamma_3} u(g_l - g_k)\ \mathrm{dx} \le \|u\|_G \|g_l - g_k\|_G \le 2C_g\|u\|_U$$
Thus as u_k minimizes I_{g_k}, the boundedness of $\{I_{g_k}(u_k)\}_{k\in\mathbb{N}}$ results from:
$$\begin{aligned} I_{g_k}(u_k) &\le I_{g_k}(u_l) \\ \Leftrightarrow I_{g_k}(u_k) - I_{g_l}(u_l) &\le I_{g_k}(u_l) - I_{g_l}(u_l) \le 2C_g\|u_l\|_U \\ I_{g_k}(u_k) &\le 2C_g\|u_l\|_U + I_{g_l}(u_l) < \infty \qquad \text{for some fixed } l \in \mathbb{N} \end{aligned}$$
Now with Lemma 4.1 follows the boundedness of $\{u_k\}_{k\in\mathbb{N}}$, i.e. there exists constants $\tilde{\gamma} > 0$, $\tilde{\beta} \in \mathbb{R}$ such that
$$\tilde{\gamma}\|u_k\|_U^p \le I_{g_k}(u_k) - \tilde{\beta} \le 2C_g\|u_l\|_U + I_{g_l}(u_l) - \tilde{\beta}$$
Again reflexivity implies the existence of a subsequence $u_k \rightharpoonup \tilde{u}$ in $W^{1,p}(\Omega;\mathbb{R}^3)$.

2. *Minimizing property of the weak limit*:
As the embedding $W^{1,p}(\Omega;\mathbb{R}^3) \hookrightarrow L^2(\Gamma_3;\mathbb{R}^3)$ is compact for $p \ge 2$, the strong convergence $u_k \to \tilde{u}$ in $L^2(\Gamma_3;\mathbb{R}^3)$ implies $\int_{\Gamma_3} g_k u_k\ \mathrm{ds} \to \int_{\Gamma_3} \bar{g}\tilde{u}\ \mathrm{ds}$. Then Lemma 4.2 gives $I_g(\tilde{u}) \le \liminf_{k\to\infty} I_g(u_k)$ and hence
$$\begin{aligned} I_{g_k}(u_k) &\le I_{g_k}(\tilde{u}) \le \liminf_{j\to\infty} I_{g_k}(u_j) \\ \Leftrightarrow W(u_k) &\le W(\tilde{u}) - \int_{\Gamma_3} (\tilde{u} - u_k)g_k\ \mathrm{ds} \le \liminf_{j\to\infty} W(u_j) - \limsup_{j\to\infty} \int_{\Gamma_3} (u_j - u_k)g_k\ \mathrm{ds} \\ &\le \liminf_{j\to\infty} W(u_j) - \int_{\Gamma_3} (\tilde{u} - u_k)g_k\ \mathrm{ds} \\ &\le \liminf_{j\to\infty} W(u_j) + \|\tilde{u} - u_k\|_{L^2(\Gamma_3;\mathbb{R}^3)}\|g\|_{L^2(\Gamma_3;\mathbb{R}^3)} \end{aligned}$$
The strong convergence of u_k in $L^2(\Gamma_3;\mathbb{R}^3)$ then gives
$$\limsup_{k\to\infty} W(u_k) \le W(\tilde{u}) \le \liminf_{j\to\infty} W(u_j) \quad \Rightarrow \lim_{k\to\infty}\inf W(u_k) = W(\tilde{u})$$

and with $\int_{\Gamma_3} g_k u_k \,\mathrm{ds} \to \int_{\Gamma_3} \bar{g}\tilde{u} \,\mathrm{ds}$ holds

$$I_{g_k}(u_k) \to I_{\bar{g}}(\tilde{u})$$

Now let $\bar{u}$ be a minimizer of $I_{\bar{g}}(u)$. Then holds

$$\lim_{k\to\infty} I_{g_k}(\bar{u}) = I_{\bar{g}}(\bar{u}) \leq I_{\bar{g}}(\tilde{u}) = \lim_{k\to\infty} I_{g_k}(u_k) \leq \lim_{k\to\infty} I_{g_k}(\bar{u}) = I_{\bar{g}}(\bar{u}) \quad \Rightarrow I_{\bar{g}}(\bar{u}) = I_{\bar{g}}(\tilde{u})$$

So $\tilde{u}$ is a minimizer of $I_{\bar{g}}(u)$ and thus the pair $(\tilde{u}, \bar{g})$ is an admissible candidate for a minimizer of $J(u, g)$. The strong convergence of u_k in $L^2(\mathbb{S}; \mathbb{R}^3)$ gives

$$\|u_k - u_{ref}\|_{L^2(\mathbb{S};\mathbb{R}^3)} \to \|\tilde{u} - u_{ref}\|_{L^2(\mathbb{S};\mathbb{R}^3)}$$

and with Theorem A.8 follows that the operator $g \mapsto \int_{\Gamma_3} |g|^2 \,\mathrm{ds}$ is weakly lower semi-continuous. Set $j := \inf\limits_{u\in\mathrm{argmin}\ I_g} J(u, g)$. Then

$$J(\tilde{u}, \bar{g}) \leq \liminf_{k\to\infty} J(\tilde{u}, g_k) = \liminf_{k\to\infty} J(u_k, g_k) = j$$

Thus it has been shown that the pair $(\tilde{u}, \bar{g})$ is a minimizer of (2) s.t. (46).

3. *Show that* $\tilde{u} \in U_{ad}$:
What has not been proved yet is the property $\det(I + \nabla\tilde{u}) > 0$ a.e. This can be seen as follows. From Theorem A.6 follows that the mapping

$$W^{1,p}(\Omega; \mathbb{R}^3) \to L^{\frac{p}{3}}(\Omega; \mathbb{R}) : \, u \mapsto \det(I + \nabla u)$$

is continuous. Therefore the boundedness of u_k in $W^{1,p}(\Omega; \mathbb{R}^3)$ implies the boundedness of $\det(I+\nabla u_k)$ in $L^{\frac{p}{3}}(\Omega; \mathbb{R})$. Consequently there exists a weakly convergent subsequence $\det(I+\nabla u_{k_n}) \rightharpoonup \delta$ in $L^{\frac{p}{3}}(\Omega; \mathbb{R})$ and it holds $\delta = \det(I+\nabla\tilde{u})$ (also Theorem A.6). Now the theorem of Mazur gives the existence of a strongly convergent subsequence

$$v_m = \sum_i a_i^m \det(I+\nabla u_k) \geq \epsilon_0 \quad \sum_i a_i^m = 1,\, a_i \geq 0 \quad v_m \to \det(I+\nabla\tilde{u}) \text{ in } L^{\frac{p}{3}}(\Omega; \mathbb{R}).$$

Hence there exists a subsequence $v_{m'}$ of v_m that converges almost everywhere to $\det(I + \nabla\tilde{u})$ and therefore $\det(I + \nabla\tilde{u}) \geq 0$ a.e. Assume that there exists a subset $\mathcal{A} \subset \Omega$ with $|\mathcal{A}| > 0$ and $\det(I + \nabla\tilde{u}) = 0$ on $\mathcal{A}$. By definition of the weak convergence and $\det(I + \nabla u_k) > 0$

$$\lim_{k\to\infty} \int_{\mathcal{A}} |\det(I + \nabla u_k)| \,\mathrm{dx} = \lim_{k\to\infty} \int_{\mathcal{A}} \det(I + \nabla u_k) \,\mathrm{dx} = \int_{\mathcal{A}} \det(I + \nabla\tilde{u}) \,\mathrm{dx} = 0$$

i.e. $\det(I + \nabla u_k) \to 0$ in $L^1(\mathcal{A}; \mathbb{R})$. Consequently there exists a subsequence again denoted by $\{u_n\}_{n\in\mathbb{N}}$, $n = n(k)$ such that $\det\Big(I + \nabla u_n(x)\Big) \to 0$ a.e. on $\mathcal{A}$. Now consider the sequence $F_n : \mathcal{A} \ni x \mapsto F_n(x) := f\Big(x, \nabla u_n(x)\Big)$. By Assumption 3 of Theorem A.1 the sequence $\{F_n\}_{n\in\mathbb{N}}$ is bounded from below and one can apply Fatou's Lemma in order to get

$$\int_{\mathcal{A}} \liminf_{n\to\infty} F_n(x) \text{ dx} \le \liminf_{n\to\infty} \int_{\mathcal{A}} F_n(x) \text{ dx}$$

Then Assumption 2 of Theorem A.1 gives

$$\liminf_{n\to\infty} F_n(x) = \liminf_{n\to\infty} f\Big(x, \nabla u_n(x)\Big) = \lim_{\det(F)\to 0^+} f(x,F) = \infty \qquad \text{a.e. on } \mathcal{A}$$

and thus

$$\infty = \int_{\mathcal{A}} \liminf_{n\to\infty} f\Big(x, \nabla u_n(x)\Big) \text{ dx} \le \liminf_{n\to\infty} \int_{\mathcal{A}} F_n(x) \text{ dx}$$

With the coerciveness inequality of Lemma 4.1 this contradicts

$$\lim_{n\to\infty} I_{\bar{g}}(u_n) = \inf_{u\in \text{argmin } I_{\bar{g}}} I_{\bar{g}}(u) < \infty$$

Hence if holds $\det(I + \nabla\tilde{u}) > 0$ a.e. on Ω and therefore $\tilde{u} \in U$.

■

Remark 14.

1. *The above proof clearly works for more general cost functionals $J(u,g)$. It is sufficient that the following assumptions are satisfied:*

   a) There exists constants $c, r > 0$ such that $J(u,g) \ge c\|g\|_G^r \quad \forall (u,g) \in U \times G$.

   b) J is weakly lower semi-continuous.

2. *Also the constraints must not be given through a polyconvex stored energy function. Any other constraint from elasticity theory may be used, that admits the following properties:*

   a) Lemma 4.2 must hold.

   b) The boundedness of any sequence $\{g_k\}_{k\in\mathbb{N}}$ in G implies the boundedness of the corresponding sequence of displacements $\{u_k\}_{k\in\mathbb{N}}$ in U.

   c) For the weak limit $\hat{u}$ of $\{u_k\}_{k\in\mathbb{N}}$ in U holds $\det(I + \nabla\hat{u}) > 0$ a.e. in Ω.

3. *The argumentation in [Ci88, Thm. 7.9-1] shows that the incorporation of the additional restriction $\int_\Omega \det(\nabla\Phi) \text{ dx} \le \text{vol}(\Phi(\Omega))$ allows to prove the weak injectivity condition $\text{card}\Big(\Phi^{-1}(x)\Big) = 1$ for almost all $x \in \Phi(\bar{\Omega})$ for $p > 3$.*

4. *If desired one can also incorporate the incompressibility condition $\det(\nabla\Phi) = 1$. In order to prove this property for the minimizer $\hat{u}$ a simplified version of the strategy for the prove of $\det(I + \nabla\hat{u}) > 0$ can be used. It is a special case of the technique of compensated compactness, introduced and studied by F. Murat and L. Tartar. In the present case the lack of compactness is compensated by the continuity of the mapping $W^{1,p}(\Omega;\mathbb{R}^3) \ni u \to \det(I + \nabla u) \in L^{\frac{p}{3}}(\Omega : \mathbb{R})$ with respect to weak convergence.*

4.3. Lack of regularity

After having proven the existence of solutions of the optimal control problem (40) s.t. (41) the next interesting point would be the well-posedness with respect to the control and the necessary optimality conditions. For nonlinear constraints the strategy for the derivation of the optimality conditions starts with the linearization of the constraints. Then one tries to prove the existence of Lagrange multipliers in order to get a KKT-System. Finally it must be shown that the necessary optimality conditions of the linearized problem are also necessary optimality conditions for the original problem.

In the considered context of polyconvex stored energy functions $f : \Omega \times U \to \mathbb{R}$, i.e. there exists a convex function $\mathbb{F}(x, \cdot) : \mathbb{M}^3 \times \mathbb{M}^3 \times]0, +\infty[\to \mathbb{R}$, such that

$$\mathbb{F}\Big(x, F, \operatorname{adj}(F)^T, \det(F)\Big) = f(x, F) \quad \forall F \in \mathbb{M}^3_+,$$

it is already difficult to derive the well-posedness with respect to the control. More precisely it is even a problem to derive the optimality conditions for the constraint $u \in \arg\min_{v \in U_{ad}} I_g(v)$. While $\mathbb{F}(x, \cdot)$ is, as a consequence of its convexity, continuous and its subdifferential is nonempty at every $F \in \mathbb{M}^3_+$, the occurrence of $\operatorname{adj}(\cdot)$ and $\det(\cdot)$ does not admit to transfer these properties, except continuity, to f. Considering the properties of the corresponding energy functionals as mappings on $W^{1,p}$-spaces with $p < \infty$ implies even less regularity as continuity gets lost. Even if f is continuously differentiable, as is the case for Ogden-type material laws as in [We07] this property does not hold for the energy functional. This is due to the condition $\lim_{\det(F) \to 0^+} f(x, F) = \infty$, which is, in[We07], incorporated using the function $\Gamma(s) = \ln(s)$, $\forall s > 0$. Considering the strain energy $W(u) = \int_\Omega f\Big(x, \nabla u(x)\Big)$ dx implies that $W(u) = \infty$ on a dense subset of $\mathbb{W}^{1,p}(\Omega; \mathbb{R}^3)$. This problem can be ruled out by the minimizing property and the assumption that minimizers $\bar{u}$ satisfy $W(\bar{u}) < \infty$, that also allows for $u_1 = \arg\min_{u \in U} I_{g_1}(u)$ and $u_2 = \arg\min_{u \in U} I_{g_2}(u)$ the estimate

$$\|u_2\|_U \leq W(u_2) + \|u_1\|_U \|g_2 - g_1\|_G$$

Nevertheless it does not seem possible to derive the necessary regularity for the optimality conditions without additional hypothesis, i.e. suitable growth conditions are necessary resp. for the differentiability of W it is necessary to get a lower bound on $\det(\nabla u)$ (see also [Ci88, Ma83, Ba02]). As noted 2002 in John Ball's paper "Some open problems in elasticity" ([Ba02, Problems 5 and 6]) it is not yet clear if, and under which conditions, a minimizer of the energy functional W satisfies the weak formulation of its Euler-Lagrange equation

$$\int_\Omega f'(\nabla u) \nabla \psi \ \mathrm{dx} = 0 \quad \forall \psi \in C^\infty(\Omega; \mathbb{R}^3) \, \text{with} \, \psi|_{\Gamma_1} = 0$$

For approaches using the implicit function theorem it is necessary to consider sufficiently smooth function spaces, i.e. $C^{2+\delta}(\Omega; \mathbb{R}^3)$, $\delta > 0$ or $W^{2,p}(\Omega; \mathbb{R}^3)$, $p > 3$ and that the linearized solution operator is invertible in the considered spaces. As for $\Phi \in W^{2,p}(\Omega;\mathbb{R}^3)$, $p > 3$ the deformation gradient $\nabla\Phi$ is in $W^{1,p}(\Omega;\mathbb{R}^3)$, that forms a Banach-algebra, the displacement as well as its gradient are continuous. This facilitates the handling of point-wise conditions, i.e. one can assume that a solution $\bar{u}$ of the optimal control solution satisfies $\det\Big(I + \nabla\bar{u}\Big) \geq c > 0$ a.e. on Ω and gets sufficient regularity in an ϵ- environment of $\bar{u}$ in $W^{1,\infty}$. The drawbacks of this approach are on one side the natural restriction to small perturbations and on the other side the necessary regularity of the linearized solution operator in the considered spaces, which is in general, especially for mixed boundary value problems with nonempty intersections of the different parts of the boundary, not easy resp. impossible to proof.

Using the direct method of calculus of variations as done in the existence proof in the last section for $u \in W^{1,p}$, $p < \infty$ it is necessary to derive sufficiently general assumptions, that can be justified from a physical point of view and guarantee the desired regularity. Computational experiments performed in this thesis, the success of the current "by rule of thumb" approach used in practice and the experiments performed by Fung support the assumption that in the context of implant shape design the solution operator near the optimal solution satisfies sufficient regularity properties. The problem is to derive assumptions that admit the desired regularity, without restricting the underlying elasticity theory inappropriately.

Another problem stated in [Ba02] is the occurrence of the Lavrentiev phenomenon, i.e. the minimum of the energy functional is dependent on the chosen function spaces. One dimensional examples in [Ba85] show that the Lavrentiev phenomenon can occur for continuous deformations Φ that have unbounded gradients. Another example is the possibility to construct function spaces that do or do not allow cavitation to occur. The more general question under which additional hypothesis the Lavrentiev phenomenon can be excluded in elastostatics is again unsolved ([Ba02, Problem 4]). Obviously the occurrence of the Lavrentiev phenomenon implies difficulties in the numerical treatment and the choice of the adequate function space (see [Ba85]).

This thesis will be concluded by the observations, that in the context of material laws satisfying the assumptions of Theorem A.1 it is necessary to derive additional assumptions, as described above, that admit sufficient regularity such that the necessary and possibly also the sufficient optimality conditions can be derived. Alternatively it may be reasonable to model the biological soft tissue as Fung-elastic material. As derived only for quasi-incompressible, resp. incompressible, biological soft tissue this material law allows to drop condition (11): $\lim_{\det(F)\to 0^+} f(x,F) = \infty$. Therefore it does not imply the problems induced by the orientation-preserving condition and thus may be easier to treat mathematically. The examination of both approaches is subject to future research.

A. Appendix

A.1. Elasticity theory

The following existence theorem is taken from [Ci88] and follows the existence results of John Ball in [Ba77, Thm. 7.3 and Thm. 7.6]. It holds for mixed displacement-traction problems as well as for pure displacement problems with dead loads.

Theorem A.1. *Let Ω be a domain in $\mathbb{R}^3$, and let $\hat{W} : \Omega \times \mathbb{M}^3_+ \to \mathbb{R}$ be a (stored energy) function with the following properties:*

1. *Polyconvexity: For almost all $x \in \Omega$ there exists a convex function $\mathbb{W}(x, \cdot) : \mathbb{M}^3 \times \mathbb{M}^3 \times]0, +\infty[\to \mathbb{R}$ such that*

$$\mathbb{W}\Big(x, F, \operatorname{adj}(F)^T, \det(F)\Big) = \hat{W}(x, F) \qquad \forall F \in \mathbb{M}^3_+$$

   and the function $\mathbb{W}(\cdot, F, H, \delta) : \Omega \to \mathbb{R}$ is measurable for all $(F, H, \delta) \in \mathbb{M}^3 \times \mathbb{M}^3 \times]0, +\infty[$.

2. *Behaviour as $\det(F) \to 0^+$: For almost all $x \in \Omega$ holds $\lim_{\det(F)\to 0^+} \hat{W}(x, F) = +\infty$.*

3. *Coerciveness: There exist constants $\alpha > 0$, $\beta \in \mathbb{R}$, $p \geq 2$, $q \geq \frac{p}{p-1}$, $r > 1$ such that*

$$\hat{W}(x, F) \geq \alpha(|F|^p + |\operatorname{adj}(F)|^q + |\det(F)|^r) + \beta$$

   for all $F \in \mathbb{M}^3_+$ and almost all $x \in \Omega$.

Let $\Gamma = \Gamma_0 \cup \Gamma_1$ be a measurable partition of the boundary of Γ of Ω with $|\Gamma_0| > 0$, and let $u_0 : \Gamma_0 \to \mathbb{R}^3$ be a measurable function such that the set

$$\begin{aligned} U :=& \{u \in W^{1,p}(\Omega; \mathbb{R}^3) : \operatorname{adj}(\nabla u) \in L^q(\Omega; \mathbb{R}^{3,3}),\ \det(\nabla u) \in L^r(\Omega; \mathbb{R}), \\ & \det(\nabla u) > 0 \text{ a.e. in } \Omega,\ u = u_0 \text{ a.e. on } \Gamma_0\} \end{aligned}$$

is nonempty. Let $f \in L^p(\Omega; \mathbb{R}^3)$ and $g \in L^\sigma(\Gamma_1; \mathbb{R}^3)$ such that the linear form

$$L : u \in W^{1,p}(\Omega; \mathbb{R}^3) \to L(u) := \int_\Omega fu \ \mathrm{dx} + \int_{\Gamma_1} gu \ \mathrm{ds}$$

is continuous. Set

$$I(u) = \int_\Omega \hat{W}\Big(x, \nabla u(x)\Big) \ \mathrm{dx} - L(u)$$

and assume that $\inf_{u\in U} I(u) < +\infty$.

Then there exists at least one function $\bar{u} \in U$ such that $I(\bar{u}) = \inf_{u\in U} I(u)$.

Proof. See [Ci88, Thm. 7.7-1]. ∎

Theorem A.2. *(Korn's First Inequality)*

Let Ω be a domain in $\mathbb{R}^n$ with piecewise smooth boundary. Define the symmetric gradient ∇^s by $\nabla^s u := \frac{1}{2}(\nabla u + \nabla u^*)$. Then there exists a constant $c = c(\Omega) > 0$ such that

$$\int_\Omega \nabla^s v : \nabla^s v \ \mathrm{dx} + \|v\|^2_{L^2(\Omega;\mathbb{R}^3)} \geq c\|v\|^2_{H^1(\Omega;\mathbb{R}^3)} \qquad \forall v \in H^1(\Omega;\mathbb{R}^3)$$

Proof. See [Ba07, Thm. 3.1] for a short sketch of the proof and a reference to the complete proof. ∎

Theorem A.3. *(Korn's Second Inequality)*

Let $\Omega \subset \mathbb{R}^3$ be a domain with piecewise smooth boundary. Let $\Gamma_0 \subset \partial\Omega$ with $|\Gamma_0| > 0$. Then there exists a constant $c = c(\Omega, \Gamma_0) > 0$ such that

$$\int_\Omega \nabla^s v : \nabla^s v \ \mathrm{dx} \geq c\|v\|^2_{H^1(\Omega;\mathbb{R}^3)}$$

Proof. See [Ba07, Thm. 3.3]. ∎

A.2. Functional Analysis

Theorem A.4. *(Theorem of Mazur)*

Let X be a Banach space and suppose $u_n \rightharpoonup \bar{u}$ in X. Then there exists a function $N : \mathbb{N} \to \mathbb{N}$ and a sequence of sets of real numbers $\{\alpha(n)_k\}_{k=n}^{N(n)}$ such that $\alpha(n)_k \geq 0, \forall k$ and $\sum_{k=n}^{N(n)} \alpha(n)_k = 1$ such that the sequence

$$v_n := \sum_{k=n}^{N(n)} \alpha(n)_k u_k$$

converges strongly to $\bar{u}$ in X.

Proof. See [Be83, Thm. III.7]. ∎

Theorem A.5. *Let Ω be a domain in $\mathbb{R}^3$. For each $p \geq 2$ the mapping*

$$W^{1,p}(\Omega;\mathbb{R}^3) \ni u \to \mathrm{adj}(\nabla u) \in L^{\frac{p}{2}}(\Omega;\mathbb{R}^{3,3})$$

is well defined and continuous. Furthermore holds

$$\left.\begin{array}{rl} u_k \rightharpoonup u & \text{in } W^{1,p}(\Omega;\mathbb{R}^3),\ p \geq 2 \\ \mathrm{adj}(\nabla u_k) \rightharpoonup H & \text{in } L^q(\Omega;\mathbb{R}^{3,3}),\ q \geq 1 \end{array}\right\} \Rightarrow H = \mathrm{adj}(\nabla u)$$

Proof. See [Ci88, Thm. 7.5-1]. ∎

Theorem A.6. *Let Ω be a domain in $\mathbb{R}^3$. For each number $p \geq 2$ and each number q such that $s^{-1} := p^{-1} + q^{-1} \leq 1$, the mapping*

$$W^{1,p}(\Omega;\mathbb{R}^3) \times L^q(\Omega;\mathbb{R}^{3,3}) \ni \Big(u, \operatorname{adj}(\nabla u)\Big) \to \det(\nabla u) \in L^s(\Omega;\mathbb{R})$$

is well defined and continuous. Furthermore holds

$$\left.\begin{array}{lc} u_k \rightharpoonup u & \text{in } W^{1,p}(\Omega;\mathbb{R}^3),\ p \geq 2 \\ \operatorname{adj}(\nabla u_k) \rightharpoonup H & \text{in } L^q(\Omega;\mathbb{R}^{3,3}),\ p^{-1}+q^{-1} \leq 1 \\ \det(\nabla u_k) \rightharpoonup \delta & \text{in } L^r(\Omega;\mathbb{R}),\ r \geq 1 \end{array}\right\} \Rightarrow \left\{ \begin{array}{c} H = \operatorname{adj}(\nabla u) \\ \delta = \det(\nabla u) \end{array}\right.$$

Proof. See [Ci88, Thm. 7.6-1]. ■

Theorem A.7. *(generalized Poincaré's inequality)*

Let Ω be a domain in $\mathbb{R}^n$, and let $1 \leq p < \infty$. Let Γ_0 be a measurable subset of the boundary Γ with $|\Gamma_0| > 0$, Then there exists a constant $c_{gP} > 0$ such that

$$\int_\Omega |u|^p \,\mathrm{dx} \leq c_{gP}\Big(\int_\Omega |\nabla u|^p \,\mathrm{dx} + \left|\int_{\Gamma_0} u \,\mathrm{ds}\right|^p\Big) \qquad \forall u \in W^{1,p}(\Omega;\mathbb{R}^3)$$

Theorem A.8. *(Tonelli)*

Let Ω be a domain in $\mathbb{R}^n$ and $m \geq 1$. For functions $u : \Omega \to \mathbb{R}^m$ and continuous $f : \mathbb{R}^m \to \bar{\mathbb{R}}$ define the nonlinear function

$$\mathcal{F}(u) := \int_\Omega f\Big(u(x)\Big) \,\mathrm{dx}$$

Then the function $\mathcal{F}$ is weakly lower semi-continuous on $L^p(\Omega)$, $1 < p < \infty$ and weak-star lower semi-continuous on $L^\infty(\Omega)$ if and only if $u \mapsto f(u)$ is convex.

Proof. For a sketch of the proof see [Re04, Thm. 10.16]. For the complete proof see [Ev98, Thm. 1] or [Ma83, Box 4.1]. ■

Theorem A.9. *Let G and U be two real Hilbert spaces with norms $\|\cdot\|_G$ and $\|\cdot\|_U$ and let $G_{ad} \subset G$ be closed, bounded and convex. Let $u_{ref} \in U$ and $\alpha > 0$. Moreover let $S : G \to U$ be a linear and continuous operator. Then the quadratic optimization problem*

$$\min_{g \in G_{ad}} \frac{1}{2}\|Sg - u_{ref}\|_U^2 + \frac{\alpha}{2}\|g\|_G^2$$

has a unique optimal solution $\bar{g} \in G$.

Proof. See [Tr09, Thm. 2.14]. ■

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Notation

Φ	deformation
u	displacement
C	Cauchy-Green strain tensor ($= \nabla\Phi^*\nabla\Phi$)
$E(u)$	strain tensor ($= C - I$)
∇^s	symmetric gradient/linearization of the strain tensor $\left(\frac{1}{2}(\nabla + \nabla^*)\right)$
U_{ad}	set of admissible displacements
G	set of admissible controls/boundary forces
g	control/boundary force
λ, μ	Lamé constants
E	Young's modulus
ν	Poisson's ratio
α	Tichonoff regularization parameter
$\mathbb{M}^n$	set of all real square matrices of order n
$A : B$	$= \mathrm{tr}(A^T B)$
$\mathbb{M}^n_+$	$= \{A \in \mathbb{M}^n : \ \det(A) > 0\}$
$\mathbb{O}^n$	set of all orthogonal square matrices of order n
$\mathbb{O}^n_+$	$= \mathbb{O}^n \cap \mathbb{M}^n_+$
$\mathbb{S}^n$	set of all symmetric matrices of order n
$\mathbb{S}^n_>$	set of all positive definit matrices of order n

List of Figures

The Figures have been created with Matlab (Figures 9-13), ZIBAmira (Figures 1, 6, 7 & 8, 14-20), GIMP and Open Office (Figures 2-5). Figure 21 has been taken from [We07].

Eidesstattliche Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit selbständig und ohne Benutzung anderer als der angegebenen Hilfmittel angefertigt habe.

Berlin, den 21.12.2010