Doctoral Thesis

Investigation of the Mechanical Behavior of Facial Soft Tissues

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Investigation of the Mechanical Behavior of Facial Soft Tissues

A thesis submitted to attain the degree of DOCTOR OF SCIENCES of ETH ZURICH
(Dr. sc. ETH Zurich)

presented by

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Abstract

The present thesis deals with the mechanical characterization of the highly non-linear, time-dependent, and isotropic behavior of facial soft tissues and their interaction within tissue structures. Theoretical and experimental approaches are combined to provide the basis for improved finite element (FE) modeling of complex facial tissue response, such as skin wrinkle formation in facial expressions and active muscle contraction in mastication. The theoretical work addresses the need for constitutive model equations capable of describing the active and passive behavior of individual tissues and their numerical implementation within the FE environment. The experimental investigations comprise the characterization of facial tissues at different length scales and include the visualization of interactions between soft tissue constituents. Experimental data are used for determination of mechanical tissue properties, i.e. for material parameter optimization and validation of numerically predicted tissue response.

Finite element modeling of facial tissues considers the development of constitutive equations, their numerical implementation within the FE environment, and the generation of anatomy based model representations of soft tissue structures. The first part of the present work focuses on the numerical implementation of an elastic-viscoplastic material model particularly suitable for facial soft tissues and a skeletal muscle model representing the contractile properties of active tissues. In the case of the soft tissue model, a strongly objective integration scheme and a new mixed finite element formulation were developed based on the introduction of the relative deformation gradient- the deformation mapping between the last converged and current configurations. Numerical verification of the proposed integration scheme and the consistent linearization of the Hu-Washizu functional demonstrated mandatory objectivity under superposed rigid body motion and quadratic convergence, respectively. The numerical implementation of the skeletal muscle model based on the decoupled approach- so the additive split of the strain energy function into a dilatational and a distortional part- revealed unphysical volume growth and negative eigenvalues of the tangent moduli. Consequently, a different functional form of the constitutive equations was proposed which avoids the additive split of the strain energy function and considers muscle as a nearly incompressible material, allowing for an adequate physical approximation of the mechanical response.

Physically relevant simulations of facial tissues require the development of anatomy based FE models. Magnetic resonance imaging (MRI) measurements of the head of a 29 year old male provide the basis for the development of two FE models- a multilayered
forehead model and a reconstruction of the mastication system. These models are used for simulations of the wrinkle formation in the forehead and the biting process during mastication.

The second line of research followed in this thesis is concerned with an extensive experimental characterization of active and passive facial soft tissue response. An experimental setup was developed for the suction based quantification of time- and history-dependent response of superficial tissues in multiple regions of the face and for various loading cases. The extensive experimental data on the two most superficial layers, skin and subcutaneous tissue/SMAS (superficial musculoaponeurotic system), were used in an inverse FE analysis for the identification and validation of corresponding material parameter sets for the Rubin and Bodner model.

A specific experimental setup for ultrasound based visualization of soft tissue behavior in general and tissue layer interactions in particular, enabled the qualitative determination of location dependent interaction properties in the forehead region. The experimental observations provided significant improvements for the FE forehead model allowing more realistic and location specific interaction properties to be defined in the region of the so-called glide plane space and the temporal fusion zone. Moreover, the proposed measurement system was shown to be promising as a diagnostic tool for the clinical examination and monitoring of full-thickness skin tissue changes related to age and disease, such as scleroderma.

Finally, in collaboration with the Nestlé Research Center, a measurement system was developed for simultaneous ultrasound imaging of masseter muscle deformations and location specific bite force measurements. Muscle shape was visualized in various horizontal and one vertical cross section while maintaining a set bite force. The measurement protocol included three physiological bite forces (50N, 100N, and 200N) and two biting locations (molar and incisor) in order to provide an approximate geometric reconstruction of masseter shape during the mastication process. Accompanying numerical simulations of molar and incisor biting with the FE mastication model showed remarkable agreement with experimental data for maximum bite forces.
Zusammenfassung


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The work presented in this thesis was carried out at the Institute for Mechanical Systems in the Department of Mechanical and Process Engineering at ETH Zurich.

I would like to thank my supervisor Prof. Dr. Edoardo Mazza for giving me the opportunity to work in the exciting field of experimental continuum mechanics. I deeply appreciate the great support and guidance of my research, all the insightful discussions, valuable advice, and academic freedom throughout the years.

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Zurich, February 2015
Johannes Weickenmeier
Structure of the work

The investigation of facial soft tissues presented in this thesis involves both, the experimental and numerical characterization of the mechanical behavior of tissues and tissue structures. This led to a division of the thesis into four parts in order to distinguish between the work associated with the development of finite element technologies and the experimental investigations of facial tissues. These respective Parts II and III are enclosed by a general introduction in Part I and the general conclusions and appendices in Part IV.

More precisely, Part I contains a brief motivation demonstrating the evident need for the numerical modeling and experimental characterization of soft biological tissues in view of an increasing interest in medical and industrial applications. A literature review on state-of-the-art facial modeling and a brief summary of anatomical features of the face and forehead provides the motivation for the individual contributions in this thesis aiming at increasing the understanding of the highly interesting biomechanics of soft tissues and tissue structures.

The second part of this work focuses on the numerical investigation of facial soft tissues. In particular, a new element formulation is developed especially suitable for elastic-viscoplastic material models governed by evolution equations. Additionally, the implementation of a physically based skeletal muscle model within an ABAQUS user subroutine is derived. This part of the thesis provides several different numerical verifications analyzing objectivity of integration schemes under rigid body motions, optimal convergence, and enforcement of the tissue incompressibility constraint. A specific outline is given on page 21.

The third part of this thesis is dedicated to the experimental campaigns aiming at the visualization of tissue deformation and the quantification of the mechanical response of superficial tissue layers and mastication muscle. These investigations tie in with previously presented work by Barbarino (2011) and extends the suction based characterization of superficial skin layers to time and history dependent behavior. Moreover, three ultrasound measurement campaigns are presented that provide new insight into the interaction properties of tissue layers in the forehead and the contractile properties of muscle tissue. An overview of specific chapters in Part III is given on page 77.
The presented work is concluded by a general summary of both Parts II and III and provides the key contributions of all investigations. The presented work provides distinct improvements over existing facial finite element models and allows for the simulation of complex medical and industrial applications. Related extensions of the finite element model as well as useful additional experimental work are recommended for future investigations. The remaining sections of this thesis contain the bibliography, a list of publications, and a curriculum vitae.
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Part I

Introduction
Motivation

The mechanical behavior of facial soft tissues defines our outer appearance and determines how we are perceived through our facial expressions. The face, including the forehead region, is characterized by a highly complex tissue structure that experiences significant changes during lifetime. Tremendous effort has been invested in the experimental characterization, material modeling, and numerical simulation of facial tissues, providing increasingly physical and realistic descriptions of the mechanical behavior of soft tissues across several length scales.

Understanding facial soft tissue mechanics is of profound interest in medicine and industry. In particular, clinicians rely on the mechanical characterization of soft tissues and the change of their properties under consideration of age, gender, ethnicity, and most relevant for clinical diagnostics, the transformation of tissue behavior due to disease. Quantifying pathological developments in soft tissues provides means for early diagnosis, reliable monitoring of the course of a disease, and the development of effective treatment strategies. In recent decades, interest in surgical planning tools which incorporate several different disciplines in biomechanics, ranging from the experimental characterization and patient specific model development to realistic predictions of surgery outcome, has grown substantially.

The cosmetic and medical technology industry relies on physically based material modeling for the development, optimization, and validation of new products for the external treatment of superficial tissues, as well as prosthesis and implants for the reconstruction of functionally degraded tissue structures. Numerical simulations of aging, the process and results of surgical interventions, and the tissue response to implants provide measures for the evaluation of biocompatibility, risks, and efficacy of new products. Along these lines, the food industry shows increasing interest in taking advantage of anatomy based mastication models for the simulation of mastication and swallowing to test new food textures and their behavior in the oral cavity.

Reliability and physically based predictive capability of facial models require the comprehensive investigation of soft tissues. This encompasses the analysis of soft tissue composition, the corresponding mechanical behavior, as well as their interaction within multilayered or entangled tissue structures.
The experimental characterization of soft tissues comprises the assessment of numerous influencing factors such as (i) time and history dependent material response, (ii) differentiation of in- and ex-vivo tissue properties, (iii) measurement technique, and (iv) intra-and inter-subject variability. Geometrical reconstructions of anatomy based models are generally based on computer tomography (CT) or magnetic resonance image (MRI) data and subsequent (semi-)automatic segmentation techniques. The finite element (FE) method represents a sophisticated tool for the analysis of these geometrically complex structures and provides a means for the integration of material models representing the highly non-linear material behavior of soft biological tissues. FE modeling includes the anatomy based definition of kinematic boundary conditions and tissue layer interaction properties.

Given the range of model assumptions, there is an evident necessity for the verification of FE simulations. The physically based description of soft tissue behavior is usually presented within the theory of continuum mechanics. The corresponding implementation of constitutive model equations within the FE environment represents a major challenge. Several different element formulations have been developed to enforce such material properties like incompressibility or to avoid often observed element locking including both, shear and volumetric locking, for lower order elements. These strategies include mixed finite element methods and several enhanced strain finite element formulations. The verification of numerical simulations requires careful consideration of the numerical material model implementation, the correct representation of kinematic, kinetic, and contact constraints, and the predicted overall tissue response. Direct comparison with experimental data allows for the evaluation of the predictive capabilities of a FE model. In particular, based on a properly verified FE model, sensitivity analysis of the given model allows to reliably validate several different hypotheses regarding material properties, modeling assumptions, and different deformation mechanisms underlying the respective model problem.

The work presented in this thesis aims at providing new insight into (i) the development of FE models of the face and the numerical implementation of physically based constitutive model equations and (ii) the experimental characterization of superficial tissue behavior. The following sections present an overview of current literature on these two topics.

Facial FE modeling

The emergence and availability of medical imaging techniques gave way to the development of anatomy based FE models which allow for a detailed description of soft tissue structures and a realistic differentiation between specific tissue layers. Especially the face is characterized by geometrically complex structures including multiple tissues and bone. Previously mentioned biomechanical applications have motivated the development of several different facial FE models for the simulation of aging, facial expressions, and surgical interventions. Hannam (2011) provides an extensive overview of computational modeling of craniomandibular mechanics and differentiates between individual modeling strategies
(FE, rigid body, and mixed approaches) and individual regions (face, jaw, craniomandibular skeleton, and tongue). Zachow et al. (2002), Gladilin et al. (2004), and Chabanas et al. (2003) were among the first to present patient specific FE models for simulations of craniomaxillofacial surgery in order to predict post-operative outcome and related implications on facial expressions. The growing interest in computational tools supporting surgery planning and real-time monitoring of optimal bone repositioning during surgery lead Mollemans et al. (2007) to develop computationally significantly cheaper mass-tensor models (MTM). In their work they compare several different computing strategies including a mass-spring model and linear and nonlinear FE models to assess the computational efficiency and numerical accuracy for predicting surgical outcome. Besides several modifications proposed by Chabanas and co-workers to enhance above-mentioned models (Chabanas et al., 2004a,b; Luboz et al., 2005; Swennen et al., 2009), Stavness et al. (2011) presented a three-dimensional dynamic model of the jaw-tongue-hyoid complex in order to simulate the impact of an active tongue muscle on jaw kinematics. The model considers muscle as a point-to-point connector that shortens upon activation. In their work, they combine the rigid body model presented by Hannam et al. (2008) and a FE tongue model by Bucaillard et al. (2009) in order to simulate the mechanical behavior of the entire oral cavity. In view of several medical conditions associated with the oral cavity such as dysphagia, sleep apnea, and CMF surgery, several other FE models have been proposed. Pelteret and Reddy (2012) simulated the upper airway system and, in particular, the interaction between breathing pressure and individual tongue muscle subgroups to investigate the impact of tongue involvement in apnea and related diseases. In an enhanced version of the tongue model, Kajee et al. (2013) discussed the impact of muscle activation patterns on tongue deformation in dependance of obstructive sleep apnea.

The mechanical behavior of the mastication system has been investigated for many decades. Primarily, mathematical representations and one-dimensional muscle models were used to investigate muscle forces, bite forces, and respective loading states of the temporomandibular joint. These studies provide valuable insight into the mechanics of the mandible by determining the effect of jaw opening angle, biting position, jaw kinematics in biting and speech, temporomandibular disorders, and individual muscle involvement (see Chapter 8). To the author’s best knowledge, up to this day however, the only three-dimensional mastication model has been presented by Röhrle and Pullan (2007). It incorporates a realistic representation of the masseter muscle shape and considers a constitutive model formulation for a physically based muscle description. They provided a model for muscle force and joint loading simulations in which they pay special attention to an anatomy based representation of muscle fiber orientation and its influence on model predictions.

There is an ever increasing interest in physically based simulations of facial expressions and transformations in the morphology of the face related to soft tissue changes. Respective FE models are generally based on medical images, but differ significantly in the subsequent representation of soft tissues with respect to number of layers, layer thicknesses, incorporation of muscle structures, and especially the choice of the constitutive material models. Nazari et al. (2010) presented a three layer soft tissue model derived
from work presented by Chabanas et al. (2003) and considered superficial muscles of the face. Muscles, being responsible for tissue deformation in facial expressions, are treated as one-dimensional cable-elements whose contractile properties are mimicked by a thermal expansion model. The FE model allows to investigate soft tissue deformation upon activation of distinctive muscles or muscle groups to reproduce facial expressions. Similar work was presented by Wu et al. (2013a,b), who proposed a different modeling approach to incorporate muscle tissue. Their modeling strategy is based on a one layer FE mesh that represents the individual facial soft tissues as a homogeneous continuum. Muscle geometries of 15 facial muscles however, are reconstructed from medical images and embedded into the face continuum. Nodal kinematic coupling between boundary nodes of the muscle and corresponding insertion points in the face transmits the contractile response of activated muscles to the overall facial mesh. In a modified version, the presented face model is applied to determine distinctive muscle activation patterns to achieve a more realistic prediction of facial expressions (Wu et al., 2013a,b).

As a next step in improving the physicality of these facial models, Flynn et al. (2015) presented a facial model, based on the work by Chabanas et al. (2003), for the simulation of facial expressions considering orthotropic tissue behavior and in vivo tension in the skin layer. Despite the significant simplifications with respect to the soft tissue layer structure, muscle geometry, and the respective constitutive model equations, the model provides new insight into the prediction of outer appearance based on specific muscle activation patterns.

An essential feature of facial expressions and aging is the formation of skin wrinkles. Previously presented face models are often limited in the prediction of tissue behavior on this scale due to considerable homogenization across multiple tissue layers of varying mechanical properties and very coarse meshes which do not allow to represent wrinkles or folds. Warburton and Maddock (2013) proposed a novel multilayer forehead model capable of representing wrinkling upon frontalis muscle activation. The model solver is based on the total Lagrangian explicit dynamic FE method (Miller et al., 2007) and was optimized for GPU implementation for interactive graphics applications. In comparison to the forehead model presented in this thesis (Weickenmeier, 2014; Weickenmeier et al., 2014b) the soft tissue model is based on the simple hyperelastic neo-Hookean constitutive equation and uses a muscle model that builds on an additive split of passive and active muscle stress as presented by Röhrle and Pullan (2007).

Wrinkle simulations using implicit FE solvers require a more physical representation of the facial soft tissue structure in order to achieve the buckling like tissue response upon (muscle induced) compression. Several simplified skin models have been proposed in order to investigate the impact of layer thickness, tissue stiffness, and compression mechanism (Flynn and McCormack, 2008, 2010; Herlin et al., 2014; Hung et al., 2009; Kuwazuru et al., 2008; Lévéque and Audoly, 2013). With respect to skin biomechanics, Limbert (2014) provided a comprehensive review on state-of-the-art constitutive model equations based on physical material behavior and phenomenological observations and challenges in the numerical implementation of these models, especially with respect to FE models considering complex geometries and boundary conditions.
In summary, considerable effort has been invested in the development of anatomy based FE models and their use for the characterization of soft tissue behavior. However, several of these FE models share common model assumptions related to material modeling, geometric approximations of tissue structure, and incorporation of simplified muscle structures including their interaction with surrounding tissue. This raises questions regarding the physicality and predictive capabilities of these models. A great part of the work presented in this thesis is dedicated to the experimental characterization of tissue layer interactions and the development of numerically robust model implementations of a skeletal muscle model and a soft tissue model. For one, the consideration of proper tissue interaction is shown to improve the predictive accuracy of the presented anatomy based and subject specific FE model. For the other, it is shown that the consideration of physically based constitutive model equations and their numerical implementations allows to represent experimentally observed material behavior in terms of deformation and forces remarkably well.

Experimental characterization of superficial facial tissue layers

The mechanics of biological soft tissues are determined by numerous material properties, ranging from the individual constituents to the interactions with surrounding tissue structures, on top of which all of these properties experience substantial changes over time and show a significant dependence on their loading history. In particular, superficial tissues are extensively exposed to environmental factors (e.g. the impact of sun) and undergo clearly visible changes in morphology in the form of loss of elasticity, deposition of fat, and the formation of permanent wrinkles. Besides age related transformation in skin and subcutaneous tissue properties, there are several pathological tissue alterations affecting either one of the constituents or their interplay within the entire tissue structure.

The mechanical characterization of tissue behavior in its healthy state and, ideally, the quantitative assessment of pathological and age related property changes provide means for developing preventative and healing treatment strategies in clinical applications. Anatomy based FE models of soft tissue structures including appropriate material modeling based on experimental findings, will gain increasing importance in patient specific medical treatments.

Experimental characterization of soft biological tissue includes a large number of measurement methods which depend on the property of interest. In general, based on the accessibility and availability of individual tissues, measurement methods are either in-vivo, in-situ, or ex-vivo investigations. The state in which tissues are analyzed has a significant impact on the physicality of corresponding measurement data and its relevance for clinical applications. A typical ex-vivo measurement method is uniaxial tensile testing on excised tissue samples (Jacquemoud et al., 2007; Ní Annaidh et al., 2012) or the testing in a bi- or multi-axial stress state such as in indentation and inflation tests (Geerligs et al., 2011; Tonge et al., 2013). Ní Annaidh et al. (2012) presented uniaxial tension tests on excised back skin samples under consideration of Langer Lines (Langer, 1862) and the corresponding principal orientation of collagen fibers. Their measurement results indi-
cated a clear correlation between elastic modulus, ultimate tensile strength, and tensile strain failure with the orientation of the Langer lines. Moreover, histological analysis provided additional evidence for a significant correlation between Langer line orientation and preferred direction of collagen fibers in the dermis. In comparison to that, Tonge et al. (2013) aimed at quantifying the anisotropic behavior of full-thickness skin through bulge tests of excised planar tissue samples. The inflation setup allows to visualize tissue deformation and, in particular, to quantify the anisotropy related asymmetric, elliptical bubble shape. While these two methods allow to investigate anisotropic material properties of full-thickness skin, the in-vitro indentation method presented by Geerligs et al. (2011) focused on epidermis consisting of stratum corneum and viable epidermis (which includes the other layers of the epidermis: stratum basale, stratum spinosum, and stratum granulosum) and provided isotropic material parameters in the form of Young’s modulus. This work is motivated by increasing interest in transdermal drug delivery which requires data on the mechanical properties of the most superficial tissue layer.

While the above works focus on the characterization of individual skin layers, other measurement techniques allow to address full-thickness skin properties by means of visualizing skin layers deformations. Lamers et al. (2013) applied large amplitude oscillatory shear measurements to quantify the shear properties of skin across multiple tissue layers. Their findings suggest to consider full-thickness skin as a homogeneous layer with gradually changing shear properties much rather than distinguishing between individual layers. The most superficial layer of skin is characterized by the largest shear modulus and decreases exponentially with increasing tissue depth. In a similar setup, Gerhardt et al. (2012) presented an experiment for visualization and quantification of tissue deformation in shear displacement measurements. By means of digital image correlation, through-plane skin layer deformations are quantified and allow for the determination of a skin stiffness profile across the individual layers. The experimentally observed shear strain and shear modulus profile differ from the previously mentioned study. In fact, there is a distinct difference between epidermal and dermal behavior in terms of a rather homogeneous shear modulus within each layer and a difference in the absolute values. Moreover, there is a noticeable transition in the strain profile for the interface between epidermis and dermis. Especially the latter method plays a significant role in the work related with this thesis as presented in Chapter 6.

In view of physically based modeling of soft biological tissues and the simulation of full-thickness skin response such as skin wrinkling or facial expressions, in-vivo measurement methods of superficial tissue structures provide relevant data for the calibration of numerical predictions. The calibration process involves material parameter identification, the validation of the presumed deformation mechanism explaining observed tissue behavior, and the verification of numerically predicted tissue deformations and forces by direct comparison with experimental data. Despite potential similarities in ex- and in-vivo measurement techniques, the observed tissue response is generally different.

The uniaxial tensile method presented before has been adopted for in-vivo measurements in different works. Khatyr et al. (2004) developed an experimental setup for extension and compression measurements on the inside of the forearm. By recording relative dis-
tance and load on tweezers connected to the skin surface, the mechanical response upon deformation was quantified. By varying the displacement direction, tissue anisotropy is clearly visible in the mechanical response. In a similar approach, Flynn et al. (2011, 2015) presented a single tip extension test setup which allows for multiple directions of skin displacement. Based on various in- and out-of-plane displacement vectors, the three-dimensional tissue response was determined. Measurements in six different regions (five in the face and one on the forehead) provided a location specific characterization of the full-thickness skin response. Despite the three-dimensional displacement vector and a clear tissue anisotropy, the experimental data is used for determining material parameters for an isotropic Ogden strain energy function based on a planar FE skin model. In comparison to work presented in Chapter 5, the proposed numerical representation of the experimental setup seems unsuitable for a parameter optimization for later FE simulations with geometrically more realistic models.

Several experimental campaigns aim at characterizing skin tissue changes related to age. Batisse et al. (2002) investigated age related wrinkle formation by means of a newly developed device. The DensiScore\textsuperscript{R} produces standardized compression of 42\% in the plane of the skin and allows for a distinct categorization of wrinkle size. In addition to wrinkle measurements, tissue extensibility and elasticity of skin were measured using a Dermal Torque Meter\textsuperscript{R}. Subsequent ultrasound based visualization of skin layer thicknesses at the measurement sites allowed to correlate age dependent mechanical properties of the skin with layer thicknesses and the degree of skin wrinkling. The results clearly indicate a pronounced increase of the wrinkle score for aged skin, a significant negative correlation between wrinkle score and skin extensibility (for stratum corneum as well as full-thickness skin), and a clear relation between full-thickness skin stiffening for increasing wrinkle scores. These results are very much in line with data obtained in similar torsional extension tests presented much earlier by Escoffier et al. (1989), with the main difference of observing a later onset of age related tissue changes in the latter study.

As regards the experimental characterization of superficial tissue layers, suction based measurements reproduce the most physically relevant state of deformation which skin exhibits in every day life (Fujimura et al., 2007; Hendriks et al., 2006; Iivarinen et al., 2013; Luboz et al., 2014; Piérard et al., 2013a,b; Tarsi et al., 2013). In literature, different suction devices have been presented which differ primarily in the probe opening diameter. The opening diameter and shape controls the depth of tissue involvement as well as the shape of the deformed tissue (usually spherical or otherwise elliptical tissue bubble) upon suction. Among many experimental studies, Fujimura et al. (2007) used the suction method to assess age related changes in skin elasticity. More recently, Luboz et al. (2014) presented a newly developed aspiration setup, specifically designed for clinical use, in order to provide patient specific linear elastic properties of facial soft tissues.

Due to a significant interest in location dependent and subject specific quantification of skin properties in biomechanics and surgery simulation, a substantial suction based experimental campaign is presented within this thesis. Well-known measurement errors related to the control of repeated probe placement, minimal contact pressure, and the impact of probe opening diameter are specifically addressed in the experimental setup and measurement protocol.
While significant focus lies on the characterization of superficial tissues, skeletal muscles (lying underneath the skin), and subdermal tissues, are just as relevant for providing new insight into the mechanics of facial expressions, mastication, and changes of facial morphology with respect to age, ethnicity, and inter-subject variability. Muscle architecture and anatomy has been thoroughly documented in literature for several decades. With increasing complexity of face and forehead models as well as constitutive muscle models, there is a need for experimental characterization of muscle tissue behavior during active contraction. In particular, the relation between muscle force and corresponding muscle shape change is of key importance for improving realistic numerical predictions of muscle behavior in FE models.

In view of the work presented in this thesis the following aspects related to muscle mechanics are most relevant. For one, there is a clear need to understand the interaction between individual tissue layers including the interaction of muscle with its surrounding tissues. Wu et al. (2010) presented an ultrasound based measurement on the relative deformation behavior at the muscle-tissue interface upon masseter muscle contraction. Of similar importance is the experimental determination of masseter muscle shape change when clenching as presented by Kubo et al. (2006). Finally, physically based modeling of muscle tissue requires muscle specific architecture which refers to such properties like sarcomere length, fiber length, the ratio between contractile tissue and tendinous tissue weight, pennation angle, physiological cross-sectional area, and insertion points. For the example of the mastication muscles, Van Eijden and Raadsheer (1992) and Van Eijden et al. (1997, 1995, 1996) provided a full characterization of the respective muscles.

Concluding Remarks

The numerical and experimental investigations presented within this work aim at improving existing FE model representations and their predictive accuracy, which tend to miss sufficient physicality in terms of a proper geometric reconstruction of facial tissue structures, the use of simple constitutive model equations, or disregarding tissue interactions. The observations and achievements presented by Barbarino (2011) represent the starting point of this work and motivate the specific investigation of time, history, and location dependent behavior of superficial layers, the activation of muscle tissue, and the specification of tissue layer interactions for more realistic FE modeling assumptions.

In summary, the work presented here, represents state-of-the-art soft tissue characterization and numerical modeling for advanced FE based simulations of facial expressions, skin wrinkling, and mastication.
Anatomy of facial tissues

Facial anatomy is well documented and numerous anatomy textbooks provide a very high level of detail in the representation of tissue layer structures with respect to their thicknesses, muscle shapes, and the course of facial nerves and blood vessels (Gosling et al., 2008; Prendergast, 2013; Schünke et al., 2012; Wulc et al., 2012). The anatomy of the face as it is relevant to the finite element (FE) modeling presented within this thesis has been thoroughly described by Barbarino et al. (2009b, 2011) and is extended here by a detailed description of the forehead region.

The human face is characterized by a strong interplay of several different muscles and the surrounding soft tissues, which account for our outer appearance and drives our perception of one another. In general, facial muscles are separated into two groups of superficial muscles and deep muscles. While superficial muscles are primarily associated with facial expressions and speech, deep muscles are responsible for controlling the position of the jaw as in speech, jaw movements, and most importantly for the generation of bite force in mastication. Van Eijden et al. have studied muscles of mastication for several decades and have provided substantial insight into their architecture and their physiological properties Van Eijden and Raadsheer (1992) and Van Eijden et al. (1997, 1995, 1996). Individual muscles are different with respect to their average sarcomere and overall fiber length, their physiological cross-sectional area, and insertion points on top of which location dependent variations within each muscle provide optimized functionality.

Facial aging is among the most observable indicators for the continuous transformation of soft biological tissues driven by anatomical, biochemical, and genetic factors. Changes in outer appearance are three-dimensional processes and involve multiple different tissue layers and their interactions (Farage et al., 2007; Knize, 2001; LaTrenta, 2004; Wulc et al., 2012). Superficial tissue layers, and especially skin (being the body’s barrier to the environment), are exposed to external factors such as sun or UV light, chemicals, and mechanical loading. Most soft tissues experience a progressive gravimetric descent over time leading to the sagging of superficial layers (Knize, 1996a,b; Mazza et al., 2007). Actinic damage and solar elastosis from repeated exposure to sun lead to an accelerated loss of collagen and elastin in the dermis and an associated loss of skin elasticity. Exper-
imental data revealed a significant correlation between loss of elasticity and the onset of skin wrinkles (Lee et al., 2008). At the same time, it is often observed that fat lobules in subcutaneous tissue show a pronounced tendency to grow and to accumulate more fatty tissue. Due to a progressive loss of tautness in the supporting fascial ligament network, an overall drop of facial tissues appears (LaTrenta, 2004).

In the forehead, Matros et al. (2009) described a characteristic aging phenomena around the eyebrows which is referred to as the *spastic frontalis syndrome*. With the accumulation of eyebrow ptosis in combination with an increase in excessive upper eyelid skin, the field of vision is severely constricted. However, it is observed that frontalis muscle tone increases involuntarily thus compensating for undesired sagging of tissues. This leads to two clearly visible changes generally associated with the aged face. For one, the rather arched eyebrow of a young person becomes much flatter since the lateral part of the eyebrow drops due to tissue sagging and the medial part of the brow is raised upon frontalis muscle tone increase. At the same time, involuntary and continuous frontalis muscle contraction lead to the formation of permanent forehead wrinkles.

**Anatomy of the Forehead**

The anatomic description of the forehead region is based on the substantial contributions of Dr. D. Knize to the medical community to promote the understanding of anatomy, surgical procedures for reconstruction and rejuvenation, and tissue mechanisms underlying facial expressions and aging of the forehead region (Knize, 1996a, 2009, 1996b, 2001, 2007). The anatomic organization of the forehead in presented in the following and is represented in Figure 2.1 adapted from Knize (2001).

The scalp consists of five layers which are skin, subcutaneous tissue, galea aponeurotica, loose areolar tissue, and periosteum. Forehead skin is the thickest of all facial skins and has many sebaceous and sweat glands. The underlying subcutaneous tissue has many transverse fibrous septa that reach from the frontalis muscle to the dermis. These fibers are partially responsible for the formation of transverse rhytides. The galea aponeurotica is a layer of dense fibrous tissue and is closely connected to the skin by a firm, dense, fibro-fatty layer which forms the superficial fascia of the scalp. Loose areolar tissue consists of randomly organized unconnected fibers, large number of blood vessels, and significant empty space. It is located in the subgaleal space and is often used in plastic surgery as a dissection plane.

In the region just medial to the temporal fusion line and its continuation as the superior temporal fusion line, periosteum is tightly fixed to the bone and the overlying soft tissues, and consists of dense irregular connective tissue. The five layers mentioned initially continue into the forehead region where galea interdigititates with muscles of facial expression in the eyebrow region. The soft tissue layout of the forehead depends on the region that is studied. The most general distinction can be made between the mid-forehead and the temporal fossa.
Figure 2.1: Figure adapted from Knize (2001) (see for Figure 4.10 on page 54). The zone of fixation lies at the junction of the forehead and the temporal fossa (blue). Within this zone periosteum (P) is densely fixed to bone (B). Temporalis muscle (TM) and frontalis muscle (FM) provide strong support to the entire forehead region. The deep temporal fascia (DTF) covers the temporalis muscle. The deep galea plane (DG) over the forehead becomes the outer layer of the superficial temporal fascia (STF I) over the temporal fossa. The subgalea fascia plane (Sub G) over the forehead becomes the middle (STF II) and deep (STF III) layers of the superficial temporal fascia. The superficial divisions of the supraorbital nerve (SON-S) run over the surface of the frontalis muscle and the deep division of the supraorbital nerve (SON-D) runs deep to the frontalis muscle always just medial to the zone of fixation.

The mid-forehead consists of skin, fat tissue, and galea aponeurotica. Galea aponeurotica has a similar layout as in the scalp and incorporates the superficial musculoaponeurotic system (SMAS) and very loose connective tissue. SMAS refers to a dense collagen-muscle fiber network that provides significant support to several facial and forehead regions (Ghassemi et al., 2003). The mid-forehead muscles interdigitate with galea in the supraorbital region of the eyebrow. Underneath galea periosteum extends laterally across the frontal bone all the way to the temporal fusion line. Superior to the orbital rim (over a transverse band of 2.5mm) it is tightly adherent to the bone. Over the rest of the frontal bone it is loosely attached to the bone and allows for rather large movement of soft tissue over the frontal bone (as in facial expression such as surprise) resulting in multiple horizontal rhytids.
Chapter 2. Anatomy of facial tissues

Moving laterally along the **temporal forehead**, the periosteum becomes deep temporal fascia (DTF) and temporal fascia (TF) that cover the surface of the temporalis muscle. Deep temporal fascia is a thick, dense connective tissue layer that separates into a superficial layer and a deep layer a few centimeters above the zygomatic arch. In between these two layers of DTF lies the superficial temporal fat pad. Continuing medially this superficial fascia layer fades into galea aponeurotica and SMAS over the mid-forehead. The deeper galea layers (sub-galea) over the mid-forehead become the middle (STF II) and deep (STF III) layers of superficial temporal fascia in the temporal region. The most superficial tissue layers in the temporal forehead consist of connective fatty tissue and skin.

**Muscles in the forehead and temporal fossa region** are primarily responsible for eyebrow movement, blinking, mastication, and many different facial expressions. With facial aging the muscle tone of several muscles changes in order to compensate for skin and other soft tissue laxities (LaTrenta, 2004). The frontalis muscle pair is the primary eyebrow elevator. The superior half of each pair arises from the deep galea plane and fades into the orbital portion of the orbicularis oculi muscle, which inserts into dermis under the eyebrow. The lateral end of the frontalis muscle reaches just medial to the superior temporal line of the skull. The procerus muscle originates from the dorsum of the nasal bone, splits into two parts in the glabella region before interdigitating with the medial edge of the frontalis muscle. The distal ends of the procerus muscle insert into dermis between the frontalis muscles. The paired corrugator supercilii muscles originate from the glabella and the supraorbital ridge and insert into the skin of the medial eyebrow. The depressor supercilii muscle passes upward from the dorsum of the nose to the skin of the forehead. The paired corrugator and depressor muscles are brow depressors which allow to pull the eyebrow inferiorly and medially. A contraction of this muscle group causes vertical and horizontal rhytids in the glabella region. These folds appear during facial expressions such as frowning and anger or as a response to facial aging (LaTrenta, 2004). The orbicularis oculi muscle (OOM) is the sphincter of the eye and consists of three parts: orbital, palpebral, and lacrimal. The orbital part of the OOM is responsible for a firm closure of the eyelid, the palpebral part enables blinking and the lacrimal part is concerned with the control over the lacrimal sac (i.e. moisturizing the eye, crying, and so on). The temporalis muscle is the strongest elevator and retractor of the jaw. It arises from the temporal fossa as far as the inferior temporal fusion line and from the temporal fascia. Its insertion extends on the coronoid process of the mandible to act as a muscle of mastication.

Figure 2.2 shows two high resolution magnetic resonance images of the medial forehead of a 29 year old male. Full-thickness tissue response during frowning is visualized, by fixing three wrinkles with medical tape for the course of the image acquisition time. Similarly, a suction bubble was produced to visualize the adherence between tissue layers in the mid-forehead. It can be seen, that the deepest layer clearly experiences large deformations while individual layers in the superficial tissue structure show strong interactions.
Figure 2.2: High-resolution magnetic resonance images of the medial forehead with (a) three fixed skin wrinkles and (b) a suction based tissue bubble. Visualization of individual forehead tissue layers and especially their interaction upon compression (as in frowning) and suction. Images (a) and (b) clearly visualize the glide plane space in the mid-forehead region as well as the layer of loose areolar connective tissue on top of the bone. The glide plane space enables large displacements of the whole forehead tissue structure based on large, reversible deformations of the underlying areolar tissue layer.
Chapter 2. Anatomy of facial tissues

Echogenicity of Soft Tissues

Visualization of soft tissues plays a key role in clinical applications for non-invasive, non-ionizing, and easily applicable assessment of tissue changes associated with health, age, and especially disease or injury. Medical imaging may be generally subdivided into ionizing and non-ionizing methods where X-ray and computer tomography comprise the first group and the second group includes regular digital imaging techniques, (confocal, second harmonic generation, etc.) microscopy, magnetic resonance, and ultrasound. Among the non-ionizing methods, ultrasound imaging is gaining importance in clinical examinations due to technical improvements allowing for very flexible visualization of not only deeper larger organs, but also superficial tissue layers like skin (Aspres et al., 2003; Kleinerman et al., 2012; Wortsman et al., 2013). Ultrasound imaging makes use of intrinsic differences of physical properties of individual tissues. When ultrasound waves penetrate through skin the tissues different constituents in the measurement site generate a distinct reflection pattern. The ultrasound waves are reflected at the boundaries of the individual structures and create reflections with various amplitudes.

In particular, the primary constituents of skin (including epidermis, dermis, and subcutaneous tissue) are keratin, collagen, and water which all exhibit a distinct echogenic response. Echogenicity is determined by a material’s capability to reflect incoming sound waves (Wortsman et al., 2013). The maximum frequency of the ultrasound probe determines the maximal penetration depth. Low frequency ultrasound (≤7MHz) is generally used for examining deep and large organs while high-frequency ultrasound (≤20MHz) is used to visualize superficial tissues, especially since it provides sufficient resolution to differentiate between epidermis and dermis. Very-high frequency ultrasound (>20MHz) has been used to resolve the anatomical structure of the epidermis. However, going to very high frequencies limits the observable tissue thickness to the epidermis only and additionally might lead to adverse affects for living tissue, essentially causing heat damage and cavitation (Kleinerman et al., 2012). As presented by Wortsman et al. (2013), in high-frequency ultrasound imaging, the high keratin-content in the thin epidermis layer appears as a bright hyperechoic line, while dermis continues to appear hyperechoic but noticeably weaker due to a dense but less echogenic collagen network. Even deeper layers like hypodermis or the subcutaneous layer appear as a hypoechoic band primarily due to their high fat content. Individual hyperechoic marks are associated with fibrous septa which fulfill a supportive function to the overall facial tissue stiffness.

The sonographic property of muscle tissue is primarily characterized by hypoechoic thick fascicles containing the muscle fibers and hyperechoic adipose-fibrous septa in between. Additionally, muscles are well differentiable in ultrasound images since they are encapsulated by a hyperechoic fascia.

In the attempt to determine the deformation mechanisms explaining the soft tissue behavior in facial expressions, aging, and the formation of wrinkles, visualization of different tissue configurations provides significant insight into model development. In view of the presented work in this thesis, ultrasound and magnetic resonance imaging are key...
measurement techniques in quantifying tissue behavior of muscle and soft tissues upon contraction and external loading.
Moreover, it was shown that ultrasound imaging is a strong diagnostic tool in monitoring skin diseases including cysts, scleroderma, and (solid, malignant, or inflammatory) lesions (Kleinerman et al., 2012; Wortsman et al., 2013). Ultrasound imaging is a highly flexible measurement technique that allows for dynamic imaging of tissue behavior. By recording B-mode image sequences, tissue deformation behavior is visualized and subsequently quantified by tracking of tissue motion. In summary, ultrasound imaging provides an optimal measurement technique for the investigation of soft tissue interactions and muscle deformation properties as presented in Chapter 6, 7, and 8.
Part II

Soft Tissue Modeling

Development and Implementation of Constitutive Model Equations
Overview

The numerical simulation of soft tissue behavior requires the development of constitutive model equations and their numerical implementation within the finite element (FE) environment. In particular, anatomy based FE models of soft tissue structures are often characterized by geometrically complex and highly irregular meshes and corresponding soft tissues experience large deformations which both call for robust numerical schemes to allow for appropriate convergence.

Most soft tissues are usually considered as incompressible materials which poses numerically challenging constraints on volumetric measures. Moreover, several tissue structures include active muscle tissue which enables voluntary contraction of tissue as in facial expressions and mastication. The numerical implications of an actively contracting incompressible material, together with other constraints of continuum mechanics, e.g. objectivity and convexity, stresses the necessity of reliable derivations and implementations of robust numerical routines.

Chapter 3 outlines the numerical implementation of the elastic-viscoplastic constitutive equations proposed by Rubin and Bodner (2002) in a user defined element formulation. A suction based experimental campaign on skin tissue in the jaw region allowed for the identification of a preliminary set of material parameters. The presented work is based on the following journal publication:


In order to allow for the simulation of active tissue response as in facial expressions, mastication, and muscle tone increase of frontalis muscle due to aging in the forehead region, a skeletal muscle model based on work presented by Ehret et al. (2011) is implemented within a user material subroutine. The corresponding work is presented in Chapter 4 and is based on the following journal publication:

Chapter 3

Elastic-viscoplastic soft tissue modeling

3.1 Introduction

Understanding the mechanical response of soft biological tissues is essential in the development of computational tools to enable physically based simulations for realistic applications in the medical field. This includes the planning of surgical interventions, the design of biocompatible prosthetic devices and implants, as well as the quantitative evaluation of different medical treatments with respect to faster healing of diseased and damaged tissue. Mathematical modeling in general and the finite element (FE) method in particular are crucial tools in understanding the mechanical response of soft biological tissues. Specifically, the FE method can be used in simulations of organs and systems of organs at increasing levels of complexity with respect to the level of structural representation, material models across different length scales, interaction of multiple tissue structures, and the type of medical application.

Generally speaking, soft tissues differ by their specific composition of mostly collagen, elastin and the hydrated matrix of proteoglycans, as well as other constituents depending on their individual functionality. Experimental observations have shown that soft biological tissues exhibit a highly nonlinear response, pronounced anisotropy, heterogeneous and large deformation upon physiological loading, hysteresis, and often a poroelastic and (nearly) incompressible material response (Fung, 1993). Additionally, soft biological tissues exhibit a strong time and history dependent behavior governed by fluid flow through porous fibrous networks, presence of transient fiber network connections and inherent time dependent behavior of tissue components, e.g. elastin and collagen (Bischoff et al., 2004). Alongside these effects, tissues undergo different forms of morphological changes over time leading to irreversible deformations and altered morphology. Such effects are seen in pre-conditioning in cyclically loaded soft tissues (Buerzle et al., 2013; Ehret and Itskov, 2009; Fung, 1993); stress relaxation at constant strain (Barbarino et al., 2009a); growth of skin, heart, tumor and muscle tissues (Göktepe et al., 2010; Menzel and Kuhl, 2012; Zöllner et al., 2012); softening of stretched tissue (Badir et al., 2013b; Ehret and Itskov, 2009; Maher et al., 2012); damage (Alastrué et al., 2007; Marini et al., 2012; Martin and Sun, 2013; Sáez et al., 2012); collagen turnover, remodeling, and aging (Epstein, 2009; Kuhl and Holzapfel, 2007; Mazza et al., 2005; Sáez et al., 2013).
Chapter 3. Elastic-viscoplastic soft tissue modeling

In constitutive modeling of time and history dependent material, the mechanical behavior is generally differentiated by viscoelasticity and inelasticity. Among the most frequently used formulations for rate dependent stress response of soft biological tissues are Fung-type quasi-linear viscoelastic models (Fung, 1993). The extensive flexibility with respect to constitutive formulations for the rate of instantaneous elastic stress and the reduced relaxation function in the hereditary integral of the viscoelastic stress, inspired several specific formulations for tendons (Provenzano et al., 2001; Sverdlik and Lanir, 2002), collageneous tissue (Nekouzadeh et al., 2007), skin (Bischoff, 2006), human liver (Nava et al., 2004), and ligaments (Vena et al., 2006) among many other applications. However, these models are of purely phenomenological nature and often fail to properly describe the characteristic highly nonlinear behavior (Provenzano et al., 2001).

Another common approach was adopted for studying skin tissue (Bischoff, 2006), as well as viscoelastic soft fiber reinforced composites (Nguyen et al., 2007) and the cornea (Le Tallec et al., 1993), which is based on a multiplicative decomposition of the deformation gradient into an elastic and a viscous part. In this approach, evolution equations are determined for strain-like internal variables. In contrast, work has been presented in formulating rate equations for stress-like internal variables solved by means of convolution equations, as presented by Holzapfel and Simo (1996) and Govindjee and Reese (1997). Applications of this approach were presented by Holzapfel and Gasser (2001) and Holzapfel et al. (2002) for arterial tissue, as well as by Peña et al. (2007, 2008) for ligaments.

Despite several well justified constitutive assumptions, viscoelasticity fails to describe the strongly inherent inelastic response of soft biological tissues (Fung, 1993). Literature provides experimental evidence for several different softening phenomena related to damage and loading beyond the physiological state of tissue, see e.g. (Ehret, 2011; Famaey et al., 2013; Peña et al., 2010) and references therein. Constitutive models for the description of irreversible alterations of tissue on the structural level have been proposed for fiber reinforced tissues (Balzani et al., 2012; Schröder et al., 2005) alongside above mentioned work. Respective work has revealed a similar softening behavior as it was described by Mullins (1948) for rubber-like materials, in particular for modeling tissues beyond their physiological limit (Ehret, 2011). Furthermore, softening in soft tissues is related to transient adaptation of tissue structure to certain loads, to maturation, remodeling, and fiber reorientation. Preconditioning due to cyclic loading of tissues (Buerzle et al., 2013; Hollenstein et al., 2011), as well as creep (Boyce et al., 2007) and skin relaxation experiments (Barbarino et al., 2009a) all demonstrate the necessity to include different softening mechanisms when aiming at realistic modeling of soft tissues (Buerzle and Mazza, 2013; Ehret, 2011; Ehret and Itskov, 2009; Pini et al., 2004; Sverdlik and Lanir, 2002). However, a final aspect often related to softening is residual strains accumulating not only in the pathological, but just as well in the physiological regime. Different work is presented in literature expressing tissue softening and corresponding irreversible deformations within mathematical formulations (Franceschini et al., 2006; García et al., 2013; Maher et al., 2012; Rubin and Bodner, 2002), as well as in combination with damage models (Balzani et al., 2006, 2012; Gasser, 2011; Peña et al., 2011).
To the best of the author's knowledge, few work has been presented on the basis of elastic-viscoplastic theory despite the significant freedom of capturing nearly all of the characteristic properties of soft biological tissues, see e.g. Perzyna (1971) and Rubin and Bodner (2002). In the work presented by Rubin and Bodner (2002) the elastic strain part, as well as the dissipative tissue response are governed by evolution equations. This model considers the typically observed accumulation of residual strain and softening behavior from the first loading cycle onwards. Moreover, the constitutive equations are formulated in terms of the deformed metric, recognizing the fact that elastic deformation should be associated with the current configuration during plastic flow, see Eckart (1948), Rubin and Attia (1996), Rubin (2012), and Volokh (2013). In recent years the Rubin and Bodner model was adopted for FE modeling of facial tissues (Barbarino et al., 2009b, 2011).

The objective of the present paper is the mathematical formulation of a set of generalized elastic-viscoplastic constitutive equations for the inelastic modeling of soft biological tissues within a corresponding FE formulation. In particular, constitutive equations that are based on the rate forms of the deformation measures require a strongly objective integration scheme and a proper FE formulation. For this reason, a new mixed formulation is proposed that is formulated in terms of the last converged and the current configuration. In view of those configurations the relative deformation gradient is introduced, which plays a crucial role in all subsequent derivations presented in this paper.

The outline of the paper is as follows. Section 3.2 presents a generalized framework for the elastic-viscoplastic constitutive formulation of soft biological tissues and summarizes the constitutive model equations introduced by Rubin and Bodner (2002). Section 3.3 presents the strongly objective integration scheme and in Section 3.4 the consistent spatial tangent moduli are derived. In Section 3.5 the new mixed FE formulation is introduced. Section 3.6 presents the validation for the FE formulation through standard tests and Section 3.7 describes an experimental campaign of Cutometer measurements, which is used to demonstrate a procedure to determine a set of model parameters for facial skin tissue. Finally, Section 3.8 summarizes and concludes the present study.

3.2 Constitutive model formulation

By way of background, let $X$ denote the location of a material point in the reference configuration, $x$ denote the location of the same material point in the present configuration at time $t$, and $v = \dot{x}$ denote the absolute velocity of a material point. Here and throughout the text, a superposed dot is used to denote material time differentiation, where $X$ is fixed. Furthermore, let $F = \partial x/\partial X$ be the deformation gradient, $l = \partial v/\partial x$ be the velocity gradient, $d = \left(1 + 1^T\right)/2$ be the rate of deformation tensor, and $b = FF^T$ be the total deformation tensor.

Following the work of Eckart (1948), Besseling (1968), Leonov (1976), Rubin and Bodner (2002), and Rubin and Attia (1996) it is possible to model inelastic response by introducing an elastic distortional deformation tensor associated with a dissipative response as a primary quantity governed by an evolution equation. In particular, the total
dilatation $J$, the measure of the total elastic distortional deformation $b'$, and the elastic distortional deformation associated with the dissipative component $b_{de}'$ are specified by the following evolution equations (Rubin and Bodner, 2002)

\[
\begin{align*}
\dot{j} &= J d : \mathbf{I}, \\
b' &= lb' + b' T - \frac{2}{3} (d : \mathbf{I}) b', \\
\dot{b}'_{de} &= lb'_{de} + b'_{de} T - \frac{2}{3} (d : \mathbf{I}) b'_{de} - \Gamma a_d, \quad a_d = b'_{de} - \frac{3}{b'_{de}^{-1}} : \mathbf{I}, \\
\end{align*}
\]

where the first two evolution equations in (3.1) control the elastic response, while the third evolution equation controls the inelastic response. Specifically, the term $\Gamma a_d$ in (3.1c) models the rate of inelastic deformation, with $a_d$ being the direction of inelastic flow and $\Gamma$ being the magnitude of the rate of inelasticity. In this regard it is noted that when $\Gamma a_d$ vanishes, the dissipative component responds elastically. Furthermore, the form of the symmetric tensor $a_d$ in (3.1d) is one of the simplest forms which ensures the elastic distortional deformation tensor associated with the dissipative component, $b_{de}'$, to remain a unimodular tensor and to evolve toward the value $\mathbf{I}$.

### 3.2.1 General elastic-viscoplastic constitutive equations for soft biological tissue

In this section the scalar of the rate of inelasticity as well as the hardening parameter are presented in a general form since these mechanical mechanisms are usually tissue dependent. Based on experimental observations of a specific tissue (for example the Rubin and Bodner model for facial tissue), one can propose an explicit form for the functions $\Gamma$ and $\beta$. Specifically, the nonnegative function $\Gamma$ is proposed in the following general form

\[
\Gamma = \hat{\Gamma}(\dot{\varepsilon}, \beta, \beta_{de}),
\]

where $\dot{\varepsilon}$ is the effective total distortional deformation rate and $\beta_{de}$ is the effective elastic distortion strain associated with the dissipative component. The magnitude of the rate of inelasticity $\Gamma$ serves as a continuous switch where the plastic deformation evolves continuously with a smooth transition from elastic to plastic response. In this regard, a more general form for the scalar function $\Gamma$ can be obtained by replacing $\beta_{de}$ by the two invariants of the unimodular tensor $b_{de}'$ and as well by adding the dependency over the two invariants of the unimodular tensor $b'$.

The scalars $\{\dot{\varepsilon}, \beta_{de}\}$ are, respectively, defined by

\[
\dot{\varepsilon} = \sqrt{\frac{2}{3}} \| \text{dev} (d) \|, \quad \beta_{de} = \sqrt{\frac{3}{2}} \| \text{dev} (b_{de}') \|,
\]

where $\| \cdot \|$ is the norm operator and $\text{dev} (\cdot) = \cdot - 1/3 (\cdot : \mathbf{I}) \mathbf{I}$ is the deviator operator. Furthermore, the scalar valued function $\beta$ in (3.2) is a hardening measure,

\[
\beta_{de} = \frac{3}{\beta_{de}^{-1}} : \mathbf{I},
\]
which can be associated with fluid flow through cells of the tissue for example, and is given by an evolution equation of the following general form

$$\dot{\beta} = \hat{\beta}(\dot{\varepsilon}, \Gamma, \beta, \beta_{de}).$$

(3.4)

The unspecified functional forms of $\hat{\Gamma}$ and $\hat{\beta}$ may be defined to properly represent a specific tissue response. Moreover, their unspecified form allows to derive a general numerical framework for elastic-viscoplastic models.

Now, a full set of evolution equations is formulated for $\{J, b', b'_de, \beta\}$ and appropriate initial conditions are needed in order to fully describe the initial-boundary value problem. Assuming that the material is in the virgin state at the start time $t = t_0$, then the initial conditions are specified by

$$J(t_0) = 1, \quad b'(t_0) = I, \quad b'_{de}(t_0) = I, \quad \beta(t_0) = \beta_0.$$

(3.5)

It should be noted that if equations (3.1c) and (3.4) are homogeneous of order one in time, then the model will predict rate independent elastic-plastic response.

Next, the strain energy function $W$, which accounts for the stored elastic energy per undeformed unit volume, is based on the work by Rubin and Bodner (2002) and is therefore proposed as a function of the total dilatation $J = \det(F)$, four invariants of which two are based on the total deformation tensor $\{\beta_1 = b' : I, \beta_2 = b' : b'\}$ and the other two on the dissipative component $\{\alpha_1 = b'_{de} : I, \alpha_2 = b'_{de} : b'_{de}\}$, and the stretch of the $I$'th fiber family $\lambda_I = \|m_I\|$, $I = 1, ..., N_{fib}$ (where $m_I = F \cdot M_I$ is a vector characterizing the orientation and the stretch of the $I$'th fiber family and $M_I$ is a unit vector characterizing the reference orientation of the same fiber family). The general form of the strain energy function is specified by

$$W = \hat{W}(J, \beta_1, \beta_2, \alpha_1, \alpha_2, \lambda_I).$$

(3.6)

Within the context of the purely mechanical theory that states the positiveness of the rate of material dissipation, $D = \sigma : \dot{d} - \dot{W}/J \geq 0$, the Cauchy stress tensor reads

$$\sigma = \frac{\partial W}{\partial J} I + \frac{2}{J} \frac{\partial W}{\partial \beta_1} \text{dev}(b') + \frac{4}{J} \frac{\partial W}{\partial \beta_2} \text{dev}(b'^2) + \frac{2}{J} \frac{\partial W}{\partial \alpha_1} \text{dev}(b'_{de}) + \frac{4}{J} \frac{\partial W}{\partial \alpha_2} \text{dev}(b'_{de}^2) + \sum_{I=1}^{N_{fib}} \frac{1}{J\lambda_I} \frac{\partial W}{\partial \lambda_I} m_I \otimes m_I.$$  

\[ \text{(3.7)} \]

It should be noted that a different constitutive formulation for the rate of deformation tensor $d$ would lead to a different functional form of the Cauchy stress tensor $\sigma$ as it was presented by Papes (2011).
3.2.2 Specific elastic-viscoplastic constitutive equations for soft biological tissues - Rubin and Bodner model (2002)

Rubin and Bodner (2002) developed three-dimensional constitutive equations that describe finite elastic-viscoplastic deformations which produce reasonable agreement with experimental data of facial tissue. In particular, the specific constitutive equation for the magnitude of the rate of inelasticity $\Gamma$ is given by

$$\Gamma = (\Gamma_1 + \Gamma_2 \dot{\varepsilon}) \exp \left( -\frac{1}{2} \left( \frac{\beta}{\beta_{de}} \right)^{2n} \right),$$

(3.8)

where $\{\Gamma_1, \Gamma_2, n\}$ are material parameters of which $\Gamma_1$ controls the rate dependent inelastic response, while $\Gamma_2 \dot{\varepsilon}$ controls the rate independent inelastic response, and $n$ controls the sharpness of the elastic-plastic transition. The hardening function is specified by the evolution equation

$$\dot{\beta} = \frac{r_1 r_3 + r_2 \dot{\varepsilon}}{r_3 + \dot{\varepsilon}} \Gamma \beta_{de} - r_4 \beta^{r_5},$$

(3.9)

where the constants $\{r_1, ..., r_3\}$ are material parameters. Specifically, $r_1$ controls the rate of hardening during relaxation (i.e. $\dot{\varepsilon} = 0$), $r_2$ controls the rate of hardening during loading (i.e. $\dot{\varepsilon} > 0$), and $r_3$ controls the value of strain rate associated with the transition between these two responses. Note that the first part on the right hand side of (3.9) causes $\beta$ to grow, while the second part is responsible for material recovery. The parameters $\{r_4, r_5\}$ control the rate and shape of recovery of hardening, respectively. Furthermore, it is worth noting that the rate of inelastic deformation yields a rate independent response, when the following conditions are fulfilled

$$\Gamma_2 \dot{\varepsilon} \gg \Gamma_1, \quad r_2 \dot{\varepsilon} \gg r_1 r_3, \quad \dot{\varepsilon} \gg r_3, \quad r_4 = 0.$$

(3.10)

The strain energy function proposed by Rubin and Bodner (2002) models tissue as a composite material composed of an elastic material, elastic fibers, and a dissipative elastic-viscoplastic material. The specific form of the proposed strain energy function $W$ is given by

$$W = \frac{\mu_0}{2q} (e^{ag} - 1),$$

(3.11)

where $\mu_0$ and $q$ are material parameters, and the function $g = \tilde{g} (J, \beta_1, \lambda_I, \alpha_1)$ was decoupled into four parts such that

$$\tilde{g} (J, \beta_1, \lambda_I, \alpha_1) = \tilde{g}_1 (J) + \tilde{g}_2 (\beta_1) + \tilde{g}_3 (\lambda_I) + \tilde{g}_4 (\alpha_1),$$

$$\tilde{g}_1 (J) = 2m_1 (J - 1 - \ln (J)), \quad \tilde{g}_2 (\beta_1) = m_2 (\beta_1 - 3),$$

(3.12)

$$\tilde{g}_3 (\lambda_I) = \frac{m_3}{m_4} \sum_{I=1}^{N_{fib.}} (\lambda_I - 1)^{2m_4}, \quad \tilde{g}_4 (\alpha_1) = m_5 (\alpha_1 - 3),$$

where $\{m_1, ..., m_5\}$ are additional material parameters. The individual parts of $g$ include the function $\tilde{g}_1 (J)$ accounting for total volume dilatation, $\tilde{g}_2 (\beta_1)$ accounting for the distortional deformation of the isotropic matrix, $\tilde{g}_3 (\lambda_I)$ accounting for the stretch of the $I$'th
3.3 Stress update and internal variable integration scheme

fiber family, and \( \hat{g}_4(\alpha_1) \) accounting for the elastic distortional deformation of the dissipative component of the tissue. In (3.12d), \( \langle \bullet \rangle = (| \bullet | + \circ) / 2 \) are the McAuley brackets that eliminate the response of the \( I \)’th fiber family if under compression. Now using (3.7), it can be shown that the Cauchy stress tensor is given by

\[
\sigma = \frac{\mu}{J} \left[ m_1 (J - 1) I + m_2 \text{dev} \left( \mathbf{b}' \right) + m_3 \sum_{I=1}^{N_{\text{fib}}} \frac{\langle \lambda_I - 1 \rangle^{2m_4-1}}{\lambda_I} \mathbf{m}_I \otimes \mathbf{m}_I + m_5 \text{dev} \left( \mathbf{b}'_{\text{de}} \right) \right],
\]

where \( \mu \) is the nonlinear shear modulus and is defined by

\[
\mu = \mu_0 e^{qg}.
\]

3.3 Stress update and internal variable integration scheme

Typically, the evolution equations for the elastic-viscoplastic response of metals tend to be stiff differential equations that require special methods of integration to obtain a stable response. Integration algorithms for evolution equations of the elastic measures of the deformation have been discussed in Rubin and Attia (1996). More recently, Rubin and Papes (2011) developed a strongly objective integration algorithm for viscoplastic models governed by evolution equations of the elastic measure of the deformation. In this section the strongly objective integration algorithm presented by Rubin and Papes (2011) is applied for integrating (3.1) and (3.4).

In particular, considering a time increment which begins at time \( t_n \) and ends at \( t_{n+1} \) with time interval \( \Delta t = t_{n+1} - t_n \) and assuming that the solutions of \( \{ J(t_n), \mathbf{b}'(t_n), \mathbf{b}'_{\text{de}}(t_n), \beta(t_n) \} \) at time \( t_n \) are known, the numerical algorithm must provide \( \{ J(t_{n+1}), \mathbf{b}'(t_{n+1}), \mathbf{b}'_{\text{de}}(t_{n+1}), \beta(t_{n+1}) \} \) at time \( t_{n+1} \). The strongly objective integration algorithm for the evolution equations of the measures of deformation \( \{ J, \mathbf{b}', \mathbf{b}'_{\text{de}}, \beta \} \) ensures that the values of the tensors \( \{ \mathbf{b}'(t_{n+1}), \mathbf{b}'_{\text{de}}(t_{n+1}) \} \) at time increment \( t_{n+1} \) have the same invariance properties under superposed rigid body motion (SRBM) as the exact tensors \( \{ \mathbf{b}', \mathbf{b}'_{\text{de}} \} \), when \( \{ J(t_{n+1}), \beta(t_{n+1}) \} \) are unaffected by the SRBM. To this end, use is made of the work by Rubin and Papes (2011), Simo (1992), and Simo and Hughes (1998) to develop a relative deformation gradient. Specifically, the relative deformation gradient \( \mathbf{F}_r \), its determinant \( J_r \), and the unimodular part of the relative deformation gradient \( \mathbf{F}'_r \) are defined by

\[
\mathbf{F}_r = \frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}(t_n)}, \quad \dot{\mathbf{F}}_r = \mathbf{I}\mathbf{F}_r, \quad \mathbf{F}_r(t_n) = \mathbf{I},
\]

\[
J_r = \det(\mathbf{F}_r), \quad \dot{J}_r = J_r : \mathbf{I}, \quad J_r(t_n) = 1,
\]

\[
\mathbf{F}'_r = J_r^{-1/2}\mathbf{F}_r, \quad \dot{\mathbf{F}}'_r = \text{dev} \left( \mathbf{I} \right) \mathbf{F}'_r, \quad \mathbf{F}'_r(t_n) = \mathbf{I}.
\]
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Then, the exact solutions of (3.1a, b) and the approximated solution of (3.1c) are given by

\[
\begin{align*}
J(t_{n+1}) &= J_r(t_{n+1}) J(t_n) , \\
b'(t_{n+1}) &= F'_r(t_{n+1}) b'(t_n) F'^T_r(t_{n+1}) , \\
b^{*\text{de}}(t_{n+1}) &= b^{*\text{de}}(t_{n+1}) - \Delta t \Gamma(t_{n+1}) a_d(t_{n+1}) ,
\end{align*}
\]

(3.16)

where \( b^{*\text{de}}(t_{n+1}) \) is the elastic trial solution of the elastic distortional deformation of the dissipative component and is defined by

\[
b^{*\text{de}}(t_{n+1}) = F'_r(t_{n+1}) b'_d(t_n) F'^T_r(t_{n+1}) .
\]

(3.17)

Bearing in mind that the deviatoric part of the tensor \( a_d \) is identical to the deviatoric part of \( b'_d \) (according to (3.1d)) and using (3.3b), it can be shown that

\[
\begin{align*}
de(\hat{b}'_d(t_{n+1})) &= \frac{1}{1 + \Delta t \Gamma(t_{n+1})} \left[ \frac{\beta^{*\text{de}}_d(t_{n+1})}{1 + \Delta t \Gamma(t_{n+1})} \right] , \\
\beta_{de}(t_{n+1}) &= \beta^{*\text{de}}_d(t_{n+1}) = \sqrt{\frac{3}{2} \| \text{dev}(b^{*\text{de}}_d(t_{n+1})) \|} .
\end{align*}
\]

(3.18)

In order to evaluate the value of the total rate of distortional deformation at time step \( t_{n+1} \), Papes (2011) defined a strongly objective estimate for the rate of deformation \( d \). In the present paper, we propose another strongly objective estimate for the rate of deformation \( d \), which is motivated by the time derivative of the relative deformation tensor \( C_r = F'^T_r F_r \) and is defined by

\[
d(t_{n+1}) = \frac{1}{2 \Delta t} \left( I - b^{-1}_d(t_{n+1}) \right) , \quad b_r(t_{n+1}) = F_r(t_{n+1}) F'^T_r(t_{n+1}) .
\]

(3.19)

Furthermore, the estimation for the hardening variable \( \beta \) at time step \( t_{n+1} \) can be obtained by using the backward Euler differentiation such that

\[
\beta(t_{n+1}) = \beta(t_n) + \Delta t \hat{\beta} (\hat{\varepsilon}(t_{n+1})) , \quad \Gamma(t_{n+1}) , \beta(t_{n+1}) , \beta_{de}(t_{n+1}) .
\]

(3.20)

For general functional forms of \( \{ \Gamma = \hat{\Gamma} (\hat{\varepsilon}, \beta, \beta_{de}) , \hat{\beta} = \hat{\beta} (\hat{\varepsilon}, \Gamma, \beta, \beta_{de}) \} \) it is necessary to use iterative methods to find the specific values of \( \Gamma \) and the isotropic hardening variable \( \beta \) at the time step \( t_{n+1} \). Specifically, the vector of the unknowns \( z = \{ \Gamma(t_{n+1}) , \beta(t_{n+1}) \}^T \) can be obtained by solving the following set of nonlinear algebraic equations

\[
\begin{align*}
\phi_1 &= \Gamma(t_{n+1}) - \hat{\Gamma}(\hat{\varepsilon}(t_{n+1}) , \beta(t_{n+1}) , \beta_{de}(t_{n+1})) = \frac{\beta^{*\text{de}}_d(t_{n+1})}{1 + \Delta t \Gamma(t_{n+1})} = 0 , \\
\phi_2 &= \beta(t_{n+1}) - \beta(t_n) - \Delta t \hat{\beta} (\hat{\varepsilon}(t_{n+1}) , \Gamma(t_{n+1}) , \beta(t_{n+1}) , \beta_{de}(t_{n+1})) = \frac{\beta^{*\text{de}}_d(t_{n+1})}{1 + \Delta t \Gamma(t_{n+1})} = 0 .
\end{align*}
\]

(3.21)

This system is iteratively solved by using the Newton-Raphson method with the following iterative scheme

\[
\frac{\partial \phi}{\partial z} |_{z=z^i} \Delta z^i + \phi|_{z=z^i} = 0 , \quad z^{i+1} = z^i + \Delta z^i .
\]

(3.22)
Finally, the spherical part of the elastic distortional deformation associated with the dissipative component, $b_{de}$, is obtained from the requirement that $b_{de}$ is a unimodular tensor, which leads to the following cubic equation

$$\left(\frac{\alpha_1}{3}\right)^3 - \frac{1}{2}\left(\text{dev}(b_{de}^\prime) : \text{dev}(b_{de}^\prime)\right)\left(\frac{\alpha_1}{3}\right) - \left(1 - \text{det}(\text{dev}(b_{de}^\prime))\right) = 0. \tag{3.23}$$

A discussion on the solution procedure of (3.23) can be found in Rubin and Attia (1996).

### 3.4 Spatial tangent moduli

The consistent spatial tangent moduli, which determine the sensitivity of the developed algorithmic expressions for the stresses in terms of the change of the relative deformation gradient, play a crucial role in the FE calculations since they serve as iteration operators when the Newton-Raphson method is applied. Specifically, the spatial tangent moduli read

$$a(t_{n+1}) = \frac{1}{J(t_{n+1})} \frac{\partial \tau(t_{n+1})}{\partial F_r} F^T_r(t_{n+1}) - \sigma(t_{n+1}) \oplus I, \tag{3.24}$$

where $\tau(t_{n+1}) = J(t_{n+1}) \sigma(t_{n+1})$ is the Kirchhoff stress tensor and the tensor operation $\oplus$ is defined by $(A \oplus B)_{ijkl} = A_{ij}B_{jk}$. According to (3.7), the Cauchy stress tensor and, therefore, the Kirchhoff stress tensor are functions of the invariants of the deformation and the deviatoric part of the unimodular tensors $\{b', b^2, b_{de}^+, b_{de}^-\}$. However, the Cauchy stress tensor for the Rubin and Bodner model (3.13) is a function of $\{J, \beta_1, \alpha_1, \text{dev}(b'), \text{dev}(b_{de}^\prime)\}$, therefore, the spatial tangent moduli are developed for the Rubin and Bodner model in this section, while the spatial tangent moduli are recorded in Appendix B for the generalized model (3.6). Using (3.15d,g) and (3.16a,b), it can be shown that the derivatives of the invariants $\{J(t_{n+1}) = J_r(t_{n+1}) J(t_n), \beta_1(t_{n+1}) = b'(t_{n+1}) : I, \lambda_1(t_{n+1}) = \|m_I(t_{n+1})\|, m_I(t_{n+1}) = F_r(t_{n+1}) F(t_n) \cdot m_I\}$ and the deviatoric part of the total distortional deformation $\text{dev}(b')$ with respect to the relative deformation gradient are given by

$$\frac{\partial J(t_{n+1})}{\partial F_r} F^T_r(t_{n+1}) = J(t_{n+1}) I,$$

$$\frac{\partial \beta_1(t_{n+1})}{\partial F_r} F^T_r(t_{n+1}) = 2\text{dev}(b'(t_{n+1})),$$

$$\frac{\partial \lambda_1(t_{n+1})}{\partial F_r} F^T_r(t_{n+1}) = \frac{1}{\lambda_1(t_{n+1})} m_I(t_{n+1}) \otimes m_I(t_{n+1}), \tag{3.25}$$

$$\frac{\partial \text{dev}(b'(t_{n+1}))}{\partial F_r} F^T_r(t_{n+1}) = b'(t_{n+1}) \oplus I + I \otimes b'(t_{n+1}) - \frac{2}{3} b'(t_{n+1}) \otimes I$$

$$- \frac{2}{3} I \otimes b'(t_{n+1}) + \frac{2}{9} \beta_1(t_{n+1}) I \otimes I,$$

where the special tensor operation $\oplus$ is defined by $(A \oplus B)_{ijkl} = A_{ik}B_{jl}$. Also using (3.23), the derivative of the trace of the elastic distortional deformation tensor associated with the dissipative part $\alpha_1$ with respect to the relative deformation gradient is given by
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\[ \frac{\partial \alpha_1 (t_{n+1})}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}) = \boldsymbol{\alpha}_1 (t_{n+1}), \quad \alpha_1 (t_{n+1}) = \overline{\alpha}_1 (t_{n+1}) : \frac{\partial \text{dev} (\mathbf{b}'_{de} (t_{n+1}))}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}), \]

\[ \overline{\alpha}_1 (t_{n+1}) = \frac{9}{\alpha_1^2 (t_{n+1}) - \beta_{de}^2 (t_{n+1})} \left[ \frac{\alpha_1 (t_{n+1})}{3} \text{dev} (\mathbf{b}'_{de} (t_{n+1})) - \text{cof} \left( \text{dev} (\mathbf{b}'_{de} (t_{n+1})) \right) \right]. \]

(3.26)

Next, it can be shown that the derivative of \( \text{dev} (\mathbf{b}'_{de} (t_{n+1})) \) with respect to the relative deformation gradient is given by

\[ \frac{\partial \text{dev} (\mathbf{b}'_{de} (t_{n+1}))}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}) = \frac{1}{1 + \Delta t \Gamma (t_{n+1})} \left[ \frac{\partial \text{dev} (\mathbf{b}'_{de} (t_{n+1}))}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}) \right. \]

\[ - \Delta t \text{dev} (\mathbf{b}'_{de} (t_{n+1})) \otimes \Gamma (t_{n+1}) \] \]

(3.27)

where the expression for the derivative of \( \text{dev} (\mathbf{b}'_{de} (t_{n+1})) \) is defined in a similar manner to (3.25d) by replacing \( \mathbf{b}' (t_{n+1}) \) with \( \mathbf{b}'_{de} (t_{n+1}) \). Now, taking the derivative of the two implicit equations for \( \{ \Gamma, \beta \} \) (3.21) and using equations (3.3a), (3.18c), and (3.19a), the tensor \( \Gamma (t_{n+1}) \) in (3.27) reads

\[ \Gamma (t_{n+1}) = \frac{2}{d_1 (t_{n+1})} \mathbf{b}^{-1} (t_{n+1}) \text{dev} (\mathbf{d} (t_{n+1})) \]

\[ + \frac{d_2 (t_{n+1})}{d_0 (t_{n+1})} \left[ \frac{3}{\beta_{de}^s (t_{n+1})} \text{dev} (\mathbf{b}'_{de} (t_{n+1})) \mathbf{b}^s_{de} (t_{n+1}) - \frac{2}{3} \beta_{de}^s (t_{n+1}) \mathbf{I} \right], \]

(3.28)

where the coefficients \( \{ d_0 (t_{n+1}) , d_1 (t_{n+1}) , d_2 (t_{n+1}) \} \) are given in Appendix C. Finally, multiplying the stress expression (3.13) by \( J \), substituting the result into (3.24) and using (3.25) and (3.26), the spatial tangent moduli read

\[ \mathbf{a} (t_{n+1}) = m_1 \mu (t_{n+1}) \mathbf{I} \otimes \mathbf{I} + m_2 \frac{\mu (t_{n+1})}{J (t_{n+1})} \frac{\partial \text{dev} (\mathbf{b}' (t_{n+1}))}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}) \]

\[ + \frac{\mu (t_{n+1})}{2J (t_{n+1})} \sum_{I=1}^{N_{fib}} \frac{1}{\lambda_f (t_{n+1})} \frac{d}{d \lambda_f} \left( \frac{d g_3 / d \lambda_f}{\lambda_f (t_{n+1})} \right) \mathbf{m}_f (t_{n+1}) \otimes \mathbf{m}_f (t_{n+1}) \]

\[ + \frac{\mu (t_{n+1})}{2J (t_{n+1})} \sum_{I=1}^{N_{fib}} \frac{d g_3 / d \lambda_f}{\lambda_f (t_{n+1})} \left( \mathbf{m}_f (t_{n+1}) \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{m}_f (t_{n+1}) \right) \]

\[ + m_5 \frac{\mu (t_{n+1})}{J (t_{n+1})} \frac{\partial \text{dev} (\mathbf{b}_{de} (t_{n+1}))}{\partial \mathbf{F}_r} \mathbf{F}_r^T (t_{n+1}) \]

\[ + \mathbf{\sigma} (t_{n+1}) \otimes \mathbf{g} (t_{n+1}) - \mathbf{\sigma} (t_{n+1}) \otimes \mathbf{I}, \]

(3.29)

where \( \mathbf{m}_f (t_{n+1}) \) is the current structural tensor of the \( I \)th fiber family defined by

\[ \mathbf{m}_f (t_{n+1}) = \mathbf{m}_f (t_{n+1}) \otimes \mathbf{m}_f (t_{n+1}), \]

(3.30)
and \( \{ \mu (t_{n+1}) , g (t_{n+1}) \} \) are, respectively, defined by

\[
\mu (t_{n+1}) = \mu_0 e^{\gamma g(t_{n+1})}, \quad g (t_{n+1}) = q \frac{\partial g (t_{n+1})}{\partial F_r} (t_{n+1}) = 2qm_1 (J (t_{n+1}) - 1) + 2qm_2 \text{dev} \left( \mathbf{b}' (t_{n+1}) \right)
\]

\[+ 2qm_3 \sum_{I=1}^{N_{\text{m}}} \frac{\lambda_I (t_{n+1}) - 1}{\lambda_I (t_{n+1})^2} \mathbf{m}_I (t_{n+1}) + qm_5 \alpha_1. \tag{3.31} \]

### 3.5 Finite element formulation

A new mixed FE formulation, particularly suitable for viscoplastic material models involving equations of the measures of deformation, is developed here for the numerical study of soft tissues. It turned out that the reference configuration of the body in the present development became irrelevant, and all calculations are carried out on the deformed configurations at time \( t_n \) and \( t_{n+1} \). Generally speaking, the mixed formulation for nearly incompressible materials can be derived by using the Hu-Washizu functional, where the independent variables are the deformation gradient, an assumed dilatation measure, and an assumed hydrostatic pressure. In particular, the Hu-Washizu functional can be written as

\[
\Pi (\tilde{F}, J_r, \tilde{p}) = \int_{\Omega_n} \left[ \frac{1}{J (t_n)} W (\tilde{F}) + \tilde{p} (J_r - J_r) \right] d\Omega_n - \Pi^{\text{ext}}, \tag{3.32} \]

where \( \Omega_n \) is the element domain at time \( t_n \), \( \Pi^{\text{ext}} \) is the potential energy due to external forces, \( J_r \) is a scalar related to the relative volumetric dilatation, \( \tilde{p} \) is a scalar related to hydrostatic pressure (spherical part of stress), and \( \tilde{F} \) is the modified deformation gradient that can be multiplicatively decomposed into a modified relative deformation gradient and a modified deformation gradient at time \( t_n \) such that

\[
\tilde{F} = \tilde{F}_r \tilde{F} (t_n), \quad \tilde{F}_r = \left( \frac{J_r}{J_r} \right)^{1/3} F_r, \quad \tilde{F} (t_n) = \left( \frac{J (t_n)}{J (t_n)} \right)^{1/3} F (t_n). \tag{3.33} \]

The variation of the functional (3.32) with respect to the different fields yields the following three equations

\[
\delta F, \Pi = \int_{\Omega_n} \tilde{\sigma} : \delta \mathbf{h} d\Omega - \delta \Pi^{\text{ext}}, \quad \tilde{\sigma} = \frac{J}{J} \text{dev} (\tilde{\sigma}) + \tilde{p} I, \quad \delta \mathbf{h} = \frac{\partial \delta \mathbf{u}}{\partial \mathbf{x}},
\]

\[
\delta p, \Pi = \int_{\Omega_n} (J_r - J_r) \delta \tilde{p} d\Omega_n,
\]

\[
\delta J_r, \Pi = \int_{\Omega_n} \left( \frac{J (t_n)}{J (t_n)} \tilde{p} - \tilde{p} \right) \delta J_r d\Omega_n, \quad \tilde{p} = \frac{1}{3} \tilde{\sigma} : I, \tag{3.34} \]

where \( \Omega \) is the deformed element domain at time \( t_{n+1} \), \( \tilde{\sigma} \) is evaluated according to (3.7) (or according to (3.13) for the Rubin and Bodner model) where \( \{ \tilde{F}_r, \tilde{F} (t_n) \} \) are used instead.
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of \{F_r, F(t_n)\}, and \(\delta u\) is the virtual displacement field. Now, assuming that the variables \{\(J_r, \bar{p}\)\} are constants at the element domain, the variational equations (3.34b,c) yield the following explicit equations for the determination of the fields \{\(J_r, \bar{p}\)\}, respectively,

\[
J_r = \frac{1}{\Omega_n} \int_{\Omega_n} J_r d\Omega_n, \quad \bar{p} = \frac{1}{\Omega_n} \int_{\Omega_n} \frac{\bar{J}(t_n)}{\bar{J}(t_n)} \bar{p} d\Omega_n.
\]

(3.35)

According to (3.35), the variable \(J_r\) can be interpreted as the ratio between the element volume at time \(t_{n+1}\) and \(t_n\), while the variable \(\bar{p}\) is the average hydrostatic pressure within the element domain. Also, the linearization of the variation of the functional (3.32) is given by

\[
\Delta \delta \Pi = \int_{\Omega} \left[ \delta h : \left( \tilde{a}_{uu} : \Delta h + \tilde{a}_{uJ_r} \frac{\Delta J_r}{J_r} + I \Delta \bar{p} \right) + \frac{\delta J_r}{J_r} \left( \tilde{a}_{J_r,u} : \Delta h + \tilde{a}_{J_r,J_r} \frac{\Delta J_r}{J_r} - \frac{J_r}{J_r} \Delta \bar{p} \right) + \delta \bar{p} \left( I : \Delta h - \frac{J_r}{J_r} \frac{\Delta J_r}{J_r} \right) \right] d\Omega,
\]

(3.36)

where the tensor \(\Delta h\) is defined in a similar manner to \(\delta h\) in (3.34c) by replacing the virtual displacement field \(\delta u\) with the incremental displacement field \(\Delta u\). The fourth order tensor \(\tilde{a}_{uu}\), the second order tensors \(\{\tilde{a}_{uJ_r}, \tilde{a}_{J_r,u}\}\), and the scalar \(\tilde{a}_{J_r,J_r}\) are defined by

\[
\tilde{a}_{uu} = \left( I - \frac{1}{3} I \otimes I \right) : \frac{J}{J_r} \tilde{a} : \left( I - \frac{1}{3} I \otimes I \right) - \frac{1}{3} \left( \text{dev} (\tilde{\sigma}) \otimes I + I \otimes \text{dev} (\tilde{\sigma}) \right),
\]

\[
\tilde{a}_{uJ_r} = \frac{1}{3} \left( I - \frac{1}{3} I \otimes I \right) : \frac{J}{J_r} \tilde{a} : I + \frac{1}{3} \text{dev} (\tilde{\sigma}),
\]

\[
\tilde{a}_{J_r,u} = \frac{1}{3} I : \frac{J}{J_r} \tilde{a} : \left( I - \frac{1}{3} I \otimes I \right) + \frac{1}{3} \text{dev} (\tilde{\sigma}),
\]

\[
\tilde{a}_{J_r,J_r} = \frac{1}{9} I : \frac{J}{J_r} \tilde{a} : I - \frac{2 J}{3 J_r} \tilde{\sigma},
\]

(3.37)

where the fourth order tensor \(\tilde{a}\) in (3.37) is evaluated according to (3.50) in Appendix B for the generalized model or according to (3.29) for the Rubin and Bodner model, where \(\{F_r, F(t_n)\}\) are replaced by \(\{\bar{F}_r, \bar{F}(t_n)\}\).

The ansatz spaces of the different fields have to be balanced in order to obtain a robust and stable discretization which is based on the Hu-Washizu functional (3.32). Therefore, a trilinear interpolation will be applied for the displacement field and a constant
interpolation for the assumed dilatation and pressure terms. Specifically, the deformed configurations at time $t_n$ and $t_{n+1}$ are interpolated, respectively, as follows

$$x(t_n) = \sum_{I=1}^{N_{en}} N^I \hat{x}_I(t_n), \quad x(t_{n+1}) = \sum_{I=1}^{N_{en}} N^I \hat{x}_I(t_{n+1}),$$  

(3.38)

where $N^I$ represents the ansatz functions, $N_{en}$ is the number of nodes per element, \{\hat{x}_I(t_n), \hat{x}_I(t_{n+1})\} are the nodal positions of the configurations at time $t_n$ and $t_{n+1}$. Since the incremental displacements are given by $\Delta u = x(t_{n+1}) - x(t_n)$, a trilinear interpolation is also used for the incremental displacement field such that

$$\Delta u = \sum_{I=1}^{N_{en}} N^I \Delta \hat{u}_I,$$  

(3.39)

and, therefore, the relative deformation gradient is obtained by

$$F_r = \left( I - \sum_{I=1}^{N_{en}} \Delta \hat{u}_I \otimes \text{grad} (N^I) \right)^{-1}, \quad \text{grad} (N^I) = \frac{\partial N^I}{\partial \mathbf{x}}.$$  

(3.40)

For developing the element residua and element tangent stiffness matrix, the matrix notation is used. It is worth noting that for the matrix notation, vectors and second order tensors become vectors (indicated by underline) and fourth order tensors become second order matrices (indicated by double underline). Thus, the tensors $\delta \mathbf{h}$ and $\Delta \mathbf{h}$ can, respectively, be written as follows

$$\delta \mathbf{h} = \mathbb{B} \delta \mathbf{d}_u, \quad \Delta \mathbf{h} = \mathbb{B} \Delta \mathbf{d}_u,$$  

(3.41)

where $\delta \mathbf{d}_u$ and $\Delta \mathbf{d}_u$ are the virtual and incremental nodal displacement vectors, respectively, and $\mathbb{B}$ is the standard B-matrix for finite deformation, which consists of the derivatives of the ansatz functions with respect to the deformed configuration at time $t_{n+1}$. Now, the residual forces defined as the difference between the external nodal forces (due to external forces) and the internal nodal forces (due to the constitutive equations), are obtained by substituting (3.41) into (3.33a) such that

$$\hat{\mathbf{r}} = \hat{\mathbf{f}}^{\text{ext.}} - \hat{\mathbf{f}}^{\text{int.}}, \quad \hat{\mathbf{f}}^{\text{int.}} = \int_\Omega \mathbb{B}^T \tilde{\sigma} \, d\Omega,$$  

(3.42)

and the stiffness matrix is obtained by substituting (3.41) into (3.35), using the fact that the assumed dilatation and pressure fields are constant within the element region and writing these results in a matrix form as follows

$$\Delta \delta \Pi = \begin{bmatrix} \delta \mathbf{d}_u & \delta \mathbf{J}_u & \delta \mathbf{J}_r & \delta \mathbf{p} \end{bmatrix}^T \begin{bmatrix} K_{uu} & K_{ur} & K_{up} & \Delta \mathbf{d}_u \\ K_{ur} & K_{rr} & -K_{rp} & \Delta \mathbf{J}_r \\ K_{pu} & -K_{pr} & 0 & \Delta \mathbf{J}_r \\ \Delta \mathbf{J}_r & \Delta \mathbf{J}_r & 0 & \Delta \mathbf{p} \end{bmatrix} \begin{bmatrix} \delta \mathbf{d}_u \\ \delta \mathbf{J}_u \\ \delta \mathbf{J}_r \\ \delta \mathbf{p} \end{bmatrix}.$$  

(3.43)
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The submatrix $\mathbf{K}_{uu}$, the vectors $\{\mathbf{K}_{u\mathcal{J}r}, \mathbf{K}_{u\mathcal{P}u}, \mathbf{K}_{\mathcal{J}u\mathcal{J}r}, \mathbf{K}_{\mathcal{P}u\mathcal{P}r}\}$, and the scalars $\{K_{\mathcal{J}r\mathcal{J}r}, K_{\mathcal{J}r\mathcal{P}}, K_{\mathcal{P}r\mathcal{P}r}\}$ are given by

\[
\begin{align*}
\mathbf{K}_{uu} &= \int_{\Omega} \mathbf{B}^T \tilde{\mathbf{a}}_{uu} \mathbf{B} \, d\Omega, \\
\mathbf{K}_{u\mathcal{J}r} &= \int_{\Omega} \mathbf{B}^T \tilde{\mathbf{a}}_{u\mathcal{J}r} \, d\Omega, \\
\mathbf{K}_{u\mathcal{P}u} &= \mathbf{K}_{\mathcal{P}u\mathcal{P}u} = \int_{\Omega} \mathbf{B}^T \mathbf{I} \, d\Omega, \\
K_{\mathcal{J}r\mathcal{J}r} &= \int_{\Omega} \mathbf{a}_{\mathcal{J}r\mathcal{J}r} \, d\Omega, \\
K_{\mathcal{J}r\mathcal{P}} &= K_{\mathcal{P}r\mathcal{J}r} = \int_{\Omega} \mathbf{J} \, d\Omega.
\end{align*}
\]  

(3.44)

Due to the fact that the quantities $\{\mathcal{J}_r, \mathcal{P}\}$ are not assembled over all elements but are determined at the element level, it is advantageous to perform a static condensation and eliminate the quantities $\{\mathcal{J}_r, \mathcal{P}\}$. Specifically, the tangent stiffness matrix then reads

\[
\mathbf{K} = \mathbf{K}_{uu} + \frac{1}{K_{\mathcal{P}r\mathcal{J}r}} \mathbf{K}_{\mathcal{P}u\mathcal{P}u} \mathbf{K}_{u\mathcal{J}r} + \frac{1}{K_{\mathcal{J}r\mathcal{P}}} \mathbf{K}_{\mathcal{J}u\mathcal{J}r} \mathbf{K}_{u\mathcal{P}u} + \frac{K_{\mathcal{J}r\mathcal{J}r}}{K_{\mathcal{P}r\mathcal{J}r} K_{\mathcal{P}r\mathcal{P}r}} \mathbf{K}_{\mathcal{P}u\mathcal{P}u} \mathbf{K}_{u\mathcal{P}u}.
\]  

(3.45)

3.6 Numerical verifications

The newly developed mixed FE formulation and its implementation in the commercial FE software ABAQUS (2009) are verified by considering a number of standard numerical tests including the Patch test, rate of convergence test, and objectivity test. For these simulations, a set of material parameters determined by Rubin and Bodner (2002) is used. In particular, these specific parameters are based on experimental work by Har-Shai et al. (1996), where uniaxial tension tests on strips of excised human skin were conducted allowing to determine the stress-strain relationship under cyclic loading at varying strain rates.

3.6.1 Patch test

The Patch test is considered as a fundamental test in FE technology and has been used for over five decades as a condition for convergence and as a verification tool for FE algorithms (see for example Taylor et al. (1986), Babuška and Narasimhan (1997), and Zienkiewicz and Taylor (1997)). Different variants of the Patch test have been suggested by different research works, and the force version of the Patch test has been applied in this study. To this end, a cube with edge length $a = 20.0 \text{ mm}$ and meshed by seven distorted elements is considered, see Figure 3.1a. The reference locations $\mathbf{X}_I$ ($I = 1, \ldots, 16$) of the nodes of the seven elements in Figure 3.1a are specified by
3.6. Numerical verifications

\[
\begin{align*}
X_1 &= 0, \quad X_2 = a e_1, \quad X_3 = a e_2, \quad X_4 = a e_1 + a e_2, \\
X_5 &= a e_3, \quad X_6 = a e_1 + a e_3, \quad X_7 = a e_2 + a e_3, \quad X_8 = a e_1 + a e_2 + a e_3, \\
X_9 &= 0.35 a e_1 + 0.30 a e_2 + 0.20 a e_3, \quad X_{10} = 0.80 a e_1 + 0.35 a e_2 + 0.45 a e_3, \\
X_{11} &= 0.30 a e_1 + 0.75 a e_2 + 0.15 a e_3, \quad X_{12} = 0.75 a e_1 + 0.70 a e_2 + 0.20 a e_3, \\
X_{13} &= 0.20 a e_1 + 0.25 a e_2 + 0.65 a e_3, \quad X_{14} = 0.75 a e_1 + 0.30 a e_2 + 0.70 a e_3, \\
X_{15} &= 0.25 a e_1 + 0.65 a e_2 + 0.75 a e_3, \quad X_{16} = 0.65 a e_1 + 0.75 a e_2 + 0.80 a e_3.
\end{align*}
\]

Figure 3.1: Patch test for numerical verification of the constitutive equations. (a) Geometric representation of a cube discretized by 7 initially distorted hexahedral elements. (b) Results of the Patch test. Comparison between theoretical and numerical uniaxial nominal stress \( P_{11} \). Fair agreement between experimental data and the model prediction is observed for the material parameters presented by Rubin and Bodner (2002).

Also, the cube was subjected to axial stretch in the \( e_1 \) direction that causes a uniaxial stress in the \( e_1 \) direction. In the present example, three subsequent loading and unloading cycles of axial stretch with different rates were prescribed similar to the uniaxial tests performed by Har-Shai et al. (1996).

For calculating the theoretical uniaxial stress, the relative deformation gradient \( \mathbf{F}_r \) that is evaluated at the end of a typical time step is given by

\[
\mathbf{F}_r(t_{n+1}) = \frac{\lambda_1(t_{n+1})}{\lambda_1(t_n)} \mathbf{e}_1 \otimes \mathbf{e}_1 + \frac{\lambda_2(t_{n+1})}{\lambda_2(t_n)} \mathbf{e}_2 \otimes \mathbf{e}_2 + \frac{\lambda_3(t_{n+1})}{\lambda_3(t_n)} \mathbf{e}_3 \otimes \mathbf{e}_3,
\]

where \( \{\lambda_i(t_n), \lambda_i(t_{n+1})\} \) are the stretches at time step \( t_n \) and \( t_{n+1} \), respectively.
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The lateral stretches \( \{ \lambda_2(t_{n+1}), \lambda_3(t_{n+1}) \} \) are determined by iteration to satisfy the boundary condition of vanishing lateral stress

\[
\sigma : (e_2 \otimes e_2) = 0, \quad \sigma : (e_3 \otimes e_3) = 0,
\]

while the resulting axial stress is determined by equation (3.13).

The numerical uniaxial Piola-Kirchhoff stress obtained by the FE solution and its theoretical counterpart are plotted in Figure 3.1b. It can be seen that both solutions coincide, which indicates that the derived FE formulation satisfies the Patch test. Furthermore, a comparison with the experimental data used to identify the material parameters presented by Rubin and Bodner (2002) is shown in Figure 3.1b. The generally observed agreement between experimental data and numerical prediction is a demonstration of the capability of this specific elastic-viscoplastic model to provide a fairly accurate representation of facial soft tissue response.

### 3.6.2 Rate of convergence

The objective of the rate of convergence test is to verify that the derived spatial tangent moduli (3.29) ensure quadratic convergence at each equilibrium iteration. To this end, an initially distorted element is subjected to a nodal force while the remaining nodes are fixed. Figure 3.2 provides a geometric representation of the cube at both the reference (dashed lines) and deformed (solid lines) configuration, as well as the specific nodal position of the mesh points (with \( a = 1.0 \text{mm} \)). In the simulation presented here, Node #8 is subjected to \( f_8 = f_8(e_1 + e_2 - e_3) \), with \( f_8 = 0.05 \text{N} \).

The rate of convergence is expressed in terms of the nodal residual force and is calculated based on a fixed incremental time step of \( \Delta t = 0.25 \text{s} \) with a total simulation time of \( t = 1.0 \text{s} \). The residual force after each iteration for all 4 increments is given in Table 3.1, which demonstrates quadratic convergence through the apparent decay of the order of magnitude of the residual force.

<table>
<thead>
<tr>
<th>Step</th>
<th>Iteration</th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
<th>Step 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.10000000E+01</td>
<td>0.12733532E-01</td>
<td>0.40889563E-01</td>
<td>0.40196800E-01</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0.87260426E-01</td>
<td>0.20965581E-03</td>
<td>0.17495670E-02</td>
<td>0.26096952E-02</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>0.49335789E-03</td>
<td>0.11649721E-06</td>
<td>0.94714269E-05</td>
<td>0.20913626E-04</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>0.12882890E-05</td>
<td>0.33258373E-11</td>
<td>0.33819576E-09</td>
<td>0.15121905E-08</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>0.69087549E-11</td>
<td></td>
<td>0.31721042E-12</td>
<td></td>
</tr>
</tbody>
</table>
3.6. Numerical verifications

\[ X_1 = 0, \quad X_2 = ae_1, \quad X_3 = ae_2, \]
\[ X_4 = ae_1 + ae_2, \quad X_5 = ae_3, \]
\[ X_6 = 1.15ae_1 - 1.15ae_2 + 0.9ae_3, \]
\[ X_7 = -ae_1 + 0.9ae_2 + 1.25ae_3, \]
\[ X_8 = 1.25ae_1 + 1.25ae_2 + 1.5ae_3. \]

Figure 3.2: Representation of the cube considered for the convergence test and the nodal position of the 8 mesh nodes. Node #8 is subjected to a nodal force vector \( f_8 = f_8 (e_1 + e_2 - e_3) \), with \( f_8 = 0.05N \).

3.6.3 Objectivity test

The principle of material invariance is a fundamental prerequisite in continuum mechanics and postulates that the constitutive response remains independent of the observer. Hence, the objective of this test is to confirm that the presented integration scheme in Section 3.3 properly integrates the constitutive evolution equations under superposed rigid body motion.

Specifically, an element is encapsulated by a network of slide plane elements, allowing to superpose uniaxial stretch and rotation on the cube simultaneously, see Figure 3.3a. Boundary conditions are applied to Node #1 at which translational degrees of freedom are fixed and an angular velocity given by \( \omega = \bar{\omega} (e_1 + e_2 + e_3) \) is prescribed. The cube is subjected to 6 steps of loading and unloading at different strain rates, similar to the experiments by Har-Shai et al. (1996). Additionally, a rotation angle of 60° around the direction of \( \omega \) is prescribed at each step.
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Table 3.2: Loading profile in terms of time steps, strain rates, and angular velocities for validating the strong incremental objectivity of the presented numerical integration.

<table>
<thead>
<tr>
<th>step</th>
<th>time interval [s]</th>
<th>strain rate $\dot{\varepsilon} (t)$ [Hz]</th>
<th>angular velocity $\tilde{\omega}$ [rad]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>15.4</td>
<td>$+1.0 \cdot 10^{-2}$</td>
<td>$3.925972 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>9.1</td>
<td>$-1.0 \cdot 10^{-2}$</td>
<td>$6.643954 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>50.8</td>
<td>$+2.5 \cdot 10^{-3}$</td>
<td>$1.190157 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>4</td>
<td>39.2</td>
<td>$-2.5 \cdot 10^{-3}$</td>
<td>$1.542346 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>5</td>
<td>284.0</td>
<td>$+5.0 \cdot 10^{-4}$</td>
<td>$2.128872 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>6</td>
<td>200.0</td>
<td>$-5.0 \cdot 10^{-4}$</td>
<td>$0.302300 \cdot 10^{-2}$</td>
</tr>
</tbody>
</table>

The applied loading profile for the recomputation of the experiments by Har-Shai et al. (1996) is summarized in Table 3.2. The angular velocity applied to Node #1 is given in terms of $\tilde{\omega} = \bar{\omega}/t$, with $\bar{\omega} = \alpha/\sqrt{3}$, for arbitrary rotation angle $\alpha$ ($\alpha = 60^\circ$ for example) around $\omega$ and step time $t$.

Figure 3.3b shows a comparison between the rotated cyclic test and the same example without a prescribed rotation. It can be seen that both curves coincide which leads to the conclusion that the integration scheme is objective.

![Figure 3.3: (a) FE model of objectivity test. Translational degrees of freedom at Node #1 are fixed, while a rotation is prescribed and the translator element is simultaneously stretched, which induces a uniaxial stress state in the cube. (b) Comparison between numerical results for the fixed and rotated cube under cyclic uniaxial stress.](image-url)

Figure 3.3: (a) FE model for the objectivity test. Translational degrees of freedom at Node #1 are fixed, while a rotation is prescribed and the translator element is simultaneously stretched, which induces a uniaxial stress state in the cube. (b) Comparison between numerical results for the fixed and rotated cube under cyclic uniaxial stress.
3.7 Parameter identification of facial skin tissue

In this section, a set of model parameters is derived from mechanical experiments on human facial skin using the suction method. In comparison to material parameters presented by Rubin and Bodner (2002) and Mazza et al. (2005), the measurements considered here, describe a more realistic state of strain within the tissue as for the uniaxial tests by Har-Shai et al. (1996) and allow for the identification of an improved set of model parameters. Moreover, the parameter optimization procedure presented here, can be considered as a challenging example of the implementation’s applicability.

Several different non-invasive testing methods have been used to investigate the mechanical properties of skin including suction (Hendriks et al., 2006; Iivarinen et al., 2013; Piérard et al., 2013a,b; Tarsi et al., 2013), indentation (Abellan et al., 2013; Iivarinen et al., 2014), and in-situ tensioning devices (Bhushan et al., 2010; Flynn et al., 2011; Jor et al., 2011). Specifically, suction devices such as the commercially available Cutometer MPA 580 (Courage and Khazaka Electronic GmbH (2014), Köln, DE) and the Aspiration device (developed at ETH Zurich (Badir et al., 2013b; Barbarino et al., 2011; Nava et al., 2004)) have shown to provide a reliable and repeatable testing method for the characterization of individual tissue layers. Depending on the probe aperture diameter different tissue layers are addressed, which impacts the penetration depth and hence allows to determine the properties of individual tissues through solving an inverse FE problem (Barbarino et al., 2011). In the present study, we focus on the most superficial layer of the face, i.e. skin tissue, and therefore, the Cutometer device with a probe aperture diameter of 2mm is used. However, in order to determine material model parameters valid for deeper tissue layers in the face, such as the superficial muscular aponeurotic system (SMAS) as well as superficial and deep fat, more experimental data is required that should be obtained using a suction device with a bigger probe aperture (for example the Aspiration device with an 8mm probe).

In the following, the Cutometer measurements are presented, a set of model parameters for facial skin is determined, and a sensitivity analysis on the underlying inverse FE model (including boundary conditions, model dimensions, and material parameters) is shown.
3.7.1 Cutometer measurements on facial skin

The Cutometer device is based on the suction method allowing for a quantitative measurement of tissue response. Inside the Cutometer device, a negative pressure is created causing skin tissue to be sucked into the aperture of the probe. The resulting tissue deformation is captured through an optical system that evaluates the penetration depth for the corresponding loading state. In the series of measurements presented here, two measurement protocols with different loading profiles were defined in order to assess different tissue properties respectively. In the first measurement protocol a negative pressure is applied at once and held constant for 20 seconds, thus addressing the (i) instantaneous tissue response and (ii) the time dependent creep response. In the second protocol a linearly varying negative pressure at a constant pressure rate is prescribed in order to load and unload the tissue subsequently. This second experiment allows to determine the impact of strain-rate driven (i) hardening and (ii) plastification, as well as (iii) material recovery during unloading.

Figure 3.4: Experimental data from Cutometer measurements for the case of instant loading with 4-6 repetitions per pressure level (gray curves) and average curves for each pressure level (black curves).

For both loading profiles three different levels of loading were considered. Pressure levels of 300mbar, 400mbar, and 500mbar were applied in the first measurement protocol and pressure rates of 10mbar/s, 15mbar/s, and 20mbar/s for the second. Each of the six measurements was repeated for at least four times in order to ensure repeatability.

Measurements were performed on a 29 year old male subject and measurement position was chosen based on experiments presented by Barbarino et al. (2011) to be in-between the zygomatic and nasolabial region since these were found to be closest to the facial average. Figures 3.4 and 3.5 show the results of the measurements, where the gray lines represent the individual measurements and the black lines represent the three averages for each sequence of measurements at a different pressure level. Specifically, Figure 3.4 shows the measurement series for the case of instant loading. Figure 3.5 shows the experimental data for the case of linear loading and unloading in two different ways, where the apex
height history is plotted in 3.5a and the applied suction pressure versus apex height is plotted in 3.5b. In particular, the latter visualizes the high nonlinearity and inelasticity of skin tissue.

![Graphs: Apex history and Pressure vs. apex](image)

Figure 3.5: Experimental data from Cutometer measurements for the case of linear loading and unloading. Gray curves represent 4-6 individual measurements per pressure rate, black curves are averaged data over each pressure rate (a) Apex height over measurement time (b) Suction pressure over apex height.

The magnitude of deformation is determined by a number of factors such as moisture content of skin, region of measurement, pressure applied to the skin upon probe placement, and most significantly inter-subject variability. Nonetheless, as the presented data together with previous Cutometer and other suction experiments (Badir et al., 2013b; Barbarino et al., 2011) have shown so far, sufficient repeatability is provided, which is a fundamental prerequisite when using this data for model parameter identification including multiple measurement curves.

### 3.7.2 The FE model of the inverse problem

The FE model used for this study is based on the work presented by Barbarino et al. (2011). The model consists of two tissue layers, representing the most superficial layer skin and the superficial muscular aponeurotic system (SMAS) underneath. The interaction between both layers is modeled such that no relative displacement or slipping may occur. The respective thicknesses of 1.7mm for skin and 3.0mm for SMAS were determined from ultrasound measurements in the face of the 29 year old male subject of this study. Material parameters for SMAS are taken from Mazza et al. (2005), while a new set of skin parameters is determined as presented in section 3.7.3.

The FE mesh was optimized for sufficient refinement in regions of larger strains and the contact zone between skin and probe, see Figure 3.6. Furthermore, the choice of bound-
ary conditions on the model, initial shear modulus (stiffness) and thickness of SMAS, and contact definition between probe and skin were tested in order to validate the FE model assumptions. An elaborate analysis of the model’s sensitivity to changes in these properties is presented in section 3.7.4.

Due to the nature of the Cutometer measurement with respect to the size of the probe’s small aperture diameter and its circular shape, the material’s apparent anisotropy (Khatyr et al., 2004) is assumed to have a marginal impact on the resulting apex height. Therefore and without loss of generality, skin is considered to be an isotropic material in the FE model presented here. Indeed, the evaluation of suction based experimental characterization of skin is often interpreted on the basis of assuming an isotropic material response (Delalleau et al., 2006; Diridollou et al., 2000; Hendriks et al., 2006; Khatyr et al., 2006). To the contrary, suction experiments with a large and elliptically shaped probe aperture, as presented by Iivarinen et al. (2013), were used in order to potentially capture the anisotropic tissue response and to include this information in the determination of anisotropic material properties.

Figure 3.6: FE model for the inverse problem of the Cutometer experiment shown in the deformed state. The bottom nodes are fixed against vertical displacement, while no boundary conditions are imposed on nodes on the right side of the model.

3.7.3 Parameter identification for facial skin

The identification of representative model parameters is an essential component in realistic simulation of tissue response in surgery planning, implant design, and wrinkle formation during facial expressions and aging. Based on the experimental campaign and the FE model presented in sections 3.7.1 and 3.7.2 an inverse problem is set up to determine a set of parameters, which provides good agreement between experimental data and the numerical simulation.

Out of the six different averaged measurement curves three were chosen for the optimization of parameters and the remaining other three used for verification of the set. The averaged measurement curves of instant loading at 300mbar and 500mbar, as well as the
tissue response upon linear loading and unloading at a pressure rate of 15mbar/s were used as input for the objective functions in the inverse problem. Using the \textit{fminsearch procedure} in Matlab (Matlab 10.0, The MathWorks, Inc., Natick, Massachusetts, US) with the Nelder-Mead simplex algorithm, the difference between the measurement curves and the corresponding numerical simulations was minimized. The parameters that were included in the optimization were chosen based on their relevance with respect to the two different types of measurements. The shape of initial loading is mainly determined by $\mu_0$, $q$, $m_2$, and $\Gamma_2$. $\Gamma_1$ and $r_2$ are included in order to allow for adopting the material parameters to fit the linear loading and unloading experiment at different strain rates. Furthermore, the parameter $m_5$ was chosen to be $1 - m_2$. The remaining material parameters are based on work by Mazza et al. (2005) and are chosen to exhibit a specific model response, see Table 3.3. In particular, $m_1$ was set to a sufficiently large number in order to enforce the incompressibility of the tissue and $m_3$ was set to zero because of the isotropy assumption of skin.

![Figure 3.7: Results of the least square optimization. Comparison between Cutometer measurements and numerical simulations for the (a) instant loading and (b) the linearly loading and unloading case.](image)

The optimization routine provided a set of material parameters that well represents the experimental data as it is summarized in Figure 3.7. In particular, not only is the maximum apex height of the tissue bubble well predicted in all six cases, but also the experimentally observed tissue recovery in the case of linear unloading well represented. For the measurement with linearly increasing and decreasing pressure at a constant pressure rate, the Cutometer reveals limitations in pressure control for pressures below 25mbar. During the initial phase of loading and the final phase of unloading, the pressure rate
is insufficiently controlled, leading to exaggerated loading and unloading of the tissue by the Cutometer, respectively. The experimental data presented in Figure 3.6 clearly shows this effect through a pronounced slope at the beginning and end of each measurement. For this reason, experimental and numerical data in Figure 3.7b are shown for pressures greater than 25 mbar only. This deficiency of the Cutometer explains the observed discrepancy between experimental and numerical data in the initial loading and final unloading phases.

The parameters identified with the presented routine are given in Table 3.4. The numerical value of the initial shear modulus $\mu_0 = 0.18 \text{MPa}$ is well within values presented in literature (Barbarino et al., 2011; Hendriks et al., 2006; Pailler-Mattei et al., 2009; Tran et al., 2007). Moreover, the small value of $m_2 = 3.87 \cdot 10^{-5}$ can be explained by the predominant response of skin as a dissipative elastic tissue as well as the rather short term tissue response considered in the two Cutometer measurement protocols. A longer hold period in the case of instant loading pressure and/or longer pressuring times in the case of linearly varying pressures would provide more information regarding the long term response of the tissue and influence $m_2$, which mainly controls the purely elastic distortional response.

Table 3.3: Model parameters from literature (Mazza et al., 2005)

<table>
<thead>
<tr>
<th>$m_1$</th>
<th>$m_3$</th>
<th>$m_4$</th>
<th>$n$</th>
<th>$r_1$</th>
<th>$r_3$ [Hz]</th>
<th>$r_4$ [Hz]</th>
<th>$r_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.5</td>
<td>20.0</td>
<td>$10^{-10}$</td>
<td>$10^{-4}$</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 3.4: Model parameters from parameter identification for human facial skin

<table>
<thead>
<tr>
<th>$\mu_0$ [MPa]</th>
<th>$\gamma m_2$</th>
<th>$\Gamma_1$ [Hz]</th>
<th>$\Gamma_2$</th>
<th>$r_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.18</td>
<td>43.0</td>
<td>$3.87 \cdot 10^{-5}$</td>
<td>1.46</td>
<td>67.45</td>
</tr>
</tbody>
</table>

3.7.4 Sensitivity analysis of the FE model

The FE model presented by Barbarino et al. (2011) and used in the present study has been thoroughly investigated with respect to the assumptions on boundary conditions, material properties of SMAS, thickness of SMAS, and the interaction between probe and skin tissue. The impact of these assumptions at the basis of this FE model were verified using the newly determined material parameters and the results are presented in terms of the relative error defined by

$$\text{error}_{rel} = \frac{\max [u^{\text{ref}}] - \max [u^{C_i}]}{\max [u^{\text{ref}}]} \cdot 100,$$

(3.49)

where $\max [u^{\text{ref}}]$ is the maximum apex height obtained by the reference model and $\max [u^{C_i}]$ is the maximum apex height obtained by the different simulations $C_i$, where $i = 1, \ldots, 9$ (see Figure 3.8). Both Cutometer measurement protocols considered in this study are verified here, in order to demonstrate the FE model’s wide range of applicability.
3.7. Parameter identification of facial skin tissue

Figure 3.8: Sensitivity analysis on the FE model used for the parameter identification. Results shown as relative errors of apex height for the reference simulation and the corresponding simulation with a varied parameter.

It can be seen from Figure 3.8 that the variation of fundamental FE model parameters has only a marginal impact of 5.12% the most on the overall apex response when considering a variation of the parameters in a physical range. The most crucial impact on the overall tissue behavior arises from the choice of the interaction properties between probe and skin. The relative error between both extreme cases of frictionless and rough contact is 5.12% for the linearly varying loading profile and less than 2.85% in the case of instant loading. This rather marginal variation is also reflected in an only slightly influenced shape of the apex displacement curve as shown in Figure 3.9 (Simulation $C_9$). As to be expected, a tied contact between probe and skin leads to a reduced apex height as the inward suction of tissue is restricted.

The presented results also disclose the effect of the boundary conditions on the bottom nodes of SMAS. The two extreme cases of fixing horizontal and vertical displacement ($C_1$), as well as removing any constraint on these nodes ($C_2$) leads to a minor difference in the total apex deformation (+0.26% and -2.33% for instant loading and +0.27% and -2.74% for linear loading).

The intervariability of the stiffness of SMAS was studied by reducing the initial shear modulus $\mu_0$ by 10%, 20%, and 50% ($C_3$, $C_4$, and $C_5$). It was found that such a variation has a marginal impact on the skin tissue response. In particular, a reduction by 50% resulted in an increased maximum apex height of 1.82% and 1.86% for the two different measurement protocols.

It should be noted that in our study the material properties of SMAS were adopted from Mazza et al. (2005). However, there is a need to conduct further experimental measurements to properly define the material properties of SMAS. This should include suction method based experiments with a larger probe aperture diameter in order to ensure the penetration of deeper tissue layers as presented by Badir et al. (2013b), Nava et al. (2004), and Barbarino et al. (2011). The impact of the thickness of SMAS on the overall response of skin is found to be less than 0.12% for an increased tissue thickness of up to 33%.
Figure 3.9 shows the apex displacement history of both measurement protocols for a selection of simulations within the sensitivity analysis. The two extreme cases $C_2$ (bottom nodes of SMAS free) and $C_9$ (tied contact between probe and skin) represent the upper and lower bound of the tissues mechanical response in the study presented here. The remaining simulations predict a tissue response within these two curves.

In conclusion, the FE model is broadly based on physically valid assumptions with respect to the thickness of both tissues, the choice of boundary conditions on the individual layers, and a realistic representation of the interaction between probe and skin. Moreover, the presented results strongly demonstrate that a variation in relevant model parameters has a marginal impact on the predicted tissue response independent of the type of loading profile considered in the numerical simulation.

### 3.8 Conclusion

In face of the significant challenges with respect to the numerical implementation of elastic-viscoplastic constitutive equations describing the highly nonlinear and time dependent mechanical response of soft tissues, a new mixed FE formulation based on the relative deformation gradient is developed for a generalized framework of constitutive equations of elastic-viscoplastic soft biological tissues. In the present paper, the constitutive equations proposed by Rubin and Bodner (2002) were considered as a particular case and are used for the numerical study. The introduction of the relative deformation gradient leads to a formulation that is based on the last converged and the current configuration, instead of the dependence on the reference and the current deformed configuration. Such dependence
3.8. Conclusion

is particularly suitable for constitutive equations that are formulated in terms of rate of deformation measures. The developed FE formulation was implemented in the commercial FE program ABAQUS and the implementation was validated through standard numerical tests including the Patch test, rate of convergence, and objectivity test. It was found that the formulation passed the Patch test, exhibited quadratic convergence, and the integration scheme to be unaffected by superposed rigid body rotation.

Furthermore, an experimental campaign was conducted which aims at characterizing the mechanical tissue response of facial skin by means of the multiaxial loading state resulting from suction tests. Specifically, two different loading protocols were defined in order to provide sufficient data for the determination of a set of material model parameters. This set was identified by iteratively solving the inverse FE problem. A comparison between the experimental data and the numerical simulations demonstrated the model’s capabilities to represent the highly nonlinear tissue behavior of skin. This represents a valuable improvement of the model’s applicability over previously presented material model parameters. Rubin and Bodner (2002) and Mazza et al. (2005) provide two different sets of parameters based on the same experimental data on uniaxially tested excised skin tissue strips, which have both shown to significantly overestimate the tissue’s stiffness in physically relevant multiaxial loading conditions.

The present study is conducted in the framework of realistic simulation of facial tissue during facial expressions, mastication, and aging (Barbarino et al., 2009b, 2011; Mazza et al., 2007; Weickenmeier et al., 2014a). To this end, the model implementation within a numerically robust FE formulation is a significant step in the attempt to represent the physical tissue response in complex tissue structures. Further steps should include the characterization of deeper tissue layers by means of the suction method using a larger diameter for the probe opening in order to determine material model parameters for a more physical loading state in comparison to uniaxial stress tests. Moreover, the experimental campaign should be extended to investigate anisotropy of facial skin tissue, as well as the mechanical response to cyclic loading. Consequently, the inverse FE problem model needs to be adopted to allow for the determination of corresponding material parameters. The numerical performance of the new framework for the implementation of elastic-viscoplastic material models should be further analyzed with respect to convergence behavior, especially for cases of high-rate and large deformation as in traumatic brain injury or traumatic aortic rupture.
Table 3.5: Material parameters of the Rubin and Bodner model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_0, \mu$</td>
<td>Initial and nonlinear shear modulus</td>
</tr>
<tr>
<td>$q$</td>
<td>Parameter influencing the nonlinearity of the strain energy function $W$</td>
</tr>
<tr>
<td>$m_1 - m_5$</td>
<td>Parameters of the additive function $q$ in the strain energy function $W$</td>
</tr>
<tr>
<td>$r_1 - r_5$</td>
<td>Parameters of the evolution equation of the hardening function $\beta$</td>
</tr>
<tr>
<td>$\Gamma_1, \Gamma_2, n$</td>
<td>Parameters of the rate of inelasticity function $\Gamma$</td>
</tr>
</tbody>
</table>

Table 3.6: Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X, x$</td>
<td>Location of a material point in the reference and current configuration</td>
</tr>
<tr>
<td>$F, l, d$</td>
<td>Deformation gradient, velocity gradient and rate of deformation tensor</td>
</tr>
<tr>
<td>$b, b'$</td>
<td>Total deformation tensor and total elastic distortional deformation tensor</td>
</tr>
<tr>
<td>$b_{de}'$</td>
<td>Elastic distortional deformation associated with the dissipative component</td>
</tr>
<tr>
<td>$J$</td>
<td>Total dilatation</td>
</tr>
<tr>
<td>$a_d$</td>
<td>Direction of the inelastic flow</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Magnitude of the rate of inelasticity</td>
</tr>
<tr>
<td>$\dot{\varepsilon}$</td>
<td>Effective total distortional deformation rate</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Hardening measure</td>
</tr>
<tr>
<td>$\beta_{de}$</td>
<td>Effective elastic distortion strain associated with the dissipative component</td>
</tr>
<tr>
<td>$\beta_1, \beta_2$</td>
<td>First and second invariant of the total deformation tensor</td>
</tr>
<tr>
<td>$\sigma_1, \sigma_2$</td>
<td>First and second invariant of $b_{de}'$</td>
</tr>
<tr>
<td>$M_I, m_I$</td>
<td>Orientation of the $I$th fiber family in the reference and current configuration</td>
</tr>
<tr>
<td>$\lambda_I$</td>
<td>Stretch of the $I$th fiber family</td>
</tr>
<tr>
<td>$W$</td>
<td>Strain energy function</td>
</tr>
<tr>
<td>$F_r$</td>
<td>Relative deformation gradient</td>
</tr>
<tr>
<td>$J_r$</td>
<td>Relative total dilatation</td>
</tr>
<tr>
<td>$C_r, b_r$</td>
<td>Relative right Cauchy-Green deformation tensor and relative deformation tensor</td>
</tr>
<tr>
<td>$\tilde{F}$</td>
<td>Modified deformation gradient</td>
</tr>
<tr>
<td>$b_{de}'^\ast$</td>
<td>Elastic trial of $b_{de}'$</td>
</tr>
<tr>
<td>$a$</td>
<td>Spatial tangent moduli</td>
</tr>
<tr>
<td>$\bar{J}_r$</td>
<td>Assumed relative averaged volumetric dilatation</td>
</tr>
<tr>
<td>$\bar{p}$</td>
<td>Assumed averaged hydrostatic pressure</td>
</tr>
<tr>
<td>$\delta u, \Delta u$</td>
<td>Virtual and incremental displacement vector</td>
</tr>
<tr>
<td>$\delta h, \Delta h$</td>
<td>Virtual and incremental displacement gradient</td>
</tr>
<tr>
<td>$\delta d_u, \Delta d_u$</td>
<td>Virtual and incremental nodal displacement vector</td>
</tr>
<tr>
<td>$\bar{r}$</td>
<td>Residual forces</td>
</tr>
<tr>
<td>$\bar{B}$</td>
<td>Standard $B$-matrix in finite elements</td>
</tr>
<tr>
<td>$K$</td>
<td>Tangent stiffness matrix</td>
</tr>
</tbody>
</table>
Appendix B

The spatial tangent moduli for the generalized viscoplastic model are defined by

\[ a = \left[ \frac{\partial W}{\partial J} + J \frac{\partial^2 W}{\partial J \partial J} \right] I \otimes I + 4 \frac{\partial^2 W}{\partial \beta_1 \partial \beta_1} \text{dev} (b') \otimes \text{dev} (b') \]

\[ + \frac{16}{J} \frac{\partial^2 W}{\partial \beta_2 \partial \beta_2} \text{dev} (b'^2) \otimes \text{dev} (b'^2) + 2 \frac{\partial^2 W}{J \partial \alpha_1 \partial \alpha_1} \text{dev} (b'_{\text{de}}) \otimes \alpha_1 \]

\[ + 4 \frac{\partial^2 W}{J \partial \alpha_2 \partial \alpha_2} \text{dev} (b'_{\text{de}}^2) \otimes \alpha_2 + \sum_{i=1}^{N_{\text{fib}}} \sum_{j=1}^{N_{\text{fib}}} \frac{1}{J \lambda_i \lambda_j \partial \lambda_i \partial \lambda_j} (m_i \otimes m_i) \otimes (m_j \otimes m_j) \]

\[ + \sum_{i=1}^{N_{\text{fib}}} \frac{1}{J \lambda_i \partial \lambda_i} (m_i \otimes m_i) \otimes (m_i \otimes m_i) + \frac{2}{J \partial \beta_1} \left[ \text{dev} (b') \otimes \text{dev} (b') + \text{dev} (b'_{\text{de}}) \otimes \alpha_1 \right] \]

\[ + \frac{2}{J \partial \beta_2} \left[ \text{dev} (b'_{\text{de}}) \otimes \text{dev} (b') + \text{dev} (b'_{\text{de}}) \otimes \alpha_1 \right] \]

\[ + \frac{2}{J \partial \beta_2} \left[ \text{dev} (b'_{\text{de}}^2) \otimes \text{dev} (b') + \text{dev} (b'_{\text{de}}) \otimes \alpha_2 \right] \]

\[ + \sum_{i=1}^{N_{\text{fib}}} \frac{2}{J \lambda_i \partial \beta_2} (m_i \otimes m_i) \otimes (m_i \otimes m_i) \]

\[ + \frac{4}{J \partial \alpha_1 \partial \alpha_1} \left[ \text{dev} (b'^2) \otimes \text{dev} (b') + \text{dev} (b'^2) \otimes \alpha_1 \right] \]

\[ + \frac{4}{J \partial \alpha_2 \partial \alpha_2} \left[ \text{dev} (b'^2) \otimes \text{dev} (b'^2) + \text{dev} (b'^2) \otimes \alpha_2 \right] \]

\[ + \frac{N_{\text{fib}}}{J \lambda_i \partial \alpha_3 \partial \alpha_1} (m_i \otimes m_i) \otimes (m_i \otimes m_i) + \frac{4}{J \partial \beta_1} \left[ \text{dev} (b'_{\text{de}}) \otimes \text{dev} (b') + \text{dev} (b'_{\text{de}}) \otimes \alpha_1 \right] \]

\[ + \frac{1}{J \partial \alpha_1 \partial \alpha_2} \left[ \text{dev} (b'_{\text{de}}^2) \otimes \alpha_1 + \text{dev} (b'_{\text{de}}^2) \otimes \alpha_2 \right] \]

\[ + \sum_{i=1}^{N_{\text{fib}}} \frac{1}{J \lambda_i \partial \alpha_2} (m_i \otimes m_i) \otimes (m_i \otimes m_i) + \frac{4}{J \partial \beta_1} \left[ \text{dev} (b'^2) \otimes \text{dev} (b') + \text{dev} (b'^2) \otimes \alpha_2 \right] \]

\[ + \frac{\partial W}{J \partial \beta_1} \frac{\partial \text{dev} (b')}{\partial F_r} F_r^T + \frac{4}{J \partial \beta_2} \frac{\partial \text{dev} (b'^2)}{\partial F_r} F_r^T + \frac{2}{J \partial \alpha_1} \frac{\partial \text{dev} (b'_{\text{de}}) F_r^T}{\partial F_r} \]

\[ + \frac{4 \partial W}{J \partial \alpha_2} \frac{\partial \text{dev} (b'_{\text{de}})}{\partial F_r} F_r^T + \sum_{i=1}^{N_{\text{fib}}} \frac{1}{J \lambda_i \partial \lambda_i} \frac{\partial (m_i \otimes m_i) F_r^T}{\partial F_r} \]

(3.50)
Appendix C

The coefficients \( \{d_0(t_{n+1}), d_1(t_{n+1}), d_2(t_{n+1})\} \) that are used in (3.28) are given by

\[
d_0(t_{n+1}) = 1 - \Delta t \frac{\frac{\partial \hat{\Gamma}}{\partial \beta} \left( \frac{\partial \hat{\beta}}{\partial \Gamma} + \frac{\partial \hat{\beta}}{\partial \beta_{de}} \frac{\partial \beta_{de}}{\partial \Gamma} \right)}{1 - \Delta t \frac{\partial \hat{\beta}}{\partial \beta} + \frac{\partial \hat{\Gamma}}{\partial \beta} \frac{\partial \beta_{de}}{\partial \beta} \frac{\partial \beta_{de}}{\partial \Gamma}},
\]

\[
d_1(t_{n+1}) = \frac{\partial \hat{\Gamma}}{\partial \dot{\varepsilon}} + \Delta t \frac{\frac{\partial \hat{\Gamma}}{\partial \beta} \frac{\partial \beta_{de}}{\partial \dot{\varepsilon}}}{1 - \Delta t \frac{\partial \hat{\beta}}{\partial \beta}},
\]

\[
d_2(t_{n+1}) = \left( \frac{\partial \hat{\Gamma}}{\partial \beta_{de}} + \Delta t \frac{\frac{\partial \hat{\Gamma}}{\partial \beta} \frac{\partial \beta_{de}}{\partial \beta_{de}}}{1 - \Delta t \frac{\partial \hat{\beta}}{\partial \beta}} \right) \frac{\partial \beta_{de}}{\partial \beta_{de}}.
\]

(3.51)
Chapter 4

Modeling of skeletal muscle contraction

4.1 Introduction

Skeletal muscle fulfills several different functions in the human body providing support to the skeletal system, enabling body movement, or any other voluntary active tissue response such as in facial expressions, speech, and mastication. Skeletal muscle in humans differs from other muscle tissue types such as smooth or cardiac muscle through its ability to be activated voluntarily by the somatic nervous system. Similarly to most soft biological tissues, a muscle may undergo large deformations and is characterized by a highly nonlinear deformation response. Its hierarchical structure, consisting of fascicles of myocytes or muscle cells on the macro level reaching down to the basic functional unit of muscle, i.e. the sarcomere, spans across several length scales (Fung, 1993; Standring, 2008).

Unlike most other soft tissues, the ability to actively contract allows muscle to produce tensile force upon neural stimulation. Extensive mechanical characterization of muscle properties began with Hill’s phenomenological three element model (Hill, 1938). This formulation captures the fundamental relationship between contraction velocity and tensile force in the fully tetanized muscle observed in pioneering experiments on individual muscle fibers. However, the underlying contraction mechanism was not understood until Huxley proposed the micromechanically based cross-bridge theory (Huxley, 1957). The Hill model provides a simple formulation of the active properties of muscle on the tissue level and has been used and extended in many different model formulations (Ettema and Meijer, 2000; Fung, 1993; Meijer et al., 1998; Zajac, 1989). Most constitutive laws proposed in literature consider a one-dimensional formulation in order to describe the interaction between muscle, tendons, and joints within the musculoskeletal system (Chao et al., 1993; Delp et al., 1990; Dong et al., 2002; Nussbaum et al., 1995; Semwal and Hallauer, 1994). However, appropriate modeling of the interaction between muscle and its surrounding tissue requires a three-dimensional (3D) representation allowing for a physical prediction of transverse and volumetric material response. Several models describing the contractile properties on a continuum level have been proposed in recent years of which most make use of a phenomenological description of the underlying tissue behavior.
Chapter 4. Modeling of active skeletal muscle contraction

(Blemker and Delp, 2005; Chi et al., 2010; Ehret et al., 2011; Grasa et al., 2011; Hedestrierna et al., 2008; Johansson et al., 2000; Oomens et al., 2003; Röhrle and Pullan, 2007; Sharifimajd and Stålhand, 2013). Moreover, constitutive models were proposed describing the electromechanical coupling in skeletal muscle (Böl et al., 2011b; Röhrle, 2010; Shorten et al., 2007) and skeletal muscle fatigue (Böl et al., 2011a; Shorten et al., 2007; Tang et al., 2007). Representation of the electromechanical coupling was applied to model active behavior of cardiac muscles (Dal et al., 2013; Lafortune et al., 2012; Rossi et al., 2012). Other work aims at describing phenomena such as stretch induced muscle growth (Zöllner et al., 2012) and muscle damage (Ito et al., 2010).

In general, a 3D continuum approach provides the basis for an effective description of nonlinear anisotropic material behavior including the possibility to represent different muscle fiber distributions and pennation angles. Alongside the advances in mathematical modeling of muscle tissue, new experimental methods allow for more comprehensive validation procedures of the proposed constitutive formulations. These recent developments include improved experimental setups to characterize the passive properties of muscle (Böl et al., 2012), visualization of muscle deformation behavior during contraction (Böl et al., 2013; Siebert et al., 2012), as well as the application of the elastography method to determine stiffness properties of muscle (Debernard et al., 2011, 2013).

The development of mathematical muscle models provided substantial understanding of active tissue behavior in the human body. Examples are the simulation of muscle driven locomotion where rigid body systems together with one-dimensional muscle formulations (Anderson and Pandy, 2001; Delp et al., 1990; Praet et al., 2012) are implemented in the finite element (FE) environment to improve our understanding of muscle response and its interaction with surrounding tissues (Röhrle et al., 2012; Spyrou and Aravas, 2012; Ting et al., 2012). Other examples are given by detailed FE simulations of the tongue (Kajee et al., 2013), the human upper airway (Pelteret and Reddy, 2012) or the forces during mastication (Röhrle and Pullan, 2007).

FE simulations require the implementation of active or passive constitutive models. Hence, on the basis of constitutive equations governing the material response at a continuum level, the consistent linearization of the strain energy function, the stress tensor, and the associated material tangent must be provided for numerical calculation, which is missing in all previously mentioned publications. The muscle model considered here is based on the work of Böl and Reese (2008), Ehret (2011), and Ehret et al. (2011). Most constitutive material laws for muscle proposed so far make use of an additive split of muscle tissue stress into a passive and an active part. This approach is mainly due to experimental practice where the muscle responses are compared in the resting and activated states. However, this modeling approach ignores experimental evidence that the sarcomere system is not a purely active muscle component (Ehret et al., 2011; Linke and Granzier, 1998; Magid and Law, 1985). Ehret et al. (2011) avoid this explicit additive split of muscle stress and presented a phenomenologically based material model that provides significant control of several different contractile characteristics of skeletal muscle. This model assumes muscle tissue as incompressible. Model implementation in a FE program using a material subroutine is shown to prohibit the enforcement of volume preservation. For this reason, a modified formulation is introduced here without incompressibility.
condition. We first present the implementation of the new set of equations in the FE environment. Next, the consistent linearization of the strain energy function, the Cauchy stress tensor $\sigma$, and the associated spatial form of the material tangent $C$ are derived. The implementation of the strain energy function was carried out for two functionally different formulations of the muscle model allowing for a direct comparison between the so-called coupled and decoupled approach. The decoupled approach refers to the additive split of the strain energy function into a volumetric and a purely isochoric part as proposed by Flory (1961). This widely used approach is compared to a formulation avoiding this decomposition. It is shown, that the volumetric-isochoric split leads to negative eigenvalues of the spatial tangent modulus $C$ and to an unphysical volume behavior for the activated muscle state. This unphysical volumetric response has already been observed for different material models of passive fiber-reinforced soft tissues by Helfenstein et al. (2010).

Finally, our FE implementation is applied in a realistic simulation of muscle force resulting from the contraction of the masseter muscle. This example is used to demonstrate the predictive capabilities of the model implementation with respect to shape changes of geometrically complex muscles and the development of bite force during mastication.

### 4.2 Finite element implementation

On the basis of a muscle model presented in Ehret (2011) and Ehret et al. (2011) a constitutive model formulation is proposed for the passive and active behavior of skeletal muscles. The formulation makes use of the generalized invariants representation including a term that controls the muscle activation. While the constitutive model proposed by Ehret et al. (2011) considers muscle as a fully incompressible tissue, there is no experimental evidence found in literature that would indicate such behavior. Moreover, the numerical implementation of a fully incompressible material within the FE environment entails significant challenges in providing adequate approximation schemes and cannot be realized using a material subroutine. Hence, muscle tissue is considered here as a nearly-incompressible material, thus allowing for an adequate physical approximation of the mechanical response. For comparison reasons, two different functional forms for the constitutive formulation of muscle tissue with and without the additive volumetric-isochoric split of the strain energy function are presented. To the best of the author’s knowledge, the derivations of the stress tensor and the consistent material tangent for both approaches are presented here for the first time.

#### 4.2.1 Active skeletal muscle model

The first functional form of the strain energy function presented here is given as a function of the right Cauchy Green tensor $C = F^T F$ as

$$W = \frac{1}{4\mu} \left\{ \frac{1}{\alpha} \left( \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] - 1 \right) + \frac{1}{\beta} \left( \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] - 1 \right) + \frac{1}{\gamma} \left( III_C^{-\gamma} - 1 \right) \right\},$$

$$\tilde{I} = C : \left( \tilde{\mathbf{L}} + w_a \mathbf{M} \right), \quad \tilde{J} = \text{cof}(C) : \tilde{\mathbf{L}}, \quad III_C = \text{det}(C),$$

(4.1)
where \( \mu, \alpha, \beta, \gamma \) are material parameters. \( \tilde{I}, \tilde{J} \) and \( III_C \) are three invariants of \( C \) expressed in terms of the structural tensor \( \tilde{L} \) given by

\[
\tilde{L} = \frac{w_0}{3} I + w_p M. \tag{4.2}
\]

Material anisotropy is governed by the structural tensor \( M = m \otimes m \), where \( m \) is the unit vector parallel to the preferred muscle fiber direction in the reference configuration. The identity tensor of second order \( I \) serves to describe the passive isotropic properties of muscles. The weighing parameters \( w_0 \) and \( w_p \) govern the ratio between muscle matrix material (\( w_0 \)) and muscle fibers (\( w_p \)), with \( w_0 + w_p = 1 \). In this formulation an activation parameter \( w_a \) is introduced which affects the generalized invariant \( \tilde{I} \). The magnitude of \( w_a \) is correlated to the current level of the muscle activation and is governed by a physically based activation function described below.

The second functional form which makes use of the volumetric-isochoric split of the strain energy function is given by

\[
\bar{W} = \bar{W}_{iso}(C) + \bar{W}_{vol}(J),
\]

\[
\bar{W}_{iso}(C) = \frac{\mu}{4} \left\{ \frac{1}{\alpha} \left( \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] - 1 \right) + \frac{1}{\beta} \left( \exp \left[ \beta \left( \tilde{K} - 1 \right) \right] - 1 \right) \right\}, \tag{4.3}
\]

\[
\bar{W}_{vol}(J) = \frac{\kappa}{4} \left[ J^2 - 1 - 2 \ln(J) \right],
\]

where \( \mu, \alpha, \beta, \kappa \) are material parameters and

\[
\tilde{I} = C: \left( \tilde{L} + w_0 M \right), \quad \tilde{K} = C^{-1}: \tilde{L}, \quad J = \det F. \tag{4.4}
\]

In this formulation \( C \) represents the unimodular right Cauchy Green tensor which renders a pure measure of distortion and is defined by

\[
C = J^{-2/3} C. \tag{4.5}
\]

The choice of the volumetric part \( \bar{W}_{vol} \) in (4.3) is based on the strong polyconvexity condition and sufficient growth for large strains in order to penalize considerable volume changes. Substantial work on this topic has been carried out by Hartmann and Neff (2003) and Schröder and Neff (2003).

Both formulations presented in equations (1-5) represent new constitutive models describing the active tissue response. It can be shown that these two formulations coincide only for the case of ideal incompressibility. In this special case, these strain energy functions correspond to the ones presented by Ehret et al. (2011).

In the following, the strain energy function \( W \) (4.1) will be referred to as the \textit{coupled formulation} and the strain energy function \( \bar{W} \) (4.3) as the \textit{decoupled formulation}. Relevant components of the active elements in both model formulations are presented here based on the corresponding equations in Böl and Reese (2008) and Ehret et al. (2011). This set of equations constitutes the basis for the derivation of the stress tensor and the consistent
4.2. Finite element implementation

material tangent. As mentioned above, the activation level of the muscle is governed by the parameter $w_a$ determined by (Ehret et al., 2011)

$$w_a = \begin{cases} 
0 & \text{if } P_{act} = 0, \\
\frac{W_0(\chi^*)}{\alpha \lambda_m} - \frac{I_p}{2 \lambda_m} & \text{else}, 
\end{cases}$$

(4.6)

where $W_0(\chi^*)$ denotes the solution for the principal branch of the Lambert-$W$ function and $\chi^*$ is given by (Corless et al., 1996; Ehret et al., 2011)

$$\chi^* = P_{act} \frac{2 \alpha \lambda_m}{\mu} \exp \left[ \left( \frac{\alpha}{2} \right) \left( 2 - 2 I_p + \lambda_m \bar{I}_p \right) \right] + \frac{\alpha}{2} \lambda_m \bar{I}_p \exp \left[ \left( \frac{\alpha}{2} \right) \lambda_m \bar{I}_p \right].$$

(4.7)

Here, the squared fiber stretch $\lambda_m$, the passive part of the first generalized invariant $\bar{I}_p$, and its first derivative with respect to fiber stretch $\lambda_m$, $\bar{I}_p'$, are defined by (Ehret et al., 2011)

$$\lambda_m = \sqrt{C : \mathbf{M}},$$

(4.8)

$$\bar{I}_p = \frac{w_0}{3} \left( \lambda_m^2 + \frac{2}{\lambda_m} \right) + w_p \lambda_m^2,$$

(4.9)

$$\bar{I}_p' = \frac{\partial \bar{I}_p}{\partial \lambda_m} = \frac{w_0}{3} \left( 2 \lambda_m - \frac{2}{\lambda_m^2} \right) + 2w_p \lambda_m.$$

(4.10)

The nominal stress $P_{act}$ due to the activation of the muscle is expressed in terms of an activation function as (Böl and Reese, 2008; Ehret et al., 2011)

$$P_{act} = f_\zeta f_\nu Na \sum_{i=1}^{n_{MU}} \rho_i F^i_t,$$

(4.11)

where $Na \sum_{i=1}^{n_{MU}} \rho_i F^i_t$, $f_\zeta$ and $f_\nu$ are functions (of time $t$) accounting for the activation, sarcomere length and velocity dependencies, respectively. The total active muscle stress is the result of a superposition of the twitch force of each of the $n_{MU}$ motor unit types present in the muscle fiber, where $\rho_i$ indicates their corresponding fraction. The scalar factor $Na$ is a measure of the total number of activated muscle units per reference cross-sectional area. The twitch force of a single motor unit of type $i$ is determined by (Böl and Reese, 2008; Ehret et al., 2011)

$$F^i_t = G_i(T_i/I_i) \sum_{j=1}^{n_{IMP}} g_{ij} \left( t - t_{ij} \right),$$

(4.12)

with $n_{IMP}$ equal to the number of impulses sent to the recruited muscle fibers. The above formulation for $F^i_t$ is based on the sum over the mechanical response of each single motor unit twitch $g_{ij}$ multiplied by a dimensionless gain function $G_i$.

The latter function inherits the experimentally observed nonlinear relation between single muscle fiber force and normalized stimulus rate $T_i/I_i$ through a sigmoid relationship.
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\[ S_i(T_i/I_i) = 1 - \exp \left[ -2 \left( \frac{T_i}{I_i} \right)^3 \right]. \]

Twitch contraction time \( T_i \) and interstimulus interval \( I_i \) are experimentally determinable muscle properties. The gain function and the single twitch force response are of the form (Böl and Reese, 2008; Ehret et al., 2011)

\[ G_i(T_i/I_i) = \frac{S_i(T_i/I_i)}{T_i/I_i} = 1 - \exp \left[ -2 \left( \frac{T_i}{I_i} \right)^3 \right], \]

\[ g_{ij}(t-t_{ij}) = \frac{(t-t_{ij})}{T_i} \exp \left[ 1 - \frac{(t-t_{ij})}{T_i} \right], \]

where \( F_i \) is the twitch force of motor unit type \( i \) determined experimentally.

The expressions \( f_\zeta \) and \( f_\nu \) in (4.11) are physically motivated and account for the microscopic state of the muscle. From experiments by Gordon et al. (1966) and others the dependence of the overlap between actin and myosin filaments on the muscle force produced by a single twitch is well understood. In the formulation described here, \( f_\zeta \) is given by a Weibull distribution which depends on two characteristic constants \( \lambda_{\text{min}} \) and \( \lambda_{\text{opt}} \), where \( \lambda_{\text{min}} \) denotes the lower bound for the fiber stretch at which myofilaments still overlap and \( \lambda_{\text{opt}} \) refers to the fiber stretch at which maximum twitch force is reached. The asymmetric shape of the Weibull distribution properly describes the experimentally observed muscle response (Böl and Reese, 2008; Ehret et al., 2011). Accordingly,

\[ f_\zeta(\lambda_m) = \begin{cases} \frac{\lambda_m-\lambda_{\text{min}}}{\lambda_{\text{opt}}-\lambda_{\text{min}}} \exp \left[ \frac{(2\lambda_{\text{min}}-\lambda_m-\lambda_{\text{opt}})(\lambda_m-\lambda_{\text{opt}})}{2(\lambda_{\text{min}}-\lambda_{\text{opt}})^2} \right] & \text{if } \lambda_m > \lambda_{\text{min}}, \\ 0 & \text{else}. \end{cases} \]

The hyperbolic character of the relation between the force due to concentric muscle contraction and the fiber stretch velocity \( \dot{\lambda}_m \) observed in experiments by Hill (1938) is included in \( f_\nu \). The formulation considered here distinguishes between the muscle shortening and lengthening phase as follows (Böl and Reese, 2008; Ehret et al., 2011)

\[ f_\nu(\dot{\lambda}_m) = \begin{cases} \frac{1-\dot{\lambda}_m/\lambda_{\text{min}}}{1+k_c\dot{\lambda}_m/\lambda_{\text{min}}} & \text{if } \dot{\lambda}_m \leq 0, \\ \frac{1+k_c\dot{\lambda}_m/\lambda_{\text{min}}}{1-k_c\dot{\lambda}_m/\lambda_{\text{min}}} & \text{if } \dot{\lambda}_m > 0, \end{cases} \]

where \( k_c \) and \( k_e \) are constants referring to the concentric and eccentric contraction and \( \dot{\lambda}_{\text{min}} \) denotes the minimum stretch rate.

4.2.2 Implementation in the finite element program ABAQUS

In order to simulate the mechanical response of individual muscles the model was implemented into the commercial FE program ABAQUS (2009) (Dassault Systèmes, Providence, RI, USA). It allows users to program a user subroutine called \textit{UMAT}, where general material constitutive equations can be implemented. In the \textit{UMAT} subroutine, the deformation gradient \( \mathbf{F} \) represents an input while the Cauchy stress tensor \( \mathbf{\sigma} \) and the spatial tangent stiffness \( c' \) (Miehe, 1996; Sun et al., 2008) are output variables. The latter one
is consistent with the objective Jaumann-Zaremba stress rate. In particular, the Cauchy stress tensor and the spatial tangent stiffness are given by

\[ \sigma_{ij} = \frac{1}{J} F_{il} S_{IJ} F_{jJ}, \quad (4.17) \]

\[ c_{ijkl}^J = \frac{1}{J} F_{il} F_{jJ} C_{IJKL} F_{kK} F_{lL} + \frac{1}{2} \left( \sigma_{ik} \delta_{jl} + \sigma_{il} \delta_{jk} + \delta_{ik} \sigma_{jl} + \delta_{il} \sigma_{jk} \right), \quad (4.18) \]

where \( S_{IJ}, C_{IJKL} \) are components of the second Piola-Kirchhoff stress tensor and material tangent modulus tensor, respectively.

The derivations of the individual terms for the second Piola-Kirchhoff stress and material tangent modulus tensor for the functional form \( W \) (4.1) are presented in the following while the corresponding set of equations for the second formulation \( \tilde{W} \) (4.3) is derived in Appendix 4.5.2.

The second Piola-Kirchhoff stress tensor based on (4.1) reads as

\[
S = 2 \frac{\partial W}{\partial C} = \frac{1}{\mu} \left\{ \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \left( \tilde{L} + w_a M \right) - \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] C^{-1} \tilde{L} C^{-1} \right.
\]

\[
+ \left( \tilde{J} \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] - III_C^{-\gamma} \right) C^{-1} \right\}. \quad (4.19)
\]

Taking the dependence of \( w_a \) on the right Cauchy Green tensor \( C \) into account, the corresponding material tangent can be given by

\[
C = 2 \frac{\partial S}{\partial C} = \mu \left\{ \alpha \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \left( \tilde{L} + w_a M \right) \otimes \left( \tilde{L} + w_a M \right) \right.
\]

\[
+ \alpha \lambda_m^2 \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \left( \tilde{L} + \frac{1 + w_a \alpha \lambda_m^2}{\alpha \lambda_m^2} M \right) \otimes \frac{\partial w_a}{\partial C}
\]

\[
+ \beta \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] III_C^2 \left( C^{-1} \tilde{L} C^{-1} \otimes C^{-1} \tilde{L} C^{-1} \right)
\]

\[
- \left( \beta \tilde{J} + 1 \right) \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] III_C \left( C^{-1} \otimes C^{-1} \tilde{L} C^{-1} + C^{-1} \tilde{L} C^{-1} \otimes C^{-1} \right)
\]

\[
+ \left( \beta \tilde{J} + 1 \right) \tilde{J} \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] + \gamma III_C^{-\gamma} \right] C^{-1} \otimes C^{-1}
\]

\[
+ \left( \tilde{J} \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] - III_C^{-\gamma} \right) \frac{\partial C^{-1}}{\partial C} - \exp \left[ \beta \left( \tilde{J} - 1 \right) \right] III_C \frac{\partial C^{-1} \tilde{L} C^{-1}}{\partial C} \right\}, \quad (4.20)
\]

where

\[
\frac{\partial w_a}{\partial C} = \frac{d w_a}{d \lambda_m} \frac{\partial \lambda_m}{\partial C} = \left\{ \begin{array}{ll}
0 & \text{if } P_{act} = 0, \\
\left( \frac{1}{2 \alpha \lambda_m^2} \frac{d W_a(\chi^*)}{d \lambda_m} - \frac{W_a(\chi^*)}{\alpha \lambda_m^2} - \frac{1}{4 \lambda_m^2} \frac{d^2 r_p}{d \lambda_m} + \frac{1}{4 \lambda_m^2} \frac{d r_p}{d \lambda_m} \right) & \text{otherwise.} 
\end{array} \right. \quad (4.21)
\]
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The derivatives of $C^{-1}$ and $C^{-1}\tilde{L}C^{-1}$ with respect to $C$ are given in Appendix 4.5.1. It should be noted that the second term on the right hand side of (4.20) causes the material tangent modulus $C$ to be unsymmetrical.

The derivative of the Lambert-$W_0$ function with respect to the muscle stretch appearing in (4.21) is given by

$$dW_0(\chi^*) = \frac{1}{(1 + W_0) \exp[W_0]} \frac{d\chi^*}{d\lambda}$$(4.22)

$$d\chi^* = \frac{2\alpha}{\mu} \exp \left[ \frac{\alpha}{2} \left( 2 - 2\tilde{I}_p + \lambda_m \frac{d\tilde{I}_p}{d\lambda_m} \right) \right] \left\{ P_{act} + \lambda_m \frac{dP_{act}}{d\lambda_m} \right\} + \frac{\alpha}{2} P_{act} \lambda_m \left( \lambda_m \frac{d^2\tilde{I}_p}{d\lambda_m^2} - \frac{d\tilde{I}_p}{d\lambda_m} \right) + \frac{\alpha}{2} \left( 1 + \frac{\alpha}{2} \right) \exp \left[ \frac{\alpha}{2} \lambda_m \frac{d\tilde{I}_p}{d\lambda_m} \right] \left\{ \frac{d\tilde{I}_p}{d\lambda_m} + \lambda_m \frac{d^2\tilde{I}_p}{d\lambda_m^2} \right\}.$$(4.23)

The additional active muscle stress $P_{act}$ resulting from impulses sent to the muscle is a function of $\lambda_m$. Thus, we can write

$$\frac{dP_{act}}{d\lambda_m} = Na \sum_{i=1}^{n_{act}} \rho_i F_t^i \left( f_\nu \frac{df_\nu}{d\lambda_m} + f_\zeta \frac{df_\zeta}{d\lambda_m} \frac{\partial \hat{\lambda}_m}{\partial \lambda_m} \right),$$ (4.24)

where the derivatives of the functions $\{f_\zeta, f_\nu\}$ with respect to $\lambda_m$ are given by

$$\frac{df_\zeta}{d\lambda_m} = \begin{cases} 0 & \text{if } P_{act} = 0, \\ \frac{(\lambda_{min} - \lambda_m)^2 - (\lambda_{min} - \lambda_{opt})^2}{(\lambda_{min} - \lambda_{opt})^4} \text{exp} \left[ \frac{2(\lambda_{min} - \lambda_m - \lambda_{opt})}{(\lambda_{min} - \lambda_{opt})^2} \right] & \text{otherwise}, \end{cases}$$ (4.25)

$$\frac{df_\nu}{d\lambda_m} = \begin{cases} 0 & \text{if } \hat{\lambda}_m \leq 0, \\ \frac{1 + k_e \lambda_m (\lambda_{min} / \lambda_m)^{1 + k_e}}{\lambda_m (1 + k_c \lambda_m / \lambda_{min})^{1 + k_c}} \frac{\partial \lambda_m}{\partial \lambda_m} & \text{if } \hat{\lambda}_m > 0. \end{cases}$$ (4.26)

Finally, using the backward Euler differentiation, the time derivative of the muscle stretch $\hat{\lambda}_m$ and its derivative with respect to the muscle stretch can be approximated by

$$\dot{\lambda}_m \approx \lambda_m \frac{(t_{n+1}) - \lambda_m(t_n)}{\Delta t}, \quad \frac{\partial \lambda_m}{\partial \lambda_m} \approx \frac{1}{\Delta t}.$$ (4.27)
4.3 Numerical verification

The descriptive capabilities of the proposed muscle models and the reliability of the two different constitutive formulations are evaluated in this section by direct comparison of their performance. A uniaxial tension test is used to investigate the basic mechanical response of the passive and the active components of the muscle models. Finally, a benchmark example is introduced in order to study mesh dependent effects, convergence behavior and the model response for different modes of muscle contraction.

4.3.1 Passive and active uniaxial behavior

The two different implementations were tested in a numerical example of a unit cube meshed by one element and subjected to uniaxial tension. A single fiber family is considered with its preferred direction aligned in the uniaxial loading direction. Boundary conditions were chosen such that only axial stretches are applied and lateral surfaces of the cube are traction free. The material parameters used within this analysis are taken from Ehret et al. (2011) and are given in Table 4.1 for the passive components and in Table 4.2 for the active components.

Table 4.1: Material parameters of the muscle’s passive material response

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$ (kPa)</td>
<td>0.1599</td>
</tr>
<tr>
<td>$\alpha$ (-)</td>
<td>19.69</td>
</tr>
<tr>
<td>$\beta$ (-)</td>
<td>1.190</td>
</tr>
<tr>
<td>$w_0$ (-)</td>
<td>0.7388</td>
</tr>
<tr>
<td>$\kappa/\gamma$ (kPa)</td>
<td>1000.0</td>
</tr>
</tbody>
</table>

Table 4.2: Microstructural parameters of the activation functions governing $w_a$

<table>
<thead>
<tr>
<th>Motor unit type</th>
<th>Fiber Type</th>
<th>Index i (-)</th>
<th>$\rho_i$ (%)</th>
<th>$\bar{F}_i$ (N)</th>
<th>$T_i$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slow (S)</td>
<td>I</td>
<td>1</td>
<td>5</td>
<td>0.025</td>
<td>0.020</td>
</tr>
<tr>
<td>Fast resistant (FR)</td>
<td>IIa</td>
<td>2</td>
<td>29</td>
<td>0.044</td>
<td>0.011</td>
</tr>
<tr>
<td>Fast fatigue (FF)</td>
<td>IIb</td>
<td>3</td>
<td>66</td>
<td>0.768</td>
<td>0.011</td>
</tr>
</tbody>
</table>

The passive material parameters from Table 4.1 were determined by least squares optimization to fit the muscle model to experimental data from Hawkins and Bey (1994). These experiments quantified the purely passive and fully activated muscle response of rat *tibialis anterior* muscle. For this muscle microstructural properties are available in literature.

Note, that in comparison to Ehret et al. (2011) the parameters $\bar{F}_i$ (twitch force of motor unit type $i$) have been multiplied by a factor 10 in order to reproduce the data presented by Hawkins and Bey (1994). Additional material parameters: $I_i = 4.0\, ms$ ($i = 1, 2, 3$), $Na = 52.07\, cm^{-2}$, $\lambda_{\text{min}} = 0.682$, $\lambda_{\text{opt}} = 1.192$, $\lambda_m = 0.0$. 

1
In uniaxial tension simulations of the active muscle presented here, the muscle is fully activated to contract to its minimal length first, before the external stretch is applied through a prescribed displacement. The simulations using the decoupled formulation show a nonphysical volume growth for rather small axial stretches, as it can be seen in Figure 4.1. This observation has been reported by Helfenstein et al. (2010) for the very same numerical example but for other fiber-reinforced material models implemented according to the decoupled formulation. In their work, Helfenstein et al. showed that the additive split of the strain energy function might lead to undesired material responses even though the strain energy function is polyconvex. It was concluded, that for deformation modes at which the fiber contribution to the total strain energy is sufficiently large, effective fiber stretch is reduced through increasing spherical deformations.

The results of the present study (Figure 4.1) also demonstrate that the decoupled formulation for fiber-reinforced material models lacks to preserve volume also for active materials such as muscle. At the same time, it can be shown that the coupled formulation based on the strain energy function $W$ (4.1) adequately constrains volume changes for stretches far beyond the physiological range of soft biological tissues.

The nonphysical volumetric response was further analyzed by an eigenvalue analysis of the two different spatial tangent modulus tensors derived from $W$ and $\bar{W}$. For each time increment in the above mentioned simulation, the six eigenstates and corresponding eigenvalues provide a measure of corresponding stiffness. For the two implementations compared here, $t^{(1)}$ points along the space diagonal of the cube, $t^{(2)}$ points predominantly in the direction of the fiber and $t^{(3)}$ lies in the plane perpendicular to the
fibers. Eigenstates $t^{(4)}$, $t^{(5)}$, $t^{(6)}$ are associated with the shearing modes and are of less interest for the case of uniaxial tension presented here (see e.g. Annin and Ostrosablin (2008) and Mehrabadi and Cowin (1990)).

Figure 4.2 shows the evolution of the first three eigenvalues of the spatial tangent modulus tensor for (a) the purely passive muscle and (b) the active muscle using the decoupled formulation. In the passive case, the $\lambda_1$- and $\lambda_2$-curves cross. This means, that the principal direction of stiffest material response changes from being along the space diagonal of the cube to the vector mainly in direction of the fiber. This happens in the stretch range where uncontrolled volume growth begins as seen in Figure 4.1. To the authors knowledge, this behavior has not been presented before and provides significant information on the unphysical material response due to the decoupling of the strain energy function into a distortional and dilatational part.

For the activated muscle, the similar crossing of eigenvalue curves is observed again as shown in Figure 4.2(b). Additionally, we also observed that for fiber stretches $\lambda_m < 0.682$ there is no contribution of the active components to the overall mechanical response of the muscle. For fiber stretches $\lambda_m \geq 0.682$, however, the material parameter $w_a$ becomes non-zero, which results in a discontinuous evolution of $\lambda_2$ and $\lambda_3$. Only the eigenvalue associated with the element space diagonal ($\lambda_1$) behaves continuously and is almost constant. However, the behavior of $\lambda_2$ is most important since it becomes negative for fiber stretches $\lambda_m$ between 1.1 and 1.18 while all other eigenvalues remain positive. Negative eigenvalues of the spatial tangent modulus tensor indicate a non-positive definite tangent stiffness which is unphysical for the case presented here.
Much to the contrary, the coupled formulation does not exhibit either of the problems revealed for the decoupled formulation as shown in Figure 4.3 for the (a) passive and (b) active muscle behavior. For the passive muscle stretching the eigenvalues evolve continuously, are always positive and do not cross.

![Figure 4.3: Evolution of the first three eigenvalues of the spatial tangent modulus tensor based on the coupled formulation.](image)

The simulation of active uniaxial tension using the coupled formulation based on the strain energy function \( W \) (4.1) including the active material response renders only positive eigenvalues of the spatial tangent modulus tensor.

Based on the performance analysis of both functional forms it can be concluded that the split of the strain energy into a volumetric and distortional part (4.3) leads to unphysical phenomena. Especially, the inadequately constrained volume as well as the negative eigenvalues present significant limitations to the applicability of this approach for the implementation of fiber-reinforced anisotropic passive as well as active tissue models. Hence, further verification of the muscle model implementation is carried out for the coupled functional form \( W \) (4.1).

### 4.3.2 Benchmark simulations

There are different modes of muscle tissue contraction depending on the activation and the kinematic boundary conditions. Generally, a distinction is made between (i) concentric or eccentric contraction, (ii) isometric contraction, (iii) isotonic contraction, and (iv) isokinetic contraction. In the first case the force produced upon activation is either greater or lower than the load applied to the muscle and thus the muscle either shortens (concentric contraction) or lengthens (eccentric contraction). Under isometric contraction the muscle remains at constant length, so that the force produced by the muscle balances
the applied load. For the isotonic case, the contraction force of the muscle is constant and independent of changes in muscle length. Finally, the isokinetic contraction refers to the case of constant contraction velocity.

In order to understand the model response to different contraction modes, a benchmark example is considered. The geometry is defined such that all the above mentioned modes can be simulated and combined. The setup is shown in Figure 4.4 where the muscle is represented by a rectangular block with a width of 100 mm, a length of 500 mm, and a thickness of 20 mm. The muscle fibers are aligned in the longitudinal direction of the block. Both ends of the muscle are tied to rigid bodies which can only move in the longitudinal direction of the block and cannot penetrate each other.

![Figure 4.4: Geometry of benchmark model (n = 2).](image)

In the simulation, the rectangular block contracts upon activation until both rigid bodies are in contact (free contraction). Then, the contraction force increases until it reaches the maximal value corresponding to the current state of the muscle (isometric contraction). The material parameters used for this simulation are given in Tables 4.1 and 4.2. The muscle model was meshed by dividing the longitudinal, transverse, and height directions into $10n$, $2n$, and $n$ segments, respectively. Therefore, the parameter $n$ controls the level of mesh refinement. For this simulation selective-reduced integration 8-noded hexahedral elements (C3D8) were used.

Figure 4.5 shows the evolution of the contraction force predicted in the simulation. The tetanic force is reached approximately at time $t = 0.08$ seconds and remains constant for the rest of the activation time. There is no loss in tetanic force since muscle fatigue is not considered in the muscle model presented here. The gap between the two rigid bodies closes within the first millisecond and remains closed for the remainder of the simulation time. In order to investigate the homogeneity of force in the muscle, three different levels of mesh refinement were investigated. As expected for this simple uniaxial tension case, the maximum muscle force differed by less than 1% when comparing meshes with $n = 1, 2, 5$. Although the inhomogeneity of the force field at the boundaries, where the muscle is attached to the rigid bodies, showed a dependency on mesh refinement, it had a minor impact on the overall response of the muscle.
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Figure 4.5: Tetanic muscle force in the benchmark example.

The convergence behavior of the implemented material model is expressed in terms of residual force in Table 4.3. A fixed step size of $\Delta t = 1.0 \cdot 10^{-6}$ seconds was defined in order to evaluate the equilibrium equations. The evident quadratic convergence confirms the correct implementation of the material tangent for the proposed muscle model.

Table 4.3: Convergence rate of the first four loading steps in the benchmark simulation.

<table>
<thead>
<tr>
<th></th>
<th>Increment #1</th>
<th>Increment #2</th>
<th>Increment #3</th>
<th>Increment #4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iteration #1</td>
<td>$7.380 \cdot 10^{-2}$</td>
<td>$5.811 \cdot 10^{-3}$</td>
<td>$6.508 \cdot 10^{-3}$</td>
<td>$7.185 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Iteration #2</td>
<td>$1.352 \cdot 10^{-3}$</td>
<td>$8.512 \cdot 10^{-6}$</td>
<td>$1.051 \cdot 10^{-5}$</td>
<td>$1.261 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>Iteration #3</td>
<td>$4.756 \cdot 10^{-7}$</td>
<td>$2.172 \cdot 10^{-11}$</td>
<td>$3.111 \cdot 10^{-11}$</td>
<td>$4.338 \cdot 10^{-11}$</td>
</tr>
</tbody>
</table>

The muscle response due to a variation in individual twitch forces $F_i$ as well as interstimulus rate $I_i$ is analyzed on the example of isometric contraction, as shown in Figure 4.6. For this purpose, both rigid bodies are fixed and the total muscle length of 500mm is thus prescribed. Apart from the values of $F_i$ and $I_i$, material parameters are the same as in the previous simulations. The impact of the twitch force variation is investigated by varying the values of $F_i$ (reported in section 4.3.1) by $\pm 10\%$. Thus, a weaker and stronger muscle response is simulated.

It can be seen from Figure 4.6 that the magnitude of muscle force differs from previous simulations due to the different fiber stretches at which the muscle contracts isometrically (present case $\lambda_m = 1.0$, previous simulations $\lambda_m = 0.8$ due to the isotonic contraction until both rigid bodies are in contact). It can be observed that the force-time history is similar to the previous example. A variation of twitch forces by $\pm 10\%$ results in a corresponding variation on the tetanic forces by $\pm 11\%$. Furthermore, the maximum force level drops significantly for longer interstimulus times. Increasing the interstimulus rate by a factor six causes a drop in the maximum force by 80%.
4.4 Simulation of masseter muscle response

The human mastication system consists of the masseter, the temporalis, the medial pterygoid, and the lateral pterygoid muscles. All of these except for the temporalis muscle originate from the skull and insert into the mandible. Moreover, the temporomandibular joint builds a connection point between mandible and temporal bone. Due to the shape of the joint, movements in all planes are possible, thus allowing to open and close the mouth, to move sidewise, and to grind during mastication and speech. The lateral pterygoid muscle allows to open the jaw, while the other three muscles mainly act in closing and sidewise movements of the jaw. The mastication muscle group is innervated by the mandibular branch of the trigeminal nerve.

Barbarino et al. (2008, 2009b) presented an anatomically detailed FE model of the face of a 27 year old male. In their work, most facial soft tissue structures including muscles of the mastication system were semi-automatically reconstructed from magnetic resonance images. The mechanical interactions between different tissues were represented, and the nonlinear force-deformation characteristic of soft biological materials was governed by three dimensional constitutive equations that are valid for finite elastic-viscoplastic deformations (Rubin and Bodner, 2004, 2002).

The geometric representation presented here is based on the segmentation proposed in Barbarino et al. (2009b). Other examples aiming at the reconstruction of such tissue structures are presented in literature (Böl et al., 2011a; Flynn et al., 2015; Kajee et al., 2013; Röhrle and Pullan, 2007; Taylor et al., 2013). The mastication system is reduced to the masseter muscle only due to the fact that during mastication, the masseter muscle is dominantly responsible for the generation of bite force to be simulated in this example. The physiological resting position of the mandible (the relaxed state of the masseter muscle) is characterized by a mouth opening of 4.0mm at the incisors (Manns et al., 1979).
A homogeneous muscle fiber alignment in the longitudinal muscle direction is assumed. The muscle insertion points are modeled by boundary conditions applied to the superior end of the muscle where it inserts into the zygomatic arch and the inferior end. Here, it is connected to the inferior posterior region of the mandible. The jaw rotates around the transverse axis, while the sagittal and vertical axes are locked. Bone structures are modeled as rigid bodies and the masseter mesh consists of selective-reduced integration 8-node elements (C3D8). A representation of the mastication system considered in this example is shown in Figure 4.7.

Figure 4.7: Anatomical reconstruction of the masseter muscle, skull and mandible (left); the displacement magnitude of the masseter muscle at the end of the activation time (right).

When activating the masseter muscle, the jaw rotates around the temporomandibular joint causing the mouth to close. Once the teeth are in contact, the total muscle length is fixed while the muscle continues to increase the contraction force until it reaches the maximum value. The bite strength of the human mastication system has been investigated in several different ways. For example, Van Eijden (1991) provided a setup allowing to determine bite force values for various bite positions and force directions. By least squares optimization, we determined material parameters based on the maximal muscle force of 500 N- according to the range of muscle forces recorded by Van Eijden (1991).

The microstructural parameters entering the active part of the model are derived from physical properties of human masseter. The experimental work by Eriksson and Thornell (1983), Fuglevand et al. (1999), and Yemm (1977), allows to determine the distribution of muscle fiber type I (62%) and IIb (38%), as well as their respective twitch forces and
4.5. Conclusion

contraction times. According to Eriksson and Thornell (1983), the human masseter muscle has a negligible amount of fast twitch muscle fiber type IIa. Tables 4.4 and 4.5 summarize the material parameters used in the numerical example, while \( \text{Na} = 7.384 \text{cm}^{-2} \) in (4.11).

Table 4.4: Material parameters of the passive model determined by the least squares optimization.

<table>
<thead>
<tr>
<th>( \mu ) (kPa)</th>
<th>( \alpha ) (-)</th>
<th>( \beta ) (-)</th>
<th>( w_0 ) (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.165</td>
<td>19.96</td>
<td>2.02</td>
<td>0.736</td>
</tr>
</tbody>
</table>

Table 4.5: Microstructural parameters obtained from experiments on masseter muscle fibers by Eriksson and Thornell (1983), Fuglevand et al. (1999), and Yemm (1977).

<table>
<thead>
<tr>
<th>Motor unit type</th>
<th>Fiber type</th>
<th>Index i (-)</th>
<th>( \rho_i ) (%)</th>
<th>( \bar{F}_i ) (N)</th>
<th>( T_i ) (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slow (S)</td>
<td>I</td>
<td>1</td>
<td>62.5</td>
<td>0.0829</td>
<td>0.0656</td>
</tr>
<tr>
<td>Fast fatigue (FF)</td>
<td>IIb</td>
<td>2</td>
<td>37.5</td>
<td>0.0536</td>
<td>0.0459</td>
</tr>
</tbody>
</table>

The numerical model proposed here provides not only a way to predict muscle forces but also allows to realistically estimate the 3D geometric changes in the muscle shape based on the current state of contraction. As a consequence of the nearly incompressible behavior, the contraction will result in a shortening and thickening of the masseter muscle. Figure 4.7 shows the magnitude of displacement at the end of the contraction period. The activation will cause a rotation of the jaw until the teeth are closed. Note that the teeth opening of 4.0mm of the incisors corresponds to a vertical displacement of about 3.3mm in the region of the molar teeth.

The predicted muscle force-time curve is plotted in Figure 4.8. The muscle force continuously increases up to a peak force level of 500N. The time to reach tetanic force is around 0.4 seconds which is in line with Röhrle and Pullan (2007). Moreover, the shape of the muscle force curve over time closely follows data found in literature (Koolstra and Van Eijden, 2001).

4.5 Conclusion

In the present paper, two FE implementations of a continuum constitutive model with and without the volumetric-isochoric split of the strain energy function of skeletal muscle tissue are compared. The decoupled approach is often favored in cases where volumetric and distortional material response can be expressed in terms of two individual parts in the strain energy function (Holzapfel, 2000). The passive part and the physically based active part were selected such that polyconvexity and coercivity are guaranteed. The derivation of the two corresponding Cauchy stress tensors \( \sigma \) and the consistent spatial tangent stiffness \( C^J \) are provided and implemented in the user-defined ABAQUS subroutine UMAT.
A direct comparison of the two functionally different formulations revealed substantial numerical limitations of the decoupled approach. Significant volume growth takes place within a physical range of the muscle deformation and results in an unphysical representation of muscle tissue behavior. On the other hand, the coupled formulation is shown to properly predict the nearly-incompressible nature of the tissue as well as its active response. Based on the eigenvalue analysis of the spatial tangent modulus tensor, it is concluded that the decoupled approach is unsuitable for anisotropic fiber-reinforced materials, both passive and active. This observation provides strong motivation to formulate the strain energy function in terms of the full right Cauchy Green tensor. In a benchmark example, the coupled model demonstrated quadratic convergence and good predictive capabilities in different loading configurations.

Finally, an anatomically based representation of the human masseter muscle was used to investigate the predictive capabilities of the model with respect to shape changes and muscle force production during the biting phase of mastication. This example shows the possibility to simulate geometrically complex structures and highly nonlinear problems including active material response.

Experimental verification of the three-dimensional prediction of muscle shape changes during contraction is planned as a next step. Future work will also consider an anatomically based representation of muscle fiber orientation.

![Masseter muscle force response during an activation period of 600ms.](image)
APPENDIX

4.5.1 Derivation for the coupled formulation

The components of the derivatives of $C^{-1}$ and $C^{-1}\tilde{L}C^{-1}$ with respect to $C$ as in (4.20) are given by

$$
\left( \frac{\partial C^{-1}}{\partial C} \right)_{IJKL} = -\frac{1}{2} \left( C^{-1}_{IK}C_{JL} + C^{-1}_{IL}C_{JK} \right),
$$

(4.28)

$$
\left( \frac{\partial C^{-1}\tilde{L}C^{-1}}{\partial C} \right)_{IJKL} = -\frac{1}{2} \left( C^{-1}_{IK}C_{JL} \tilde{L}_{MN}C_{NL} + C^{-1}_{IL}C_{JM} \tilde{L}_{MN}C_{NK} \right) - \frac{1}{2} \left( C_{JK}C_{IL} \tilde{L}_{MN}C_{NL} + C_{JL}C_{IM} \tilde{L}_{MN}C_{NK} \right).
$$

(4.29)

4.5.2 Derivation for the decoupled formulation

The equations presented here follow general concepts of continuum mechanics (as presented in e.g. Holzapfel (2000)). However, due to the active elements entailed in the constitutive equations presented in Section 4.2.1 the standard forms of the decoupled approach include additional terms. Hence, for the sake of completeness, we present the full set of equations in the following.

The second Piola-Kirchhoff stress tensor $S$ resulting from the strain energy function $\bar{W}$ (4.3) reads as

$$
S = 2 \frac{\partial \bar{W}}{\partial C} = 2 \frac{\partial \bar{W}_{\text{iso}}}{\partial C} \cdot \frac{\partial \bar{C}}{\partial C} + 2 \frac{\partial \bar{W}_{\text{vol}}}{\partial J} \frac{\partial J}{\partial C},
$$

(4.30)

where the derivatives of $\bar{C}$ and $J$ with respect to $C$ are given by

$$
\frac{\partial \bar{C}}{\partial C} = J^{-2/3} \left[ \bar{\Pi} - \frac{1}{3} \bar{C} \otimes \bar{C}^{-1} \right], \quad \frac{\partial J}{\partial C} = \frac{1}{2} JC^{-1}.
$$

(4.31)

Here, the fourth-order projection tensor $P$ and the fourth-order unit tensor $\Pi$ have been introduced as follows

$$
P = \Pi - \frac{1}{3} \bar{C}^{-1} \otimes \bar{C}, \quad (\Pi)_{ijkl} = \frac{1}{2} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right).
$$

(4.32)

Thus, (4.30) can be rewritten by

$$
S = \tilde{S}_{\text{iso}} + J \frac{\partial \bar{W}_{\text{vol}}}{\partial J} \bar{C}^{-1}, \quad \tilde{S}_{\text{iso}} = J^{-2/3} P : \tilde{S},
$$

(4.33)

where

$$
\tilde{S} = \frac{\partial \bar{W}_{\text{iso}}}{\partial C} = \frac{\mu}{2} \left\{ \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \left( \tilde{L} + w_a M \right) - \exp \left[ \beta \left( \tilde{K} - 1 \right) \right] \left( \tilde{C}^{-1} \tilde{L} \tilde{C}^{-1} \right) \right\}.
$$

(4.34)
Again, considering the dependence of $w_a$ on the right Cauchy Green tensor $C$ the material tangent corresponding to the strain energy function $\bar{W}$ (4.3) is

$$
\mathcal{C} = 4 \frac{\partial^2 \bar{W}}{\partial C \partial C} = 2 \frac{\partial}{\partial C} \left[ 2 \frac{\partial \bar{W}_{iso}}{\partial C} : \frac{\partial C}{\partial C} + 2 \frac{\partial \bar{W}_{vol}}{\partial J} \frac{\partial J}{\partial C} \right]
$$

$$
= J^{-4/3} \mathbf{P} : \bar{\mathbf{C}} \mathbf{P}^T + 2 \frac{\partial \left( J^{-2/3} \mathbf{P} \right)}{\partial C} : \bar{\mathbf{S}}
$$

$$
+ 4 \frac{\partial^2 \bar{W}_{vol}}{\partial J \partial J} \frac{\partial J}{\partial C} \otimes \frac{\partial J}{\partial C} + 4 \frac{\partial \bar{W}_{vol}}{\partial J} \frac{\partial^2 J}{\partial C \partial C},
$$

where

$$
\bar{\mathcal{C}} = 2 \frac{\partial \bar{\mathbf{S}}}{\partial C} = \mu \left\{ \alpha \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \left( \tilde{\mathbf{L}} + w_a \mathbf{M} \right) \otimes \left( \tilde{\mathbf{L}} + w_a \mathbf{M} + \mathbf{C} : \mathbf{M} \frac{\partial w_a}{\partial C} \right) 

+ \exp \left[ \alpha \left( \tilde{I} - 1 \right) \right] \mathbf{M} \otimes \frac{\partial w_a}{\partial C}

- \beta \exp \left[ \beta \left( \tilde{K} - 1 \right) \right] \left( \mathbf{C}^{-1} \tilde{\mathbf{L}} \mathbf{C}^{-1} \right) \otimes \left( \mathbf{C}^{-1} \tilde{\mathbf{L}} \mathbf{C}^{-1} \right)

- \exp \left[ \beta \left( \tilde{K} - 1 \right) \right] \frac{\partial}{\partial C} \right\}.
$$
Part III

Experimental Characterization of Facial Soft Tissues
Overview

Physically based simulation of facial tissue response requires the development of constitutive model equations, the experimental characterization of deformation mechanisms, the relation between tissue deformations and internal forces, and underlying changes in the mechanical properties of tissue constituents.

The following part is concerned with the experimental characterization of the mechanical behavior of active and passive soft facial tissues and discusses three different experimental campaigns.

Chapter 5 contains the suction based characterization of the superficial layers of the face and forehead. The experimental data presented therein is used for the identification of material parameters sets for skin and subcutaneous tissue/SMAS.

Chapter 6 presents the experimental characterization of interaction properties of individual tissue layers in the forehead. The experimental results are used for the definition of interaction properties in the anatomically based finite element model of the forehead. This chapter is based on the following publication:


Work presented in Chapter 7 is concerned with the visualization of changes in tissue interaction properties with respect to aged and diseased skin tissue based on the previously developed ultrasound imaging method. Two additional subjects volunteered in this study allowing for the investigation of changes in tissue interaction due to morphological transformations.

And finally, Chapter 8 summarizes an experimental study to visualize the mechanical response of masseter muscle tissue during contraction. This study was carried out in collaboration with the Nestlé Research Center and is part of the overall effort of physically based modeling of the mastication process. It includes the development of an anatomy based finite element model of the mastication system in order to predict muscle shape changes during biting. Numerical simulations are compared with the experimentally observed muscle response.
Chapter 5

Suction based mechanical characterization of superficial soft tissues

5.1 Introduction

The increasing need for physical simulations of tissue behavior as in facial expressions or medical applications, ranging from the planning of surgical procedures to the prediction of age related tissue changes, requires improved numerical modeling of tissue structures and reliable experimental characterization of the mechanical response of individual soft tissues.

Following the numerical implementation of the constitutive equations of Rubin and Bodner (2002) presented in Chapter 3, the next step towards realistic simulations involves the determination of material model parameters which are capable of representing experimentally observed tissue behavior. The suction based characterization of superficial facial soft tissues and the material parameter optimization represent the two main objectives of the following work. The present study builds up on the experimental method for suction experiments on skin tissue in the jaw region presented in Chapter 3 and elaborates on the location, time, and history dependent behavior of skin and, especially, the underlying tissues in the face and forehead.

In general, besides suction based measurements several other testing methods have been used for the mechanical characterization of facial tissues such as tension, torsion, shearing, and indentation measurements. The choice of suction based testing is strongly motivated by (i) simple applicability and flexibility with respect to testing locations, (ii) non-invasive in-vivo characterization of soft tissue, (iii) targeted characterization of specific tissue layers through adaptation of the probe opening diameter, (iv) the multiaxial state of deformation in contrast to the less relevant deformation modes of other testing methods (i.e. uniaxial tension or torsion), and (v) comparability of results with existing data such as (Weickenmeier and Jabareen, 2014).

Due to locally varying anatomical features in the face and forehead, a location dependent tissue response is expected. Measurements of the superficial tissue properties in three functionally different regions, i.e. jaw, parotid, and forehead, are related to the overall tissue structure in order to improve the understanding of the mechanical behavior of relevant facial structures. The jaw region is characterized by a soft tissue structure al-
allowing increased deformability to enable speech, facial expressions, and other movements of the mouth. The forehead region has a layered anatomical structure of several different tissues including highly active muscle tissue. Finally, the parotid region provides significant support to the tissue of the cheek due to its dense connective tissue including the superficial musculoaponeurotic system (SMAS). In the presented experimental campaign two measurement devices are used which differ in probe opening diameter by a factor of four. This allows to quantify the impact of tissue structures which are deeper than the most superficial skin layer. In the following, when referring to the layered structure of facial tissues, the most superficial layer is associated with skin (including dermis and epidermis), while the second layer is denoted as subcutaneous tissue. In dependence of the facial region the subcutaneous layer consists of rather fatty tissue, dense fibrous connective tissue and fascia, or SMAS. For this reason, the finite element (FE) model of the Cutometer device differentiates between skin and subcutis, while the three layers of the tissue model for the Aspiration measurements are associated with skin, subcutis, and muscle/SMAS (depending on the measurement site).

The suction method allows for different loading profiles which activate mechanical mechanisms of variable time scales, i.e. the instantaneous tissue deformation in comparison to the long term response, as well as the tissue behavior upon gradually changing loads. Moreover, cyclic loading profiles provide means of visualizing any history dependent tissue response.

The study presented here provides a broad range of experimental data which allows for the identification of material parameters for skin and subcutaneous tissue through an inverse FE problem, similar to previous work (Barbarino et al., 2011; Weickenmeier and Jabareen, 2014). The newly proposed sets of material parameters represent a significant improvement over existing work and are verified by direct comparison of experimental data and the corresponding numerical simulation. In the following, the experimental setup of the suction measurements and the experimentally observed tissue response are presented. The second part contains the parameter identification scheme and discusses the newly determined material parameter sets. Through direct comparison of the numerically predicted tissue behavior and the experimental data the predictive capabilities of the constitutive equations in combination with the new material parameters are evaluated.

5.2 Suction measurements on facial tissues

Suction based characterization of soft tissues is a well-established measurement method which provides quantitative information on the relation between a multiaxial loading state and the corresponding tissue deformation. The experimental campaign presented here might be seen as an extension of previously published data from our lab (Weickenmeier and Jabareen, 2014): it includes the location dependence of facial tissues in form of two additional measurement sites, adapted loading times for the quantification of time dependent behavior, and cyclic loading profiles for the assessment of deformation history. Moreover, the whole series of different loading profiles is conducted with two different measuring devices mainly differing by probe opening diameter in order to assess skin and deeper tissues separately.
5.2. Suction measurements on facial tissues

The experimental setup is shown in Figure 5.1 and was developed based on experience from previous studies. Main sources of measurement errors are given by the contact pressure between probe and skin, contact angle between probe and skin, and reproducibility with respect to probe placement. Hence, a headrest commonly used in ophthalmology was modified to include a fixation device for the two probes allowing for flexible positioning and alignment of the probe with respect to the subject's head as well as a reproducible contact pressure throughout individual measurements. As the measurements presented in the following sections show, intra-subject variability was minimized and consistent tissue deformation was measured for repeated application of each device.

Figure 5.1: Experimental setup for the (b) Cutometer and (d) Aspiration device. The modified headrest (a) provides high flexibility for the positioning and alignment of the suction probes. To quantify location specific material behavior three different measurements sites are tested (c).
The two devices differ in probe opening diameter where the commercially available Cutometer MPA580 (Courage and Khazaka, 2014) has an opening diameter of 2mm and the Aspiration device of 8mm. The measurement principle is based on generating a negative pressure inside the probe cavity causing tissue to be sucked in as shown in Figure 5.2. An optical system captures the deformation profile of the tissue bubble during the whole loading cycle. Two loading profiles were defined such to activate mechanical tissue properties at different time scales. Table 5.1 contains the full list of loading profiles which were measured in each location. \textit{Instant loading} refers to measurements of instantaneous loading of the tissue to the full negative load ($p_{\text{max}}$) which is held constant for the time span denoted by $t_{\text{inst}}$. The small retardation loading time to reach maximum suction pressure is predetermined by the individual controllers of the two devices. Instantaneous loading reveals the (short term) purely elastic as well as the long term tissue response. \textit{Linear loading} refers to the linearly increasing and decreasing loading of the tissue at a constant pressure rate. This loading mode activates deformation mechanisms with intermediate time scales which include fluid flow through porous tissues and temporary reorientation of the collagen network in skin and underlying tissue. Loading magnitudes are based on previously defined loading profiles and represent realistic loads as they appear in facial expressions (Barbarino et al., 2011; Weickenmeier and Jabareen, 2014). Each loading protocol is repeated at least four times to capture potential variations in tissue response. Waiting times of at least 45 seconds between individual measurements are enforced in order to allow for the tissue to return to its initial state. In a corresponding sensitivity analysis, shorter waiting times between repeated suction measurements revealed a memory effect in the soft tissues response. At the same time, for waiting times longer than 45 seconds neither significant changes in the tissue’s reference state nor history dependent tissue behavior were observed. Measurements were performed on a 29 year old male subject in the upright position as indicated in Figure 5.1.

![Figure 5.2: Suction based measurement principle. Negative pressure inside the probe-head cavity causes soft tissue to be sucked in. During the entire loading cycle an optical measurement system determines the tissue penetration depth relative to the initial deformation.](image-url)
5.2. Suction measurements on facial tissues

Table 5.1: Loading profiles for Cutometer and Aspiration measurements

<table>
<thead>
<tr>
<th></th>
<th><strong>CUTOMETER</strong></th>
<th><strong>ASPIRATION</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Instant loading</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$p_{\text{max}}$</td>
<td>300.0 mbar</td>
<td>66.0 mbar</td>
</tr>
<tr>
<td>$t_{\text{inst}}$</td>
<td>60.0 s</td>
<td>31.0 s</td>
</tr>
<tr>
<td>$p_{\text{max}}$</td>
<td>500.0 mbar</td>
<td></td>
</tr>
<tr>
<td>$t_{\text{inst}}$</td>
<td>60.0 s</td>
<td>31.0 s</td>
</tr>
<tr>
<td>$p_{\text{max}}$</td>
<td>133.0 mbar</td>
<td></td>
</tr>
<tr>
<td>$t_{\text{inst}}$</td>
<td>31.0 s</td>
<td>31.0 s</td>
</tr>
<tr>
<td>$p_{\text{max}}$</td>
<td>200.0 mbar</td>
<td></td>
</tr>
<tr>
<td>$t_{\text{inst}}$</td>
<td>31.0 s</td>
<td></td>
</tr>
<tr>
<td>$\dot{p}$</td>
<td>10.0 mbar/s</td>
<td>15.0 mbar/s</td>
</tr>
<tr>
<td>$t_{\text{lin}}$</td>
<td>35.0 s</td>
<td>10.0 s</td>
</tr>
<tr>
<td>$\dot{p}$</td>
<td>15.0 mbar/s</td>
<td>20.0 mbar/s</td>
</tr>
<tr>
<td>$t_{\text{lin}}$</td>
<td>35.0 s</td>
<td>10.0 s</td>
</tr>
<tr>
<td>$\dot{p}$</td>
<td>20.0 mbar/s</td>
<td>30.0 mbar/s</td>
</tr>
<tr>
<td>$t_{\text{lin}}$</td>
<td>35.0 s</td>
<td>10.0 s</td>
</tr>
</tbody>
</table>

The results of the Cutometer and Aspiration measurements, a comparison of individual facial regions, and an overview of the average tissue response are presented in the following sections.
5.2.1 Results of Cutometer measurements

The results of the Cutometer measurements are shown in Figure 5.3. Gray curves represent individual measurements for each loading case and black curves are the averages of all measurements \((\geq 4)\) per loading case. It is observed that the variation between individual measurements of the same loading case is very low which is a direct result of the optimized experimental setup. In particular, the full range of experimental data provides a consistent quantification of the mechanical response across all loading profiles.

The jaw region shows the softest tissue behavior of the three different regions evident from the largest displacement of the tissue bubble or rather its apex height. Parotid and forehead show a noticeably lower apex response for all loading magnitudes due to the presence of rather stiff supportive tissue layers in these regions.

The measurements of instantaneous loading show a rapid increase in apex height followed by a quick stabilization. In the case of linear loading the skin bubble increases continuously until maximum loading. Upon linear unloading for \(t > t_{\text{lin}}\) the tissue bubble shows a delayed response by remaining near the maximum displacement for around 5 seconds before decreasing due to progressive unloading. The skin bubble generally does not fully return to its initial state upon complete unloading, thus revealing the elastic-viscoplastic character of facial soft tissues. In particular, this highlights the necessity of waiting periods between individual measurements to allow for the tissue to recover its natural state.

5.2.2 Results of Aspiration measurements

The Aspiration device was developed at ETH Zurich and has been adapted for several different investigations since, including intra-operative testing of human liver (Hollenstein et al., 2013), the history of cervical tissue stiffness over the course of pregnancy (Badir et al., 2013a,b), and the testing of superficial tissue layers in the face (Barbarino et al., 2009a, 2011). The latter experimental setup was adapted in the present study for the characterization of the tissue properties of skin and SMAS as outlined above.

The experimental results are presented in terms of the evolution of apex height during the loading cycle as shown in Figure 5.5. During the Aspiration measurement an optical system inside the probe shaft captures the profile of the tissue bubble in form of an image sequence. Through subsequent image processing initial bubble height and evolution of apex displacement are extracted from the bubble profile. In order to allow for a direct comparison with the Cutometer measurements, the evolution of apex displacement is given in relative terms with respect to the initial tissue bubble height. The significant dependence of this measurement quantity on contact pressure between probe and skin surface, further motivates the employment of the new setup (Figure 5.1). For one, this setup allows to control contact pressure through optimal positioning of the probe with respect to the skin surface and for the other, it minimizes the variation of contact pressure within repeated measurements.
5.2. Suction measurements on facial tissues

Figure 5.3: Suction measurements in three different facial regions using the Cutometer device.
The determination of apex displacement is based on an image conversion from gray-scale to black-and-white images by means of a gray-value threshold. This allows to differentiate between tissue bubble and background as shown for three distinct threshold values in Figure 5.4. The black-white threshold (BWT) is determined manually by visual judgment of sample images to identify an appropriate value. This value is strongly dependent on experimental conditions such as skin type, measurement region, and lighting settings of the Aspiration device, and may vary for different measurement sites.

Figure 5.4: Sensitivity analysis on one Aspiration image with three different black-white thresholds. Hair causes measurement errors in detecting the skin tissue contour which is strongly dependent on the BWT.

The experimental results show good agreement between individual measurements with the same protocol as well as a consistent deformation behavior for the different loading magnitudes in the same measurement site. From comparison with Cutometer data, a larger variation of apex deformation is observed, which may be explained by potential inhomogeneities of the increased region of penetrated tissue and measurement inaccuracies within the data acquisition process described above. The largest scatter in measurement data is observed in the forehead as this region is characterized by (i) a curved surface increasing the challenge of proper probe alignment, (ii) the presence of skin wrinkles at a length scale similar to the penetration zone of the Aspiration device, and (iii) a tissue structure including active muscle tissue which is involuntarily affected during measurements. In the end however, the averages for each loading magnitude represent a consistent tissue behavior across the range of loading cases within this study and demonstrate the reliability and repeatability of the experimental protocol. Similar to the Cutometer measurements, jaw tissue expresses the softest response in terms of largest apex displacement. Moreover, the nonlinear and time dependent tissue response is very pronounced, especially, in the linear loading measurements due to increased tissue penetration resulting from the larger probe opening diameter.
5.2. Suction measurements on facial tissues

Figure 5.5: Suction measurements in three different facial regions using the Aspiration device.
5.2.3 Comparison of regional differences

Facial anatomy is generally characterized by a locally varying layered tissue structure in terms of present tissue types, tissue thicknesses, and interactions between individual tissues. In the face the high level of functionality enabling speech, mastication, and facial expressions is related to a pronounced diversity in the organization of varying tissue structures. The suction experiments are expected to capture this location dependent tissue response, especially when comparing measurements with the two probe opening diameters and the corresponding involvement of superficial and deeper tissue layers.

For a comparison of the two loading cases and the different loading magnitudes, Figure 5.6 visualizes all measurements in form of facial averages. The data was normalized with respect to the total measurement time which differ for the two devices. There is a consistent increase in apex height with increasing loading magnitude for both loading types and both measurement devices produce a similar evolution of tissue deformation which is of significant relevance for the subsequent parameter identification. The data shows clearly that the Aspiration measurement addresses deeper tissues and provides means for quantifying the mechanical properties of subcutaneous tissue when analyzed in combination with data for the superficial skin layer from the Cutometer.

To elaborate on the location dependent behavior, Figure 5.7 visualizes the facial average together with the location specific response for four representative measurements (Cutometer: instant 300mbar, linear 15mbar/s; Aspiration: instant 133mbar, linear 30mbar/s). In the Cutometer tests, forehead skin showed the stiffest response, while jaw skin was softest. This response is in line with anatomical data stating that skin is thickest in the forehead in comparison to parotid and jaw. In case of the Aspiration measurements, however, the parotid region showed the stiffest response while jaw tissue was significantly softer resulting in a much larger apex height. The observed behavior may be explained by the particular functionality of the subcutaneous tissue which has to (i) enable high flexibility for movements of the mouth in the raw regions, (ii) to serve as an anchoring point of lower facial tissues in the parotid region, and (iii) allow for large deformability and strong connectivity between multiple tissue layers during wrinkle formation in the forehead region. In fact, the parotid, jaw, and forehead regions differ in tissue structure, especially with respect to deeper layers, as well as their interactions. Deeper layers in the jaw region are generally fatty tissues and have no insertion points with any bone structure which provides the high level of deformability. In contrast, the deeper layers in the parotid region are characterized by dense connective tissue and SMAS which provide the increased support to the surrounding tissues. Finally, the forehead region requires both pronounced deformability and strong connectivity to surrounding tissues which is reflected in an intermediate tissue stiffness and the observed average apex height.

While the experimental data nicely captures the locally varying mechanical properties of the superficial tissue layers, most FE simulations presented in this thesis require material parameters which are capable of representing the average response of all facial tissues. For this reason, the determination of material parameters presented in the following, prioritized on parameter sets for skin and subcutaneous tissue which provide good agreement between the numerically predicted and experimentally observed tissue response of the facial average curves. The four measurements shown in Figure 5.7 are used for the
5.2. Suction measurements on facial tissues

optimization scheme as they encompass the full range of tissue behavior observed in the experimental campaign. Based on experience from the parameter identification presented in Chapter 3 it is found useful to consider both loading profiles and different loading magnitudes in order to balance the individual time scales of the tissue response associated with distinct mechanical properties of the tissues such as creep and relaxation.

Figure 5.6: Summary of all Cutometer and Aspiration measurements in terms of facial averages for the different loading profiles.

Figure 5.7: Comparison of regional differences for measurements considered in the parameter identification.
Chapter 5. Suction based characterization of superficial soft tissues

Even though a direct comparison with data found in literature is impossible due to differences in measurement protocols, measurement sites, and loading magnitudes, the absolute values of the presented apex deformation curves fall within values reported on forearm and cheek skin for similar probe opening diameters and loading conditions as reported in Table 5.2.

Table 5.2: Suction based measurements on skin reported in literature

<table>
<thead>
<tr>
<th>Authors</th>
<th>Region, probe Ø, pressure</th>
<th>Apex height</th>
</tr>
</thead>
<tbody>
<tr>
<td>Barbarino et al. (2011)</td>
<td>face, 2mm, 500mbar</td>
<td>0.52-0.63mm</td>
</tr>
<tr>
<td>Hara et al. (2013)</td>
<td>cheek, 2mm, 150mbar</td>
<td>0.12-0.42mm</td>
</tr>
<tr>
<td>Piérard et al. (2013b)</td>
<td>forearm, 2mm, 500mbar</td>
<td>0.12-0.33mm</td>
</tr>
<tr>
<td>Hendriks et al. (2006)</td>
<td>forearm, 6mm, 200mbar</td>
<td>1.10-1.60mm</td>
</tr>
<tr>
<td>Barbarino et al. (2011)</td>
<td>face, 8mm, 133mbar</td>
<td>2.25-3.70mm</td>
</tr>
<tr>
<td>Iivarinen et al. (2013)</td>
<td>forearm, elliptic 43x28mm, 200mbar</td>
<td>1.20-2.25mm</td>
</tr>
</tbody>
</table>

In literature, the experimental data from suction experiments is most often used for the determination of the Young’s modulus or the coefficients of simple nonlinear hyperelastic equations such as the Neo-Hookean strain energy function. These models, however, fall short of describing the full experimentally observed nature of superficial (facial) soft tissues.

5.3 Model parameter identification

The representation of the experimentally observed mechanical behavior of soft tissues by means of constitutive model equations is of fundamental interest in realistic simulation of tissue response in surgery planning, facial expressions, and wrinkle formation. The model equations by Rubin and Bodner (2002) were demonstrated to adequately represent typical mechanical properties of most soft facial tissues. The corresponding equations were implemented within the FE environment to allow for numerical simulation of these tissues (Weickenmeier and Jabareen, 2014). The implemented Rubin and Bodner model requires 15 material parameters in order to fully describe the tissue response. Based on experience with the properties of the material model, six of these parameters were identified to be determined through an inverse FE analysis, see Table 5.3.

The respective optimization scheme is adapted from Weickenmeier and Jabareen (2014) and extended such to include the FE model of the Aspiration experiment. The two FE models are shown in Figure 5.8. The Cutometer model is a two-layered structure with layer thicknesses of 1.7mm for skin and 3.0mm for subcutaneous tissue. The width of the rotation-symmetric model is 25mm. The Aspiration model is a three-layered model including skin and subcutis with the same thicknesses as for the Cutometer model and an additional third layer of muscle with a thickness of 5mm. The third and deepest layer accounts for the increased penetration depth resulting from the larger probe opening. The
5.3. Model parameter identification

The width of the model is defined such that the ratio between probe opening diameter and width is the same as for the Cutometer model. Boundary conditions are identical for both models in which the bottom layer of nodes is fixed for horizontal and vertical displacements and the outer side of the tissue structure is allowed to move freely. These two assumptions were shown to have a negligible impact on the deformation behavior of the tissue or apex height, respectively, for the two different loading cases.

![Finite element models of the Cutometer (top) and Aspiration (bottom) device.](image)

The optimization scheme aims at minimizing the least square error between numerically predicted apex displacement and experimentally observed tissue response. Using the \texttt{fminsearch} procedure in Matlab with the Nelder-Mead simplex algorithm, two individual parameter sets for skin and subcutaneous tissue were determined. In initial simulations using the Cutometer and Aspiration models for determining an appropriate set of initial values of the material parameters, both models revealed a significant dependence on the stiffness of the skin layer. This implies that sequential optimization of skin and subcutis parameters is unlikely to provide adequate sets of material parameters that would allow for good agreement with both, Aspiration and Cutometer experiments. There are two competing mechanisms that play a significant role in the design of the optimization scheme. On the one hand, the sensitivity analysis of the Cutometer model presented in Section 3.7.4 revealed that the optimization for skin parameters based on Cutometer measurements is rather independent of subcutis properties. On the other hand, the Aspiration model is observed to show a strong dependence on the material properties of skin. As a consequence, sequential optimization would lead either to an overestimation of skin stiffness resulting in too low apex heights in the Aspiration simulation or to an underestimation of skin stiffness yielding a too high prediction of apex displacement in the Cutometer model. The pronounced sensitivity of both models to the properties of skin requires parallel optimization of both, the skin and subcutis parameter sets.
5.3.1 Material parameters for skin and subcutaneous tissue

The model parameters of the optimization scheme are presented in Table 5.3 and represent the currently most reliable set of values for the representation of skin and subcutaneous tissue on the basis of in-vivo suction measurements including time and history dependent data on facial tissue. As shown in Figure 5.9 the numerically predicted tissue behavior well represents the experimentally observed response.

The differences of skin parameters from work presented in Chapter 3 and Table 5.3 result from the impact of subcutaneous tissue through the Aspiration measurements. Especially the numerical prediction of apex height in the Aspiration measurement shows a clear sensitivity on the ratio between initial shear modulus of skin and subcutis noticeable in the newly proposed values (and order of magnitudes) of $\mu_0$.

The observable difference in the values for the parameter $m_2$ which is predominantly associated with the purely elastic response of the tissue, may be explained by the longer hold time in the instant loading case of the Cutometer measurements in comparison to the experimental campaign presented in Chapter 3. The apex height after 60 seconds hold time at maximum load represents the steady state long term tissue response dominated by purely elastic properties. All other optimization parameters in Table 5.3 are well within the range of values presented in previous work (Barbarino et al., 2011; Weickenmeier and Jabareen, 2014).

The direct comparison of experimental and numerical curves as shown in Figure 5.9 reveals a remarkable agreement for nearly all loading cases presented within this study, thus, demonstrating the reliability of the measurement data as well as the good predictive capabilities of the constitutive model equations presented by Rubin and Bodner (2002). The concise representation of the cyclic data highlights further, the model’s capability to capture the history dependent response of skin and subcutaneous tissue. The maximum absolute error between predicted and measured apex height at $t_{\text{lin}}$ of less than 10% may be considered marginal.
5.3. Model parameter identification

Figure 5.9: Comparison of experimental data and numerical simulation based on the material parameters determined in the parameter identification optimization.
Table 5.3: Model parameters for facial tissues

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SKIN</th>
<th>SUBCUTIS</th>
<th>MUSCLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_0$ [MPa]</td>
<td>0.096</td>
<td>0.009</td>
<td>0.37$^1$</td>
</tr>
<tr>
<td>$q$</td>
<td>25.5</td>
<td>21.54</td>
<td>25.0</td>
</tr>
<tr>
<td>$m_2$</td>
<td>0.019</td>
<td>0.013</td>
<td>0.0008</td>
</tr>
<tr>
<td>$\Gamma_1$ [Hz]</td>
<td>1.245</td>
<td>5.073</td>
<td>0.005</td>
</tr>
<tr>
<td>$\Gamma_2$</td>
<td>66.44</td>
<td>10.0</td>
<td>20.0</td>
</tr>
<tr>
<td>$r_2$</td>
<td>9.85</td>
<td>1.97</td>
<td>1.3</td>
</tr>
<tr>
<td>$m_1$</td>
<td>1000.0</td>
<td>1000.0</td>
<td>1000.0</td>
</tr>
<tr>
<td>$m_3$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$m_4$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$m_5$</td>
<td>0.981</td>
<td>0.987</td>
<td>0.0</td>
</tr>
<tr>
<td>$n$</td>
<td>0.5</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$r_1$</td>
<td>20.0</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$r_3$ [Hz]</td>
<td>$1.0 \cdot 10^{-10}$</td>
<td>$1.0 \cdot 10^{-8}$</td>
<td>$1.0 \cdot 10^{-8}$</td>
</tr>
<tr>
<td>$r_4$ [Hz]</td>
<td>$1.0 \cdot 10^{-4}$</td>
<td>$1.0 \cdot 10^{-4}$</td>
<td>$1.0 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$r_5$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

$^1$The initial shear modulus of muscle presented in Barbarino et al. (2011) was adapted to preserve the order of magnitude between skin and muscle for the current optimization.
5.4 Conclusions

The presented experimental study represents an elaborate quantification of mechanical tissue response for in-vivo characterization of location, time, and history dependent properties of skin and subcutaneous tissue. The measurement method and experimental setup were proven to ensure repeatability and reliability within consecutive measurements as well as across the whole range of loading protocols which demonstrates the high quality of the experiments. Based on the well-established optimization routine presented in previous work (Barbarino et al., 2011; Weickenmeier and Jabareen, 2014) the experimental data was used to identify two sets of material parameters for skin and subcutis which provide significant agreement between the measured and numerically predicted tissue response. The results of this study present a major improvement over currently available parameter sets due to the incorporation of history and time dependence as well as the information on location specific variation in tissue response. Simulations of facial expressions, pull-up experiments, and for surgical planning will be characterized by increased accuracy with respect to the predictions of deformation and forces.

In general, suction experiments allow to analyze the soft tissue response in a physically relevant multiaxial state of deformation. The material parameters presented in this work were determined in an inverse FE analysis and were shown to represent the suction experiments very well. However, as superficial soft tissues undergo several other states of deformation during facial expressions, speech, and aging as well it is suggested to investigate the performance of the presented material parameters in such cases like uniaxial tension, torsion, and pure shear. In particular, direct comparison with corresponding experimentally observed tissue behavior would reveal the predictive capability of the material parameters in a broad range of applications.

Moreover, it is considered necessary to analyze the FE model of the Aspiration measurement with respect to model assumptions, similar to the sensitivity analysis of the Cutometer model presented in Chapter 3. This study should aim at quantifying the impact of model assumptions on the overall material response and could potentially involve a variation of the tissue parameters of the third layer, the interaction properties between individual layers, and individual boundary conditions.

Finally, given the particular interest in the soft tissues of the forehead within the presented thesis as well as the availability of respective experimental data, it is worth determining location specific material parameters of the tissues in the forehead region.
Layer interactions in facial soft tissues

6.1 Introduction

Understanding the mechanical behavior of facial soft tissues is of great importance for many clinical applications. Physically based deformation mechanisms describing the tissue response during muscle activation for facial expressions, wrinkle formation, and aging enhance the predictive capabilities of simulations for surgery planning, implant design, diagnosis, and for the animation industry. The experimental characterization of mechanical properties of individual tissues and their interactions, the development of corresponding constitutive model equations, and their implementation into a numerical framework for robust simulations represent key steps towards realistic simulations providing substantial insight into the complex nature of facial soft tissues.

The mechanical characterization of soft biological tissues aims at determining the highly nonlinear, anisotropic, time dependent, and often loading history dependent material response. Several different in- and ex-vivo measurement methods have been proposed in literature which are suitable for the assessment of individual tissues, tissue structures, and the interaction of individual facial tissue layers. Barbarino et al. (2011) applied suction experiments to evaluate skin and deeper layers. Hendriks et al. (2006) presented a combined suction based experimental and finite element (FE) modeling approach allowing to quantify the relative contribution of different skin layers (e.g. epidermis and dermis) to the overall tissue response. The specific method provided an estimation of material properties and a description of the connection between the epidermis and dermis layer of human skin. The related through-plane layer behavior of full-thickness skin tissue was investigated by Gerhardt et al. (2012) in shear experiments. Real-time video recording captured skin layer deformations used to perform a displacement, strain, and stiffness analysis as well as the assessment of tissue layer interaction.

In-vivo quantitative visualization of tissue deformation provides essential information on the mechanical interaction between individual layers. Ultrasonography is a widely used measurement method due to its highly flexible applicability, the possibility of combining it with real-time mechanical testing, and good spatial resolution. Analysis of ultrasound
images during mechanical tests provides displacement fields and corresponding strain mappings for the quantification of tissue properties as presented by Tang and Liu (2012) for porcine sclera; Vogt and Ermert (2005) and Diridollou et al. (1998) for skin tissue. Real-time ultrasound measurements allow to visualize tissue behavior due to voluntary muscle contraction in terms of tissue motion and relative tissue deformation. Such experiments were presented by Wu et al. (2010) who investigated masseter muscle tissue motion and shape changes during active contraction as well as tissue interaction between muscle and neighboring tissues.

Our work aims at improving with respect to existing FE models (Barbarino et al., 2009b; Warburton and Maddock, 2013; Wu et al., 2013a) in terms of physical relevance of soft tissue geometry and mechanical response. In recent papers we have demonstrated the implementation of advanced active and passive constitutive models of face tissue (Weickenmeier and Jabareen, 2014; Weickenmeier et al., 2014a), as well as the accurate representation of anatomical features, and realistic boundary conditions (Barbarino et al., 2009b). Our model allows to simulate facial expressions and wrinkling by incorporating experimentally quantified interaction properties of individual tissue layers. In contrast to the general assumption of tight contact between all tissue layers, there are distinct tissue interfaces that exhibit significant relative tissue movement upon shearing. The present paper describes the procedure applied to determine the mechanical properties of the interaction between specific tissue layers in different regions of the forehead by means of ultrasound based visualization of the tissue displacement field during pull experiments. The anatomy of the forehead displays a layered organization of tissues characterized by a distinct local variation in their interactions (Knize, 1996a; LaTrenta, 2004). The forehead is easily accessible for ultrasound measurements and is clearly bound by skin surface and skull ensuring sufficient repeatability and high accuracy in measurement data. The experimentally observed through-layer tissue deformation and corresponding properties of layer interaction are projected onto an anatomically detailed FE model of the forehead. This FE model serves as a benchmark for evaluating layer interaction properties in the simulation of the pull experiments and the formation of forehead wrinkles upon muscle contraction.
6.2. Experimental characterization of facial tissue layer interactions

The forehead is a layered tissue structure consisting of skin, subcutaneous fat, galea aponeurotica, loose areolar tissue, muscle, and periosteum. The two layers of skin and subcutaneous fat are present across the whole forehead and are rather constant in thickness. The distribution of the other tissues varies locally and the temporal fusion line generally divides the medial and temporal zone; it consists of stiff connective tissue that inserts onto the skull, see ultrasound images in Figure 6.1 and work by LaTrenta (2004).

The frontalis muscle is the main active tissue in the forehead and it is primarily responsible for lifting the eyebrows during facial expressions and the resulting formation of forehead wrinkles. The muscle fibers insert into the dermis in the lower forehead enabling a maximum tissue lift upon contraction. Movement of the eyebrow is enhanced by loose areolar tissue and galea fat pads surrounding the frontalis muscle which form a glide plane allowing for reversible relative movement between superficial skin and subcutaneous tissue and the deeper tissues (Hicks and Watson, 2005; Knize, 1996a; Stuzin et al., 1992).

The locally varying tissue interactions are characterized by means of ultrasound based visualization of the through-layer displacement field upon application of external skin displacement. The experimental setup is based on work presented by Barbarino et al. (2009a) and consists of a chin rest as used in ophthalmology which was modified to include a clamping device for the ultrasound probe. The experimental setup was optimized for (i) reproducible alignment of the subject’s forehead and the ultrasound probe for multiple consecutive measurements, (ii) an adjustable orientation of the transducer with respect to the curvature of the forehead for optimal image quality, (iii) minimal movement between subject and transducer during individual measurement sequences, and (iv) flexibility in measurement site and displacement magnitude. Measurements were performed on a 29 year old male subject using a GE Logiq E9 ultrasound machine with a L8-18i-D broad-spectrum linear transducer operating at 15 MHz with a field of view of 25mm. Six seconds video sequences (33 fps) were recorded to capture a full loading and unloading cycle consisting of a horizontal displacement of a tape attached to the skin. Location dependence of tissue response was assessed by measuring in the medial and temporal forehead including the temporal fusion line.

The image sequences were analyzed in order to extract the deformation field within the soft tissue structure. Based on the optical flow tracking algorithm introduced by Lucas and Kanade (1981), multiple regular grids were aligned tangentially to the surface of the skin in order to visualize the gradient of deformation through the individual tissue layers. Densely connected tissue layers show a rather homogeneous displacement field across the layer boundary, while loosely connected tissues experience a pronounced gradient. Moreover, the deformation distribution provides an indirect measure of the stiffness of individual layers. The difference in the gradient between two neighboring layers depends on the stiffness ratio between both tissues. Figure 6.1 shows the displacement field and maximum principal stretch for a representative measurement in the medial and the temporal forehead region.
Chapter 6. Layer interactions in facial soft tissues

Figure 6.1: Ultrasound measurements in the medial and temporal forehead. Tissue layer interaction is quantified through the evaluation of the displacement field and principal stretch in the measurement plane.

The measurement results are found to provide significant quantitative and qualitative information on the mechanical properties between individual layers and comprehensively visualize the effects of the highly differentiated forehead anatomy on the tissue response. The image resolution allows to distinguish between three characteristic main tissue layers (see Figure 6.1): (i) skin as the most superficial layer including the stratum corneum which appears very bright due to reflections at the boundary between gel and skin surface; (ii) SMAS or the subcutaneous tissue layer; (iii) the third layer consists of muscle fibers that are embedded in loose areolar tissue. The structure of the third layer varies significantly when moving across the forehead, i.e. the temporalis muscle lies on top of the temporal bone, the frontalis muscle covers the medial forehead, and the temporal fusion line represents the transition zone between medial and temporal forehead. The temporal fusion line is characterized by a strong interaction between all layers and provides substantial support to the whole forehead.

In general, both measurement sites show a similar behavior in terms of the deformation gradient in the two most superficial layers. Skin and subcutaneous tissue exhibit a homogeneous displacement field and a similar and almost constant deformation gradient across both layers. The difference in stiffness between skin and underlying tissue is indicated by a minor change in the slope of the displacement gradient as visible in Figure 6.1 at the transition from the most superficial to the second tissue layer. The third layer, however, shows a locally dependent but consistently pronounced drop in the displacement magnitude. The externally applied displacement of skin propagates through the rather stiff superficial layers all the way to the third layer. The much softer third layer
of loose areolar and fat tissue exhibits significant shearing to compensate for the propagated displacement. The significant shear response of the loose areolar tissue, expressed in a large relative movement between the second layer and bone, is often associated with a gliding response of individual layers (Knize, 1996a). This relative movement is fully reversible upon unloading (e.g. relaxation of the muscle after a facial expression) and is evident in the full recovery of the initial tissue state. This interaction property is evident in both medial and temporal region. However, the measurements strongly indicate that specifically in the zone of fixation (i.e. temporal fusion line) this relative motion is fully inhibited by the strong connectivity between all layers. This is most visible in the plots of the temporal region which are characterized by a homogeneous deformation field and a very smooth gradient in comparison to the medial forehead. Finally, the principal stretch provides an additional measure to quantify the individual tissue properties.

6.3 Simulation of tissue response

An anatomically detailed FE model of the forehead was reconstructed from MR images and consists of a multilayered tissue structure including skin, subcutaneous tissue, a third layer with locally dependent material properties, periosteum, and temporalis muscle. The frontalis muscle is embedded in the soft areolar tissue of the third layer and inserts into subcutaneous tissue and skin close to the region of the eyebrows enabling the lift of surrounding tissue during facial expressions and wrinkle formation due to muscle contraction and tissue compression. The lower part of the face is included in this model for visualization purposes. The forehead model introduced here was generated similar to the procedure presented by Barbarino et al. (2009b).

Skin, subcutaneous tissue, and the third layer are tied at their individual layer surfaces to form a densely connected tissue structure. Based on the experimental observations shown in Figure 6.1, the interaction between the lower surface of the third layer and periosteum varies locally. In the medial forehead and superficial to the temporalis muscle, the third layer is free to slide on top of the periosteum. In proximity of the temporal fusion line, these two tissue layers are tied together, to accurately represent the dense connectivity between all tissues in the transition zone from medial to temporal forehead as described by Knize (1996a). The mechanical behavior of the active muscle and passive soft tissue layers is based on the implementation of constitutive material models as presented by Weickenmeier et al. (2014a) and Weickenmeier and Jabareen (2014). The corresponding material parameters for facial skin were determined from suction based in-vivo experiments on the same subject.

The forehead model is used to investigate the experimentally observed tissue behavior and to validate the proposed interaction properties. The results from the numerical evaluation of the pull experiments are shown in Figure 6.2 in terms of the through-layer displacement field and the corresponding principal stretch in a sagittal cut close to the loading point. A comparison of displacement magnitudes from simulation and experiment for selected points revealed an error of less than 20% which shows the significant predictive capability of the model with respect to location dependent tissue deformation and pronounced shearing. The propagation of externally applied displacement through
Chapter 6. Layer interactions in facial soft tissues

Figure 6.2: FE model of pull-experiments (tape in experiments modeled by the rigid element in blue; black squares indicate regions of frictionless contact). Through-layer deformation and principal stretch fields for a sagittal cut close to the loading point. Full-thickness skin is visualized in the displacement field by same material points in their initial position (red) and at maximum displacement (blue). The sliding of the third layer over periostium causes enhanced mobility of all superficial layers which is clearly visible in the large displacement of material points across the entire thickness. Modeling the pronounced intergrowth of tissues in the zone of fixation as tightly connected layers attached to the layer of periosium yields good agreement with the experiments which show limited displacement close to the bone and a small displacement gradient across subcutaneous tissue and skin. The connection between tissue layers corresponds to contact conditions for which tight contact and free sliding represent limiting cases. The proposed configurations simplify the anatomical features of (i) connective collagen fibers between individual tissue layers, (ii) the embedment of frontalis muscle fibers in surrounding tissue, and (iii) the observable shearing behavior of loose areolar tissue in the forehead. However, given the predictive capabilities of the model with respect to the experimental observations, the proposed interaction properties are well justified.
6.4 Conclusions

Figure 6.3: (a) Deformation pattern of a simplified forehead wrinkling model (b) Simulation of frontalis muscle contraction (as in facial expressions) using the full benchmark forehead model.

A simulation of wrinkle formation is numerically challenging and requires a sophisticated numerical framework with respect to robust numerical implementations of material models and a suitable geometric discretization of the individual structures. Figure 6.3 shows a simplified FE model to investigate typical forehead wrinkle patterns and the simulation results based on the forehead model for the case of active frontalis muscle contraction and the resulting wrinkle formation. The model including the proposed layer interaction properties provides a suitable representation of forehead wrinkles.

6.4 Conclusions

An experimental setup for the visualization of full-thickness facial tissue deformation during external skin displacement and facial expressions was developed and allowed to determine location dependent properties of layer interaction in terms of inter-tissue displacement gradients. Our measurements suggest to differentiate between two different configurations: (i) a strong connection between two layers (i.e. for skin and subcutaneous tissue or for all tissues close to the temporal fusion line) and (ii) a very loose connection as in free sliding (i.e. for tissues above the eyebrow in order to enable maximum lift upon frontalis muscle contraction during facial expression).

An anatomically detailed forehead model was reconstructed from MR images and used in the simulation of pull-experiments to validate the proposed interaction properties between specific tissue layers. The physically based representation of tissue interaction properties made it possible to simulate the formation of wrinkles.

In future work, the experimental method will be employed to quantify age- and health-related changes in the observed tissue response. These measurements could form part of a diagnostic tool to quantify the impact of dermatological diseases such as fibrosis. Additionally, our experimental findings will be incorporated in the finite element model of the face (Barbarino et al., 2009b) to simulate the tissue response during facial expression and mastication.

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Chapter 7

Soft tissue behavior in aged & diseased skin

7.1 Introduction

Skin tissue is the outermost layer of the body and fulfills a large number of relevant functions to sustain the body. It primarily protects all body organs from the environment and provides substantial support to all inner tissue structures. Skin serves as a shield against UV light, is responsible for body heat regulation, contains a large number of different sensory cells, and possesses the capability to heal itself by continuous regeneration of new skin cells (McGrath et al., 2010). Skin tissue consists of several different tissue layers that provide individual properties to the overall organ structure.

Skin tissues exhibit characteristic changes in morphology and phenotype related to age that affect the mechanical properties, functional performance, and outer appearance especially in the region of the face. Due to extensive exposure to gravimetric forces, progressive actinic damage, and environmental factors such as UV light radiation and chemical substances, skin tissue experiences significant changes over time. The formation of wrinkles and the increase of skin ptosis are direct consequences of loss of collagen and elastin content in the dermis causing decreased skin elasticity and pronounced sagging of supportive tissue layers (LaTrenta, 2004).

Besides age related changes, skin tissue diseases cause alterations in the biomechanical response of individual tissue layers or even the full-thickness skin structure leading to potentially severe adverse effects for the affected person. Among these, scleroderma is a rare autoimmune rheumatic disease which is predominantly characterized by pronounced skin hardening. In scleroderma, fibrotic tissue develops in localized or extensive parts of the body and is associated with a massive deposition and straightening of collagen bundles leading to skin thickening and loss of distensibility (Åkesson et al., 2004). This pathophysiology consists of oedema and inflammatory cell infiltration especially around blood vessels, extensive collagen accumulation, and pronounced deposition of extracellular matrix by fibroblasts which eventually lead to fibrosis (Åkesson et al., 2004; Balbir-Gurman et al., 2002). These tissue alterations have a strong impact on the mechanical tissue properties due to increased density of the collagen network, related pronounced friction between collagen fibers in individual tissue layers, and a loss of the loose connective tissue...
Chapter 7. Soft tissue behavior in aged and diseased skin

which results in limited shear deformations within affected layers. Different types of scleroderma exist which differ in the range of the affected tissue regions, potentially including the involvement of inner organs such as lungs, heart, and kidneys with often severe effects on their functionality.

In clinical diagnostics several different strategies have been investigated to monitor the progression of age and disease related changes in skin tissue. Suction based skin tissue measurements using Cutometer or similar devices and (high frequency) ultrasound imaging are the two most commonly used techniques in dermatology today to assess the mechanical properties and health condition of full-thickness skin. Ultrasound imaging in dermatology was pioneered by Alexander and Miller (1979) who determined individual layer thicknesses in skin. This method was first applied to monitor the progression of skin thickening in scleroderma by Myers et al. (1986) and marks are very relevant clinical criterion on diagnosis today (Åkesson et al., 2004; Balbir-Gurman et al., 2002; Cole et al., 1981; Diridollou et al., 1998; Gniadecka, 2001; Gniadecka et al., 1994; Hesselstrand et al., 2008; Piérard et al., 2013a,b; Rodnan et al., 1979). However, so far the most widely used evaluation method in clinical practice to determine skin thickness is based on a subjective palpation examination of the ability to pinch skin into a fold (also known as hidebinding). This test allows to determine a so called skin score or also known as the modified Rodnan skin score (mRss) which is a 4-stage rating system. A 0-score refers to normal skin in a scleroderma patient, 1 is associated with slight but definite thickening, 2 denotes moderate thickening, and 3 indicates severe thickening of the skin (Rodnan et al., 1979).

Several studies make use of combined suction experiment and ultrasound imaging to investigate the characteristic changes in systemic and localized scleroderma (Åkesson et al., 2004; Balbir-Gurman et al., 2002; Dobrev, 1999; Enomoto et al., 1996). However, it is often reported that due to subject specificity of skin involvement, neither thickness measurements alone nor combined thickness and suction measurement allow for an inter-subject comparison (Balbir-Gurman et al., 2002; Dobrev, 1999; Enomoto et al., 1996; Hesselstrand et al., 2008). It is generally concluded that only the mRss provides the most examiner independent evaluation method to rate intra- and inter-subject specific progression of skin involvement in scleroderma.

Ultrasound imaging allows to not only quantify individual layer thicknesses but also contains the information on the echogenicity of present tissues which is directly related to tissue composition. Echogenicity describes an object’s capacity to reflect the ultrasound waves transmitted from the probehead. In particular, the well organized collagenous fiber network in dermal tissues is well represented in high frequency ultrasound images and allows to differentiate individual layers based on the visualization of tissue interfaces (De Rigal et al., 1989; Gniadecka, 2001). This property of ultrasound imaging has been used to investigate the effect of age related elastosis from UV light radiation, increase in subepidermal interstitial fluid in oedema, inflammatory reactions, and changes in the arrangement between collagen fibers. These manifestations of photodamage, elastosis, and age in the dermis lead to a reduced echogenicity in subepidermal tissue described in literature as the subepidermal low echoic band or rather SLEB (De Rigal et al., 1989; Gniadecka, 2001; Gniadecka et al., 1994) and is most often clearly visible in ultrasound images of affected skin as shown in Figures 7.3 and 7.4.
At the example of aged and sclerotic skin, the experimental method to determine tissue layer interaction presented in Chapter 6 is used to visualize the characteristic changes described above. Our method not only contains the possibility to use the existing methods of skin thickness measurements and echogenicity analysis but provides additional information of the full-thickness layer response upon external skin displacement. This extension of the ultrasound measurement allows to relate skin stiffening, thickness, and the interaction at tissue layer interfaces of which all are directly affected by scleroderma and aging, thus potentially improving diagnosis. Measurements are conducted in the forehead region for direct comparison with measurements on healthy skin as presented in Chapter 6 (Weickenmeier et al. (2014b)) as well as on the back of the hand which is a region usually severely affected by scleroderma as shown in Figure 7.1. The objective of this study is to explore the applicability of the developed experimental setup as a diagnostic tool to quantify tissue property changes during medical treatment in scleroderma patients. Additionally, this data provides several indications on how forehead tissue evolves with respect to age and disease which may be incorporated in the finite element model of the forehead when predicting the formation of wrinkles and skin ptosis in aging simulations.

![Forehead Back of the hand](image)

Figure 7.1: Measurement sites and ultrasound probe placement in the skin displacement tests.

**Experimental setup of ultrasound measurements**

Given the wide range of applicability of the ultrasound technique in terms of only few restrictions on the measurement site and the sufficiently high resolution in the most superficial layers of the body, it is a powerful tool for the visualization of tissue response within a multilayered structure such as skin. The quality of ultrasound images in biomedical applications strongly depends on probehead alignment with respect to the skin surface, frequency of the ultrasound wave, and the minimization of signal deflections at the skin surface. The experimental setup of the study presented here is shown in Figure 7.2 and has been optimized for full control of probehead alignment with skin, repeatable positioning of the probehead in the forehead and face region, and is based on work presented in Chapters 5 and 6.
Chapter 7. Soft tissue behavior in aged and diseased skin

The modified headrest shown in Figure 5.1 was adapted to hold the ultrasound probe similarly to the Cutometer or Aspiration device. The large number of degrees of freedom of the fixation device is essential in allowing a precise placement of the ultrasound probe. The probehead is placed tangential to skin in the respective measurement site and in parallel with the direction of the external displacement vector. A thick layer of ultrasound gel is placed between skin and probe in order to compensate for the curved shape in most of the measurement sites, to minimize compressive loading of the tissue structure, and to prevent a potential collapse of veins due to too high contact pressures. A medical tape attached to a carbon fiber cord is placed on the skin in order to apply the displacement vector. The ultrasound probehead is placed close to the tape in order to capture the near- and far-field deformation response of the skin tissues. The magnitude of displacement is controlled by pulling and releasing of the carbon cord.

A sensitivity analysis was performed in order to assess the individual contributions of the measurement procedure, including probe misalignment (not tangential to skin surface), as well as extreme cases of contact pressure between probe and skin, and the stability of the overall structure. Especially latter relates to an often observed error of detecting small tissue motions despite no external displacement. However, in measurements with no displacement vector, the setup proved sufficient rigidity to ensure that no artificial displacement or systemic vibrations are captured. Measurements of severe contact pressure, however, show reduced deformability of the full-thickness structure, a blocking of arteries, and artificial signal deflections at the skin surface. On the other hand, probe misalignment as well as very low contact pressures were observed to lead to reduced repeatability of the measurement, formation of air bubbles in the layer of ultrasound gel, and a loss in image quality in terms of a change in echogenicity of individual layers due to orientation changes of tissue and probehead during the displacement.

The measurement protocol was defined such that 6 seconds long videos of B-mode ultrasound images were captured during which a single cycle of loading and full unloading was performed. Maximum displacement magnitude is controlled by the person conducting the experiment and relies on this person’s capability to reproduce a similar displacement in successive measurements. Irrespective of this limitation, the protocol represents a flexible method of testing different pull directions, magnitudes, loading rates, and multiple loading cycles. The measurements were performed on a General Electric NEW LOGIQ E9 machine with a linear array 18MHz hockey stick probehead (L8-18i).

Three different measurement sites were considered in this study on layer interaction. Besides investigating the medial and temporal forehead region, measurements were performed on the back of the hand as this part of the body is strongly affected in cases of skin fibrosis. In particular, this region is often tested in the clinical examination of skin involvement in scleroderma. Besides investigating the effect of skin disease, a special interest was placed on visualizing tissue changes in aging skin. For this reason, the extended study included a 55 year old female subject with healthy aged skin and a 43 year old subject with severe progression of systemic scleroderma.
7.2 Layer interaction properties in the forehead

The experimental campaign on aged and sclerotic skin comprised multiple consecutive measurements in the medial and temporal forehead region. Representative measurements are shown in Figure 7.3 for direct comparison between young, aged, and diseased skin for both forehead regions. In all measurements in the medial forehead region the medical tape is placed in the center of the forehead, the pull direction is to the right, and the ultrasound probe is placed to the left of the tape as it is represented in Figure 7.2.

In the temporal forehead experiment, the pull directions in the aged and diseased skin cases are reversed in comparison to the healthy skin measurement because of limited adhesion of the tape due to wrinkles and hair. Nonetheless, the ultrasound probe position and the corresponding field of view remain similar as it can be seen from the presence of the same tissue structures in all three cases in the images on the right of Figure 7.3.

The ultrasound images allow to differentiate between individual tissue structures based on a variation in echogenicity which depends on the layer specific constituents. In all images the epidermis layer appears as a single hyperechoic line that allows no further distinction of layer structure. Depending on the age and health condition of skin subepidermal layers vary significantly in thickness and echogenicity. In the images of Subject 2 with aged skin, the subepidermal low echoic band characterized by a redistribution of fluid in the dermis and progressive photodamage (Gniadecka et al., 1994) is clearly visible, especially for the more exposed medial forehead region. Only little variation in echogenicity in the subepidermal layers demonstrates the strongly fibrotic state of the skin of Subject 3. The pathological thickening of the dermis layer is the predominant observation for both measurements sites. Additionally, there is a reduced differentiability between dermis and the subcutaneous tissue layer which is a result of excessive collagen deposition and pronounced thickening of collagen fibers in both layers accompanied by a loss of surrounding adipose tissue.
Chapter 7. Soft tissue behavior in aged and diseased skin

For all cases, the transverse cut through frontalis and temporalis muscle is visible as a hypoechoic structure consisting of thick fascicles separated by hyperechoic adipose-fibrous septa as reported by Wortsman et al. (2013). The transition between the deepest soft tissue layer and bone is well visible through the hyperechoic line due to the jump in acoustic impedance at the junction of the fatty fascia layer and the skull.

The skin extension tests are analyzed with respect to the deformation behavior in full-thickness skin. In the current measurement protocol the pulling force is not standardized, so that a direct comparison of maximum displacement magnitudes is implausible. However, since all presented measurements were performed by the same examiner who paid particular attention to reproduce same maximum pulling forces across all measurements, it may be assumed that pulling force in all measurements is within a tolerable interval. This permits a qualitative evaluation of the deformation response in the individual cases shown in Figure 7.3. Regardless of the repeatability of the pulling force, the analysis of the relative deformation behavior within a single subject already provides significant mechanical properties of individual tissue layers and their interactions. It is observed, that the maximum displacement of the skin surface near the medical tape is similar for young and aged skin, but that there is a noticeable drop in absolute terms in the case of scleroderma. Generally, the displacement magnitude decreases at the surface of skin when moving away from the loading zone. However, there is a significant dependence of the difference between proximal and distal deformation magnitude on the overall skin stiffness. In particular, for the case of sclerotic skin, the increased skin thickness and pathological stiffening inhibits the decay of the external skin displacement within a reasonable region. This observation is also valid for the measurements in the temporal region and visualizes the significant loss of elasticity.

A comparison of the deformation field in the temporal region confirms characteristic observations in aged and diseased skin. Primarily, the age related progressive loss of elasticity, trophic changes, and increased actinic damage in subepidermal tissue is evident in the reduced connectivity of the tissue structure in the temporal fusion zone. While for young skin this region provides increased support to the whole forehead region through strong interactions between individual layers characterized by a flat deformation profile, the supporting function is lost with age resulting in a bent deformation profile across subepidermal layers. The shape of the deformation profile at maximum skin displacement denoted by the blue dotted line (in comparison to the undeformed state shown by the red dotted line) is a qualitative measure for the strength of interaction, differences in tissue stiffness and the relative displacement between individual layers. In measurements on Subject 1, skin exhibits a strong location dependence in the deformation response which is a clear indication for a distinct differentiation in individual tissue properties and high elasticity in the tissue structure. With age, these properties weaken visibly and result in a more homogeneous response across the forehead, and a pronounced shearing behavior in the adipose layers of the subcutis. This reduction in tissue support becomes evident in the sagging of the overall tissue structure, especially above the eyebrows.
7.2. Layer interaction properties in the forehead

**Subject 1** (male, 29 years, healthy skin, same subject as in Weickenmeier et al. (2014b))

Medial forehead | Temporal region
---|---

Subject 2 (female, 55 years, aged skin)

Medial forehead | Temporal region
---|---

Subject 3 (male, 43 years, scleroderma patient)

Medial forehead | Temporal region
---|---

Figure 7.3: Ultrasound skin displacement measurements in two sites of the forehead region for a comparison of young, aged, and sclerotic skin.
7.3 Layer interaction properties of the soft tissues on the back of the hand

The measurements on the back of the hand where performed in the region on top of the middle section of the first metacarpal bone as shown in Figure 7.1. In healthy and aged skin this region allows for very large displacements and deformability of skin over the underlying bone, in order to enable the highly differentiated movability of the hand and fingers. In the case of scleroderma, however, and especially in the region of the hand and fingers, this functionality is significantly limited due to skin stiffening. The images in Figure 7.4 show the ultrasound measurements and the corresponding displacement field at maximum skin displacement for Subject 2 (aged skin) and Subject 3 (sclerotic skin). The first metacarpal bone is clearly visible and the superficial soft tissues appear as more hyperechoic structures. While the image from the measurement on Subject 2 allows to differentiate between different layers, there is a noticeable loss in differentiability for Subject 3. In particular, the left image shows the typical hyperechoic band of the epidermal layer and the previously described layer of low echoic property SLEB, typical for aged skin with progressive photodamage and the deposition of interstitial fluid in the subepidermal layer. In comparison to the skin of Subject 2 in Figure 7.3, dermis and subcutis show a pronounced hyperechoic behavior which is associated with a higher collagen fiber content in this region. This is in line with observations in aged skin which exhibits a loss of elastin and an increase in collagen fibers. Despite a corresponding reduction in elasticity, this allows for a strong deformability of the skin on the back of the hand. The remaining elastic response causes the decay of the displacement magnitude when moving away from the tape. Especially in comparison with measurements of Subject 3, the strong curvature of the deformation profile is an expression of the (remaining) reversibility of stretched skin despite age.

The ultrasound measurements visualize the apparent reduction of skin thickness with age and the progressive thickening of dermis in sclerotic tissue. Similar to the measurements in the forehead region, the deformation profile of Subject 3 is very flat across the
whole field of view, providing a clear indication for a stiffening of full-thickness skin. The deformation profile depicts a stiff and rigid motion of skin and explains the constricted movability of the wrist and fingers of patients with this degree of scleroderma.

7.4 Conclusions

This study demonstrates the applicability and usefulness of the previously developed experimental setup for a wide range of skin conditions and measurements sites. In particular, it is shown that the concept of combined ultrasound measurement and skin displacement allows to determine the biomechanical state of skin. Characteristic changes in the individual layers of skin related to age and disease (at the example of scleroderma) are made visible and enable a long term intra- and inter-subject monitoring of progressive tissue changes.

For the proposed method to provide quantitative data, it is suggested to extend the measurement protocol to control either displacement magnitude or pulling force of the skin surface. A standardized loading mechanism is required for the present measurement procedure to serve as a diagnostic tool and to improve inter-subject comparability.

The proposed method is an improvement over existing studies that use ultrasound imaging for skin thickness determination. As reported in literature, morphological changes in scleroderma are subject specific and have different consequences with respect to the severity and progression of the disease. Based on the determination of the full-thickness deformation profile, the present method provides a thickness independent indicator for skin impairment. Moreover, it is shown that there are significant differences in the behavior of young, aged, and diseased skin with respect to the loss of stiffness, changes in morphology of subepidermal layers, the progressive damage of individual layers, and the reduction of the location specific functionality of the overall soft tissue structure, especially in the temporal fusion zone of the forehead.

In order to further explore the capabilities of the measurement method, a clinical multi-subject study considering different skin types is required. Based on data presented in literature on the mechanical response in aged and diseased skin using suction tests, it is suggested to include such measurements in the corresponding regions of interest, in order to provide a quantitative measure of the local mechanical properties of skin.
Mechanical response of the masseter muscle during mastication

8.1 Introduction

Understanding the mechanical behavior of the mastication system is of great importance for several medical applications as well as the food development and animation industry. Realistic and physically based representations of the mastication system allow to simulate muscle driven speech, facial expressions, biting, as well as the mechanical impact of medical prosthesis, surgical interventions, and dentures in terms of internal loading of the temporomandibular joint (TMJ), jaw, and surrounding soft tissues. Reliable and physically meaningful simulations require an experimental characterization of muscles properties, tissue interaction between soft tissues and bone, anatomy based geometric reconstructions of the individual structures, and a reliable estimation of intra- and inter-subject variability.

Literature provides a substantial range of experimental and numerical data describing task specific muscle behavior. Several mathematical models exists which provide theoretical limits of bite forces for specific biting positions (Koolstra et al., 1988; Le Révérend and Hartmann, 2014; Osborn, 1996; Sellers and Crompton, 2004). Most of these models, however, neglect the three-dimensional properties of active muscle behavior and represent muscle forces by one-dimensional Hill-type springs. For this reason, many studies focus on determining singular points of muscle origin and insertion to establish a unique measure for muscle length Van Eijden and Raadsheer (1992) and Van Eijden et al. (1997, 1995, 1996).

The emergence of magnetic resonance imaging, computer tomography, and ultrasonography provides new means of anatomy based model reconstructions of the mastication system. Several studies investigate influencing factor of physical limits of temporomandibular joint loading, especially with respect to TMJ disorders (Cheng et al., 2013; Commissso et al., 2015), surgical reconstruction of bone structures (Narra et al., 2014), jaw movement during chewing and mastication (Commissso et al., 2015; Hirose et al., 2006), and stress distributions of cartilage tissue in the joint (Koolstra and Van Eijden, 2005).
Chapter 8. Masseter muscle response during mastication

Figure 8.1: Representation of the mastication system including the muscle of mastication, the hyoid muscle group, temporomandibular joint, mandible, and skull. The muscle of mastication system are often separated into the group of (a) jaw opening muscles consisting of the lateral pterygoid and hyoid muscle groups and (b) jaw closing muscle group comprised of masseter, temporalis, and medial pterygoid muscle. A FE model was developed for the simulation of incisor and molar biting and is shown for the respective muscle groups. Anatomical images adapted from Williams et al. (1995)

The mastication system is characterized by a high level of interaction between different muscles, as shown in Figure 8.1, and provides considerable flexibility of jaw movability for speech and mastication. The control of jaw position is provided by complex muscle activation patterns that hold the key to realistic modeling of the mastication system. Several mathematical models aim at determining muscle activation patterns based on prescribed jaw kinematic (Comimioso et al., 2015; Hannam et al., 2008; Koolstra and Van Eijden, 2001; Osborn and Baragar, 1985). Despite significant complexity with respect to the involvement of the muscles of mastication including muscle subgroups, the generalized approximation of three-dimensional tissue response by one-dimensional material models, limits the physicality of respective model predictions (Van Eijden et al., 1997). To the author’s knowledge, to this day only one FE mastication model exists which provides a fully three-dimensional representation of the human mastication system including mandible, skull, and the masseter muscle. Specifically, Röhrle and Pullan (2007) present an anatomy based reconstruction of the masseter muscle that is governed by transversely isotropic constitutive equations. The FE model allows for the incorporation of muscle fiber orientations and realistic kinematic constraints on the masseter muscle in the regions of insertions. The numerical simulation predicts muscle forces within a full biting cycle including jaw opening, closing, and biting.

In general, the predictive capability of numerical simulations with respect to the mechanical response of muscle, joint, and bite forces in the mastication system relies on the constitutive muscle model. The model governs the passive and active properties of the muscle tissue and defines the corresponding tissue deformation. The scope of constitutive model formulations for skeletal muscle tissue is discussed in Chapter 4 and includes the
numerical implementation of a proposed muscle model within the FE environment. Despite the significant amount of constitutive model formulations for skeletal muscle tissue that can be found in literature, there is almost no work presented so far which aims at validating the numerically predicted muscle deformation by means of comparison with experimental data. Böl et al. (2011) and Böl et al. (2013) introduce novel strategies for the evaluation of numerically predicted muscle deformations by comparison with MR images of the relaxed and contracted state and present an experimental setup for real-time visualization of ex-vivo muscle contraction on a live animal model.

The work presented here is based on two fundamental objectives which provide the experimental and numerical basis for the validation of the predicted mechanical response of a newly developed mastication model. The first objective concerns the anatomy based reconstruction of the mastication system including all muscles of mastication for the numerical simulation of mastication. The geometric reconstruction is based on magnetic resonance images obtained for the same 29 year old male subject, that has volunteered in other experimental campaigns presented in Chapters 5 and 6. The second objective constitutes the experimental visualization and quantification of muscle deformation upon active contraction during biting. An experimental setup is developed which enables simultaneous measurements of bite force and ultrasound imaging during bite force generation within the biting cycle.

The following numerical and experimental investigations of muscle mechanics represent fundamentally new insight into biting location and bite force magnitude dependent muscle deformations. The subject specific mastication model allows for a direct comparison between numerically predicted and experimentally observed shape changes for multiple cross sections of the masseter muscle and constitutes a reliable method for the validation of the proposed muscle model implementation presented in Chapter 4.

8.2 Materials and methods

The investigation of the mechanics of the masseter muscle includes numerical simulations and the experimental characterization of tissue behavior during active contraction. Numerical simulations are performed on the basis of a FE model representing the mastication system. Mesh generation from medical images is described in Section 8.2.1. The experimental setup for ultrasound image based quantification of muscle deformation during biting is presented in Section 8.2.3.

8.2.1 Finite element model generation

The FE model is based on magnetic resonance images of a 29 year old male, the same subject as in the previously reported experimental campaigns in Chapters 5, 6, and 7. 180 images in the transverse plane are taken at a slice distance of 1mm and an in-plane resolution of 256 pixels at a voxel size of $1\text{mm}^3$. Scan IP software (Simpleware Ltd, Exeter, UK) is used to reconstruct the 3D contour of the mastication muscles, skull and mandible. A semi-automatic procedure allows for efficient segmentation of muscles and bone structures. Manual adjustment is required in regions of intersecting muscle strands.
such as the medial and the (superior and inferior) lateral pterygoid muscle due to similar echogenicity. Figure 8.2 shows the final stage of the semi-automatic segmentation for the (a) masseter (red), (b) temporalis (green) muscle, and (c) the entire mastication system including all bone parts and medial and lateral pterygoid muscles.

Following the initial reconstruction of all volumetric shapes, a triangulated surface is generated for each object and exported in the *STL*-format. Using *Geomagic Studio* software (3D Systems, Rock Hill, SC, US) all surfaces are smoothed in order to obtain a homogeneous contour and to repair unphysical holes, as it is shown for the example of the masseter muscle in images (a) and (b) of Figure 8.3. Subsequently, the triangulated
surfaces are represented by NURBS (non-uniform rational B-splines) in form of patched surfaces. All bone structures in the finite element model are primarily included for visualization purposes and are represented by regularly shaped patches. For all muscle objects the patched surfaces are generated such that front and back face of each muscle are represented by a uniform patch network, see image (c) in Figure 8.3. This is possible due to the rather flat shape and regular thickness along the main fiber direction of all mastication muscles. Front and back surfaces of each muscle are determined manually and the surface patch network is optimized to obtain an acceptable aspect ratio of the resulting hexahedral mesh. Patch size is adopted to local muscle thickness in order to preserve a similar aspect ratio across the entire object. Here, the aspect ratio is the factor between average edge length of a single patch and the average distance to the corresponding patch on the opposite face of the muscle. In those regions where masseter muscle is thickest, the patch size on the surface is larger in comparison to more refined patch sizes where masseter is thinner. Following this step, the patched surfaces of front and back face of each muscle are exported as quadrilateral shell meshes. Based on a user subroutine corresponding quadrilateral shells of front and back faces are combined to form volumetric (hexahedral) elements, as shown in image (d) of Figure 8.3. This strategy allows for multiple uniform mesh refinement steps while preserving a favorable aspect ratio as shown in image (e).

Figure 8.3: Development of a finite element mesh. Segmentation of MR images and subsequent transformation to a hexahedral mesh.

The individual muscle and bone structures are imported into the commercial FE program Abaqus ABAQUS (2009) (Dassault Systemes, Providence, RI, USA) for numerical simulations of the assembled mastication model. Figure 8.4 shows the four muscles of mastication (masseter, temporalis, later and medial pterygoid muscle) as well as the skull and mandible. For reasons of computational efficiency, only half of the head is modeled. This assumption of symmetry must be considered when comparing numerical simulations to experiments in which unsymmetrical biting (so biting on only one side of the mouth) is present. Several studies in literature look into the effect of unsymmetrical biting on bite forces between teeth and unsymmetrical loading conditions of the temporomandibular joints (Kubo et al., 2006; Mao and Osborn, 1994; McMillan and Hammam, 1992).

The masseter muscle is refined sufficiently to justify the use of reduced integration linear 8-noded hexahedral elements (C3D8R). Muscles and skull are constrained on the
basis of anatomical findings. The relative position between skull and mandible is defined by the temporomandibular joint. In the human mastication system this joint controls the kinematics of the jaw. This includes the relative translation of the mandible when protruding or retracting the jaw, side-ways movement of the jaw during grinding of the teeth, as well as the rotation of the jaw which occurs in almost any case, especially in opening and closing of the mouth.

Insertion points of individual muscles (or muscle groups) which are well described in anatomical textbooks (Williams et al., 1995) are converted into boundary conditions to define the fixation points of muscles with respect to mandible and skull. Generally, muscles of mastication have one rigid insertion point and one insertion point with multiple degrees of freedom. In particular, the nodes on the top of the masseter muscle are fixed, while the bottom nodes are tied to the degrees of freedom of the temporomandibular joint. In the current model one fiber family per muscle is considered which follows the principal orientation of the respective muscle. In Section 8.3.1 an additional study is presented which analyzes the impact of muscle fiber heterogeneity on the bite forces during mastication.

Figure 8.4 visualizes the full FE model of the mastication system. The muscles on the medial side of the mandible show strong overlapping in the medical images and are separated for the FE model. The distal ends of (superior and inferior head) of the lateral pterygoid muscle (orange and red) are fixed (muscle is attached to the skull) and the proximal end inserts the coronoid process of the mandible enabling closing and grinding of the jaw upon contraction. The medial pterygoid muscle (yellow) is tied to the medial angle of the mandible and is fixed at its top where the muscle anchors on the maxilla. The temporalis muscle (green) has a significant impact on the mastication system being one of the predominant jaw closing muscles. Temporalis muscle is strongly attached to the coronoid process of the mandible which is pulled upwards upon contraction and causes a rotation of the jaw about the condyle head in the temporomandibular joint.

In the model presented here, no contact constraints are considered. Both contact between individual muscles and contact between muscles and bone are not included in the current model.

### 8.2.2 Material modeling

The FE model includes the muscles of mastication and bone where latter is primarily included for visualization purposes. The mechanical behavior of muscle is characterized by passive and active tissue response which depends on the level of activation and the physical state of the muscle. The constitutive model equations describing the masseter muscle in the FE model are presented in Chapter 4 including the numerical implementation within the FE environment. Material parameters are adopted from Tables 4.1 and 4.2 and are based on an inverse FE optimization to achieve a prescribed muscle force of 500N. The underlying FE model of the optimization scheme was adopted from work presented by Barbarino et al. (2009b) and modified such to simulate molar biting. Given the similarity in the dimensions and shape between the newly developed masseter representation and the model geometry by Barbarino it is considered well justified to use the same material parameters.
8.2. Materials and methods

Figure 8.4: Complete representation of the FE model of the mastication system where muscles and bone are mirrored about the sagittal plane. (left) frontal view on masseter and temporalis muscle and bone structures (right) muscles of mastication including medial (orange and red) and lateral (yellow) pterygoid, masseter (blue) and temporalis (green).

These material parameters, including muscle fiber orientation, are considered for the whole muscle structure. Only in a separate FE simulation, do we include inhomogeneous fiber orientations in the masseter and investigate the effect on bite force and muscle shape change.

8.2.3 Experimental setup

The experimental campaign aims at characterizing the mechanical behavior of the masseter muscle during active contraction in biting. The human mastication system involves several different muscles that enable the opening and closing of the mouth as well as efficient processing of food through biting and chewing motions. Among these muscles, the masseter muscle is the primary actor in jaw closing and bite force generation. For this reason, the experimental study focuses on the masseter muscle and is designed such to provide a quantitative characterization of muscle deformations during active contraction. Ultrasound imaging is used to capture cross-sectional shape changes of the muscle at various locations and at different bite forces. This requires simultaneous measurements of bite force and ultrasound imaging. A pressure sensor is placed in a specific location between the teeth to allow for the differentiation between molar and incisor biting. As these two biting cases differ noticeably in terms of muscle involvement, maximum bite force, initial muscle shape at the beginning of force generation, and muscle shape during force generation, the experimental setup is designed such that the measurements allow to differentiate between location dependent muscle properties of the masseter.

The pressure sensor is embedded in a rectangular silicon block (width 1cm, length 3cm,
and height 0.5cm) in order to protect the sensor during biting. The biting zone on the block evenly distributes the bite force exerted on the sensor by the inhomogeneous occlusal surface of the teeth and creates a gap between the teeth that mimics the chewing process of food at a physical jaw opening angle. The pressure signal is calibrated such that it is equivalent to the bite force between the teeth given in Newton [N].

Figure 8.5 shows the experimental setup for bite force measurements at the respective biting locations and simultaneous ultrasound imaging for the visualization of muscle deformation during contraction. The ultrasound images are used to determine the cross-sectional muscle shape in six different planes. The three-dimensional shape change of the muscle is approximated by five evenly spaced transverse planes ($H_1$-$H_5$) along the principal direction of the muscle and one vertical plane ($V$) in the middle of the muscle as indicated in the figure. An 8MHz linear array ultrasound probe (Siemens ACUSION 8V3 probe) is used to take B-mode image sequences with an in-plane resolution of 0.1mm/pixel (254dpi). 1520 images are taken within a 30s video sequence which visualizes the evolution of muscle shape during multiple biting cycles including repeated buildup and relaxation of a specific bite force. In order to determine bite force specific muscle response, three force magnitudes of 50N, 100N, and 200N are defined which the subject attempts to target in each of the at least three biting cycles per video sequence. Multiple biting cycles are considered in order to examine repeatability and reliability of measurement data.

Essentially, a 30s video sequence is recorded for both biting positions (molar and incisor), for each of the three target forces, and for each of the six cross-sectional muscle planes summing up to 36 measurements, see also Table 8.1.

Repeatable probehead placement for the six different measurement planes is optimized by marking these planes on the ultrasound standoff gel pad. This comes at the additional advantage of enhancing the near-field ultrasound image resolution of the masseter. The maximum frequency of the ultrasound probe determines the depth within the tissue at which optimal resolution is achieved. In particular, since masseter muscle is directly underneath the dermis and a thin layer of fatty tissue, two standoff gel pads on top of each other are used to provide for a sufficiently large distance between probehead and masseter muscle.

Simultaneous measurements of bite force and ultrasound imaging allow to determine the individual image frames at which the target forces are reached. In a subsequent image analysis the corresponding shape changes in muscle are derived using optical flow tracking as presented in previous studies in Chapters 6 and 7. Based on a manual segmentation of the muscle contour in the initial image of the video sequence, the tracking algorithm provides the evolution of tracking points throughout the biting cycles. Muscle deformation and corresponding shape changes are analyzed in form of cross-sectional areas for each measurement plane at each bite force and biting position. This analysis yields a substantial mapping of the muscle behavior during active contraction. The area is calculated as the convex hull around the tracking points defining the individual cross-sectional boundaries of the masseter muscle. Given the clearly visible muscle structure in ultrasound images, especially due to the high echogenicity of the fascia surrounding the muscle tissue, the tracking method provides reliable data.
8.2. Materials and methods

Figure 8.5: Experimental setup for the measurements of muscle deformation during contraction. The force sensor allows for real-time measurements of the current bite force in the specific biting locations. At the same time, ultrasound imaging is used to capture muscle shape changes in multiple cross-sections of the muscle depending on biting position and bite force. Three dimensional muscle shape is approximated by six measurement planes as indicated on the gel pad and FE mesh of the masseter.

Table 8.1: List of ultrasound measurements in the individual masseter cross sections which were performed for both, molar and incisor biting.

<table>
<thead>
<tr>
<th>Bite Force</th>
<th>V</th>
<th>$H_1$</th>
<th>$H_2$</th>
<th>$H_3$</th>
<th>$H_4$</th>
<th>$H_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50N</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>100N</td>
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<td>*</td>
<td>*</td>
</tr>
<tr>
<td>200N</td>
<td>*</td>
<td>*</td>
<td></td>
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</tr>
</tbody>
</table>
Chapter 8. Masseter muscle response during mastication

8.3 Results

In this section, the analysis of the numerical simulations and the experimental observations on the mechanical behavior of the masseter muscle are presented. Efficient processing of food for optimal nutritional uptake begins with scrunching and chewing in the mouth. This process includes different biting mechanisms that depend on food texture and bite size and differ with respect to bite force, biting position, and jaw motion. Kinematics of the jaw are characterized by specific muscle recruitment patterns. In the study presented here, closing and clenching in the molar and incisor biting position are analyzed.

8.3.1 Numerical simulation of the mastication system

The numerical simulation of biting as it is presented here, refers to the specific part in the biting process at which bite force is generated. This study aims at predicting the masseter muscle response for this particular step. Two different simulations are designed in order to investigate the difference in the response for the cases of incisor and molar biting. In general, the simulations differ in terms of the contact points of the teeth when the jaw closes upon muscle contraction. In the human biting process, the biting position is controlled by a superposed translation and rotation of the mandible about the temporomandibular joint. In the simulations presented here, the closing of the mouth is separated into two steps. In the first step, the mandible is translated along the sagittal plane in order to align the closing teeth. In the second step, the closing of the mouth is modeled as a pure rotation about the condyle head of the temporomandibular joint. During the first step the masseter muscle is considered to behave passively and is only activated in the second step for the actual closing of the mouth and the development of bite force between contacting teeth. The numerical model for this study, includes the masseter, the mandible, and the skull.

Electromyography (EMG) measurements of the muscles of mastication during characteristic jaw movements clearly indicate that the biting process heavily depends not only on the masseter but just as much on the temporalis and pterygoid muscles (Koolstra and Van Eijden, 1992; Mao and Osborn, 1994; Van Eijden et al., 1993). Given the fan-shaped fiber orientation and its insertion on the coronoid process, the temporalis muscle exerts large forces on the temporomandibular joint, contributing substantially to the overall biting force in the molar, but especially in the incisor biting case (Hannam et al., 2008; Hirose et al., 2006; Koolstra and Van Eijden, 2005). Despite the existing EMG measurements for determining temporalis and masseter involvement during biting, only little is known about bite location and bite force magnitude dependent muscle recruitment in terms of individual muscle activation patterns, contractability of specific muscle regions, and resulting bite forces vectors. For this reason, the current FE model omits the temporalis and focuses on the analysis of the masseter muscle.

Figure 8.6 shows two schematic representations of the numerical simulations. In the case of molar biting, the mandible is initially retracted, causing a passive stretch of the masseter muscle along its principal vertical direction. On the other hand, in the case of incisor biting, the mandible is protruded such that the frontal teeth touch when the
8.3. Results

Figure 8.6: Numerical simulation of biting including the differentiation between (a) molar and (b) incisor biting. The mechanical model described the jaw kinematics that depend on the biting location. In case of (a) molar biting the jaw must retract. In contrast, the jaw must protrude in the case of (b) incisor biting. This influences the initial shape of the masseter muscle before closing of the mouth as it is visualized by the resting state of the muscle (transparent green mesh) and the masseter shape at the beginning of biting (solid blue mesh). The FE model representation shows the temporalis muscle for visualization purposes only.

Jaw closes upon muscle activation. In this second type of simulation, the masseter muscle is passively compressed before it actively contracts in the closing step. The passive deformation of the masseter muscle influences the initial shape before the contraction step and consequently affects the overall mechanical response of the masseter in terms of muscle fiber recruitment, total bite force and shape change. The passive deformation of the muscle influences the approximation of cross-sectional area as the general orientation of the mesh tilts. When protruding the jaw, as for the case of incisor biting, the mesh tends to acquire a more upright orientation leading to increased accuracy of the approximated areas of $H_1-H_5$. The area calculation for the FE simulations is based on the convex hull encapsulating the nodes of the FE mesh closest to the measurement planes. The projection of these nodes onto the measurement planes becomes more accurate as the mesh orientation becomes more upright and assimilates with the horizontal cross sections.

The numerical simulations are analyzed with respect to the predicted muscle and bite forces as well as corresponding shape changes in the masseter muscle during biting. Bite forces between teeth are calculated from contact forces in the positions where the respective teeth come into contact.
Masseter muscle force is derived from the reaction forces in the upper anchoring points of the muscle. The variation in initial position of the masseter muscle for the two individual biting cases has a noticeable impact on the kinematic configuration at the beginning of the active biting step. Despite similar trends in the mechanical response of the masseter muscle, this effects the absolute values of both, predicted forces and shape changes as can be seen in Figures 8.7ff. The small but noticeable difference in initial muscle shape for molar and incisor biting influences the total muscle force as the maximum force is 2.5% higher in the molar biting case. The initial average fiber stretch before activation in the masseter muscle is $\lambda_m = 1.01[-]$ in the molar and $\lambda_m = 0.994[-]$ in the incisor simulation. These findings are in line with measurement data presented by Goto et al. (2001) who reported a muscle length increase upon pronounced jaw protrusion by a factor 1.04.

Based on the muscle model considered in these simulations, see Chapter 4 and work by Ehret et al. (2011), the maximum muscle fiber force depends on fiber stretch, that is the overlap of myosin and actin proteins, that build up the muscle’s force producing sarcomeres. The initial stretch of the masseter muscle in the molar biting case results in an increased myosin-actin overlap and hence in a higher muscle force.

The significant difference of maximum bite for molar biting in comparison to incisor biting is based on the respective lever arms of muscle and bite force with respect to the temporomandibular joint. In the case of molar biting, the lever arm of the bite force vector is significantly smaller than in the incisor biting case. Since maximum muscle force is similar for both cases, the maximum bite force must be smaller to fulfill the equilibrium

![Figure 8.7: Numerically predicted bite and muscle forces during biting depending on the biting position. Comparison to the maximum molar and incisor bite force (363N and 211N, respectively) measured in the experimental campaign.](image-url)
equation for the case where teeth close in the front. This observation has been shown by several mathematical models despite their simplified model representations (Le Révérend and Hartmann, 2014; Osborn, 1996; Sellers and Crompton, 2004). Numerous experimental measurements of maximum bite force exists which suggest a broad range of values (Kiliaridis et al., 1995; Palinkas et al., 2010; Paphangkorakit and Osborn, 1997; Raadsheer et al., 1999; Van Spronsen et al., 1989; Varga et al., 2011). The scattering in these values (>500N) is related to different force sensor measurement systems, measurement positions, bite force directions, age, gender, and many other factors. The experimentally measured maximal bite forces of 363N in the molar and 211N in the incisor biting case have been found to match the results presented by Palinkas et al. (2010) of 343.5N for the molar biting and by Paphangkorakit and Osborn (1997) of 210N in the incisor biting case remarkably well. This is a clear indicator for the reliability of the experimental setup and the calibration of the pressure sensor. Moreover, the considerable agreement between numerical and experimental maximum bite force values observed here, suggests that the FE model provides a reliable representation of the clenching process. Several factors allow explaining the discrepancy in contraction time to maximum bite force between experiments and simulations. For one, the experimental data shows a gradually but fluctuating increase in bite force which is caused by (i) continuous muscle recruitment and muscle fatigue leading to non-uniform muscle fiber recruitment within the masseter, and (ii) a persistent adjustment of the jaw position due to asymmetry when biting down on only one side of the teeth. For the other, the FE model is defined such that ideal kinematic constraints prevent any sliding or jaw movements during biting. Additionally, material parameters used in these simulations were not optimized for realistic fiber twitch and contraction times, see Chapter 4. The difference between numerically predicted and experimentally observed maximum bite force for the incisor biting case is attributed to the temporalis muscle which is not considered in the current FE model. It is presumed that the integration of the temporalis muscle as well as considering multiple muscle fiber directions in the model would increase the predictive accuracy. Weighted masseter and temporalis muscle involvement will noticeably affect the distribution of forces in the mastication system (Röhrle and Pullan, 2007).
Despite the rather homogeneous overall rectangular shape of the masseter muscle, the FE model predicts a varying stress distribution across the individual cross-sections, especially in the localized regions of pronounced geometric inhomogeneity. As shown in Figure 8.8, stress increases in the regions of fixation that are the anchoring points of muscle near the zygomatic arch and the mandible (\(H_1\) and \(H_5\)). Especially where masseter is attached to the mandible, nominal muscle stress peaks as the muscle becomes thinner while internal muscle force remains uniform across all horizontal planes. Stresses in the planes \(H_2\), \(H_3\), and \(H_4\) are very similar as cross-sectional areas are homogeneous in this part of the muscle.

In fact, stress inhomogeneity is a result of nonuniform muscle geometry and location dependent gradually changing muscle fiber orientations. In the current FE model, a single fiber family is considered which is aligned with the principal vertical orientation of the muscle. Fiber inhomogeneity in terms of gradually changing fiber orientation is included in a modified FE model in order to investigate its impact on stress distribution and model forces, as shown in the subsection on pages 130ff.

Figure 8.8: Vertical component (3-direction) of the nominal stresses in the individual horizontal measurement planes \(H_1\)-\(H_5\). Comparison between molar and incisor biting reveals similar trends in stress development upon contraction. However, significant variation in stress values appear across the difference measurement planes due to muscle shape inhomogeneity and different kinematic boundaries on the upper and lower end of the masseter. Stresses are calculated from the sum of all nodal stress components that fall within the individual measurement planes.
Muscle deformation is analyzed by a user subroutine which determines the cross-sectional area of the measurement planes defined in the experimental campaign. For every converged increment in the biting step the current position of all nodes on the outer muscle surface is extracted. Each measurement plane is defined by a normal vector and a reference node on the respective surface. The horizontal measurement planes $H_1$-$H_5$ are described by the same normal vector but five different intersection points at varying vertical positions evenly spread along the masseter, as indicated in Figures 8.5 and 8.8. The normal vector for the vertical measurement plane $V$ is chosen such that the resulting cross-sectional representation of the muscle captures the full masseter profile perpendicular to the transverse planes.

Nodes of the outer contour that are closest to each of the measurement planes are projected onto a horizontal plane based on which the cross-sectional area is calculated. The high level of mesh refinement for the masseter muscle ensures an accurate area approximation when the muscle shape is described by the convex hull encasing all contour nodes.

Figure 8.9 shows the evolution of the cross-sectional area changes during the biting process for (a) molar and (b) incisor biting.

It is observed that both vertical cross sections decrease similarly with increasing bite force irrespective of the biting position. There is a noticeable shift between both area curves.

Figure 8.9: Numerically predicted muscle deformation in terms of area change for increasing bite force. There is noticeable variation in the simulated shape change depending on biting position and measurement location within the masseter muscle. Cross-sectional area is approximated by the convex hull encasing the nodes of the masseter surface intersecting with the respective measurement planes. Dashed curves in image (a) visualize the cross-sectional area changes for the FE simulation of inhomogeneous muscle fiber orientations discussed in detail on pages 130ff.
which is related to the initial translation of the jaw prior to the active closing of the mouth. This causes a stretch for the molar biting and a compression of the masseter in the incisor biting case which is associated with an increased and decreased initial area, respectively.

In both simulations the muscle contour decreases in the lowest horizontal plane $H_3$, where all others increase with bite force. The area in the highest plane $H_1$ changes marginally independent of the bite force which is related to the proximity to the fixation points. The middle sections of the muscle $H_2-H_4$ show pronounced thickening as this part of the muscle is least restrained by boundary conditions.

The kinematic boundary conditions on the masseter muscle inhibit any global shortening of the muscle once the teeth are in contact. In combination with the incompressibility condition of muscle tissue enforced in the material model, muscle deformations are characterized by the observed thickening in the middle of the muscle and thinning in the boundary regions.

**Muscle fiber inhomogeneity**

Muscle fiber orientation defines the force vector during active muscle contraction and determines how the muscle will deform. Depending on muscle function, several different fiber patterns exist. From anatomical data it is known that the actual fiber orientation of the masseter changes along its vertical axis (Williams et al., 1995). Fibers are oriented horizontally at the lower end of the muscle where the muscle attaches to the mandible and changes to a fully vertical orientation when moving upwards. In order to ensure sufficient adhesion of muscle on bone, fibers are ideally aligned perpendicular to the anchoring surface. Within the lower third of the masseter muscle the fiber orientation gradually changes by 90°. In the region where the muscle is connected to tendon the fibers are primarily aligned in the principal vertical direction of the muscle for maximal muscle force generation.

Figure 8.10 provides a schematic representation of the masseter muscle and visualizes how the gradually changing fiber orientation (gray curves) are implemented within the FE model. The non-transparent half of the masseter on the right, depicts the individual sections inside the muscle mesh which have different fiber orientations. Each shade of green represents a set of elements for with the fiber direction is equal. There is a clear effect on the mastication forces and nominal stresses in the individual cross sections which suggests improved muscle functionality. In the numerical example of molar biting, the direct comparison between homogeneous and inhomogeneous fiber orientation reveals increased bite and muscle forces for the latter simulation. Besides an absolute increase in bite force, it is observed that the direction of the bite force vector remains nearly unaffected indicated by the bar plot on the right. A nearly vertical bite force vector is associated with optimal biting conditions for the type of biting simulated here as incisor teeth are primarily used for splitting bigger chunks of food into single pieces, such as in biting into an apple. At the same time, there is a noticeable change in the ratio between the normal and transverse component of the muscle force vector. The vertical force component increases less in comparison to the transverse component. These fiber orientation related changes
have a noticeable influence on the loading of the temporomandibular joint which is in line with work presented by Mao and Osborn (1994) and Koolstra and Van Eijden (1992).

Figure 8.11 visualizes the changes in nominal stresses in the transverse measurement planes when considering multiple fiber families. Planes $H_1$, $H_2$, and $H_3$ show almost no changes to the initial simulation as the fiber directions are equal and unchanged for this region of the muscle. For the lower part of the muscle, however, the gradual change from horizontal to vertical fiber direction causes a significant decrease of the vertical stress component.

Revisiting Figure 8.9 in view of considering gradually changing fiber orientations reveals one main difference in comparison to the homogeneous masseter model. Contrary to the initial observation, the second lowest measurement plane $H_4$ is found to decrease upon biting. This may be explained by the primary orientation of muscle fibers in the transverse plane causing a thinning of the muscle. Additionally, the vertical cross section experiences a pronounced decrease in comparison to the previous simulation and is directly related to the muscle thinning in $H_4$. All other measurement planes are predicted to show a slightly raised area increase.

Figure 8.10: Impact of muscle fiber inhomogeneity on the numerical bite and muscle force prediction. The non-transparent half of the FE model of the masseter shows element sets with the same fiber orientations which are differentiated by different shades of green. Gray arrows indicate the gradually changing anatomy based muscle fiber orientation which is approximated in the FE model. The bar plots on the right, depict the absolute value as well as the vertical and transverse components of bite and muscle force in the two simulations: homogeneous (HFO) and inhomogeneous (IFO) fiber orientation.
Figure 8.11: Comparison of nominal stresses in vertical direction for homogeneous and inhomogeneous fiber orientations in the masseter muscle. Dashed lines refer to the homogeneous case and solid lines are associated with changing fiber orientations. Nominal stresses in measurement planes $H_1$, $H_2$, and $H_3$ experience negligible changes, whereas stresses in $H_4$ (black) and $H_5$ (gray) vary significantly.

These initial results strongly promote to investigate further the effect of the actual fiber orientation. Diffusion tensor magnetic resonance imaging (DT-MRI) is a useful method to visualize the location dependent orientation of muscle fibers in muscle. So far, such measurements have been presented for animal models and human cadavers but no in-vivo DT-MRI measurements of the human mastication system are available in literature (Kober et al., 2004; Schenk et al., 2013). Latter is primarily related to the complex geometry of the mastication muscles and their specific location within different bone structures and air way systems leading to artificial measurement errors. Our investigatory experiment (Anliker, 2014) indicates that such measurements require a novel experimental setup to obtain reliable measurement data.
8.3.2 Experimental characterization of muscle shape changes during mastication

An exemplary ultrasound image is shown in Figure 8.12 of a measurement on the vertical cross section of the masseter muscle. The two gel pads are clearly visible which alleviate the artificial high echogenic signal at the superficial skin boundary and place the masseter muscle within the optimal focal plane of the transducer. The resolution of the ultrasound image allows to differentiate between a highly echogenic epidermal layer and a rather thick layer of dermis and subepidermal tissue characterized by a lower echogenicity. The masseter is well visible especially due to the fascia tissue that appears as a slim highly echogenic band around the muscle (Serra et al., 2008). The ultrasound images of the transverse planes $H_1$-$H_5$ provide a full representation of the masseter cross section allowing to approximate the area size with sufficient accuracy. In the vertical measurement plane the ultrasound image shows a clearly visible outline of muscle tissue. However, subsequent analysis reveals a significant difference between cross-sectional area for the FE model and the ultrasound image. It has been shown that cross-sectional area or thickness measurements based on MR images provide larger values than ultrasound based analysis (Kubo et al., 2006). It is expected that the muscle-tendon complex at the upper end of the masseter muscle is not precisely differentiable in the US image given the limitations with respect to the field of view and disturbances of the ultrasound signal by the neighboring zygomatic arch which leads to an underestimation of the muscle cross-sectional area. Raadsheer et al. (1994) suggest that a common source for larger MRI based values is related to an underrepresented aponeurotic tissue layer surrounding the muscle in ultrasound images.

![Exemplary ultrasound image of the relaxed masseter muscle (sagittal view) out of a video sequence for deformation tracking. The yellow points indicate the current outer contour of the masseter muscle. Muscle dimensions are measured for comparison with values reported in literature.](image)

Figure 8.12: Exemplary ultrasound image of the relaxed masseter muscle (sagittal view) out of a video sequence for deformation tracking. The yellow points indicate the current outer contour of the masseter muscle. Muscle dimensions are measured for comparison with values reported in literature.
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The area calculation for each of the ultrasound video sequences is based on an initial manual segmentation of muscle contour. The ultrasound image of the reference frame is used to select a sufficiently high number of points along the muscle outer surface. These points are then tracked though the sequence of images using the optical flow method presented by Lucas and Kanade (1981). The tracking algorithm provides coordinates of each tracking point for every image. Based on these nodes, the cross-sectional area of each measurement plane is approximated by calculating the area of the convex hull surrounding all contour nodes, similar to the evaluation of the numerical simulations.

Before presenting the observed muscle deformations, force measurement data captured simultaneously with the ultrasound image sequence is analyzed. For a specific measurement sequence, the repeatability of reaching and maintaining the target bite force magnitude for repeated biting cycles is verified in order to identify sources of error in the measurement protocol.

Figure 8.13: Simultaneous force and ultrasound measurements allow for a distinct association of bite force and muscle shape. The measurement data is shown for the whole investigation of the molar biting position at the bite force set value 100N. Measurement recording time includes the measurement in all six measurement planes. The pressure sensor provides the equivalent of the bite force and a synchronization signal that is visible in the ultrasound images as well. Data analysis yields the measurement initiation frame from the synchronization signal and the ultrasound image frame numbers for area calculations of muscle in the reference and contracted state.

For the example of molar biting up to 100N, Figure 8.13 shows the measurement data of the bite force sensor system for the series of measurements in all six planes. The figure contains the synchronization signal (gray line) and the actual bite force measured between the teeth (black line). In order to quantify muscle deformation for specific bite
forces values, muscle shape is determined at two characteristic time points in the biting cycle, the relaxed and the contracted state. This provides a distinctive measure for the shape changes due to contraction of the muscle and allows for comparison with experimental data in literature. At the beginning of the ultrasound image sequence the muscle is considered to be in its reference state. During repeated biting cycles within one video sequence the muscle contracts and relaxes multiple times. Determining the cross-sectional area associated with a specific bite force, requires the identification of the time point for which the bite force signal is considered most stable around the set value. The stability criterion applied in this study is based on determining the maximum number of consecutive data points for which the bite force is within a range of the target value (±0.5N). In order to establish shape and area changes of the muscle upon contraction, the cross-sectional areas associated with specific bite forces are compared to the reference area. Blue and red circles mark the time points in the force data which are associated with the reference state of the muscle and the contracted state of the muscle, respectively. The synchronization of the bite force signal and the ultrasound video is based on a trigger signal causing a spike clearly visible in the force data (indicated by green points) and on the ultrasound images. Knowing the individual sampling rates of the pressure sensor and the ultrasound device, image frame numbers can be uniquely related to the overall measurement time.

The bite force data, as shown in Figure 8.13, is considered to represent a reliable force measurement system which allows to determine the time points of the reference and the contracted state of the muscle accurately. The fluctuations of bite force around the set value is a distinct source of measurement error. However, as an analysis of corresponding fluctuations in the cross-sectional area calculation will show in the following, this error has a marginal affect on the reliability and accuracy of the newly developed experimental setup.
Along these lines, Figure 8.14 presents the experimentally measured cross-sectional area of the vertical plane for the cases of (a) molar and (b) incisor biting at three different bite force levels. Data is shown for the entire ultrasound video sequence during which multiple biting sequences are performed. There is an observable drift in the cross-sectional area that is caused by the optical flow tracker. The internal integration of the optical flow in the tracking scheme accumulates artificial errors. However, as the red lines indicates, the accumulation is observed to grow homogeneously across the entire video sequence. Reference area or the area at the relaxed state in between repeated biting cycles, respectively, is shown to drift similarly to the area during the biting cycle. The consistency in the drift is considered to justify the analysis of the first biting sequence only, instead of determining an average over all biting cycles based on drift-corrected area measurements. Latter approach is certainly recommended for a follow up study of the presented data in order to exclude certain tracking errors.

In general, it is observed that the drift increases with bite force. This is mainly attributed to increased muscle deformations and changes in the echogenicity of the muscle tissue within the image sequence due to probehead movements related to thickening of the cheek.

The analysis of bite force fluctuations related to repeated reaching (and temporary holding) of the bite force target, as well as the drift in area calculation revealed no correlation between these two measurement quantities. This result represents additional confirmation that specific consideration of the drift in the tracking data may be avoided by looking at the results of the first biting cycle only.

The experimental setup combining bite force measurements and dynamic ultrasound imaging of muscle deformations is prone to several additional sources of error. Such well known factors include (i) repeatable positioning of the ultrasound probehead, (ii) proper probehead alignment with respect to skin surface, (iii) accurate gel pad placement on the face in between measurement sequences, (iv) stable targeting of the set value bite force, and (vi) reliable manual segmentation of muscle contour in the initial frame for subsequent contour tracking (Bertram et al., 2003; Kubo et al., 2006; Raadsheer et al., 1994; Serra et al., 2008). The experimental setup presented here is based on the experience of other ultrasound based measurement campaigns and is optimized to minimize external error sources. Despite inevitable, but bounded, measurement errors, the newly developed experimental setup allows for the determination of consistent trends and characteristic mechanical properties of the masseter. The qualitative and quantitative comparison with numerically predicted masseter response requires careful consideration but provides meaningful new insight, as it is presented later on.
8.3. Results

Figure 8.14: Sensitivity analysis of the vertical cross-sectional area calculation ($V$) for (a) molar and (b) incisor biting based on the optical flow tracking results. The evolution of area over an entire ultrasound video sequence of 30s is shown and clearly visualizes a drift in the data due to the accumulation of artificial measurement error. The measurement error increases with bite force which is related to increased motion of probehead during the measurement and related changes in echogenicity of individual tissue layers.
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The optical flow algorithm tracks the nodal position of a set of nodes throughout the entire image sequence. The nodal set consists of the manually segmented outer surface of the masseter muscle and is determined for the first image of each video sequence. The synchronization with bite force measurements allows to determine the two image frames at which the biting cycle begins and where bite forces reaches the target value. The following analysis of muscle shape changes during active contraction is based on the areas at these two distinct image frames. These area values are directly compared to each other in order to derive observable trends and characteristic muscle properties. Figure 8.15 visualizes the variation of calculated reference areas for the full range of measurements. Black circles are associated with the averages of reference areas over all bite forces in the respective measurement planes for the molar biting case. Gray circles are the equivalent values for the case of incisor biting. Finally, red circles represent the overall average of all calculated reference areas in the respective measurement region.

![Figure 8.15: Evaluation of reference area variation across the entire measurement campaign. Black circles represent averages for the molar biting scenario of reference areas in the measurements with different bite forces. Gray circles correspond to the equivalent quantity but for incisor biting. Red circles are the overall average in the respective measurement plane. Black and gray circle sizes are related to the variation in reference area calculation.](image)

There is a general difference in the average reference area of the two biting positions for all the individual measurement planes. However, inter-measurement variability is considered to be very low, as circle sizes indicate. Literature reports, that variability is higher for measurements in the relaxed muscle state in comparison to the contracted state which is primarily attributed to the susceptibility of the pressure with which the probehead is held against the cheek in the relaxed state (Bertram et al., 2003; Kubo et al., 2006; Raadsheer et al., 1994) and the brightening of the muscle outline resulting from changes in the echogenicity during contraction (Kubo et al., 2006).
The biggest variation between the two biting positions is observed for the vertical cross section. The difference in average reference areas is related to the positioning of the jaw which needs to protrude in the case of incisor biting and is retracted for molar biting. Given the orientation of the masseter in the resting state (which refers to the situation with no pressure sensor between the teeth) of the jaw, the muscle is stretched in one case and compressed in the other. No measurement data is available for the masseter in its resting position which would allow for a more detailed analysis of the passive muscle deformation prior to active contraction. Within the horizontal measurement planes, $H_5$ shows the largest variation within same biting positions (Bertram et al., 2003). This is attributed to measurement errors due to variations in positioning of the probehead near the lower end of the masseter muscle. This region is particularly inhomogeneous with respect to shape resulting in larger variations of calculated area (Kubo et al., 2006; Raadsheer et al., 1994).

The experimentally observed horizontal cross-sectional areas provide a realistic representation of masseter geometry, especially, in comparison to the geometric reconstruction based on medical MR images in Section 8.2.1. In good agreement with data in literature, masseter muscle is found to be thin at the top, to thicken towards the lower end, and to rapidly decrease in size near the lower insertion points (Bertram et al., 2003; Kubo et al., 2006; Raadsheer et al., 1994).

In absolute terms, the ultrasound based calculation of horizontal cross-sectional areas along the masseter muscle ranges from $70\text{mm}^2$ ($H_5$) to $412\text{mm}^2$ ($H_3$) agree very well with data reported by Goto et al. (2002), Van Spronsen et al. (1989), and Weijs and Hillen (1985). From data presented by Kubo et al. (2006), the calculated vertical cross-sectional area is $710\text{mm}^2$ which is within reasonable variation of the presented averaged value of $620\text{mm}^2$ considering typical inter-subject variability and different measurement systems. Goto et al. (2001) report a muscle length for the intercuspal position (relaxed state) of $59\text{mm}$ which matches well with the masseter dimensions of the subject in this study, see Figure 8.12.
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Figure 8.16: Cross-sectional areas in the six different measurement planes for (a) molar and (b) incisor biting. Bite force dependent evolution of area is compared to the respective reference area before muscle activation. For the bite force of 200N no measurement data is available for horizontal cross sections $H_2$ and $H_4$ due to muscle fatigue, avoidance of sensor damage, and increased measurement uncertainty.

The contractile behavior of muscles consisting of multiple fiber strands leads to a shortening and thickening of the overall structure. Based on the principal direction of muscle fibers, the deformation behavior will vary and affect the resulting muscle force that is exerted on the respective insertion points. Specific muscle shape is the result of an optimization of functionality. In particular, muscles of the mastication system must provide sufficient movability and generate high biting forces. In fact, the masseter muscle is the strongest muscle in the human body and has been reported to allow for bite forces of up to 800N (Varga et al., 2011). For this reason, there is great interest in understanding the deformation response under such intense loads.

In order to observe general trends in muscle deformation, the evolution of cross-sectional area is determined for selected bite forces of 50N, 100N, and 200N. These values represent the typical range or mastication forces required to process most of human every day nutrition. Figure 8.16 illustrates the biting position and measurement location dependent area change for the three bite forces.

There is an overall trend, that cross-sectional area increases with respect to its reference area upon muscle contraction following usual observation presented in literature (Bertram et al., 2003; Kubo et al., 2006; Raadsheer et al., 1994) and several more reporting noticeable muscle thickening (Bakke et al., 1992; Kiliaridis and Kålebo, 1991; Pereira et al., 2007). Despite similar values of muscle thickness changes measured in the presented study and reported in literature, most studies obtain muscle thicknesses for a single measurement.
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site only which is usually defined in the middle of the muscle. Moreover, corresponding
bite forces at the time of measurement are never reported. Instead, thickness changes are
most often determined with subjects clenching their teeth which represents the physio-
logical limit of the masseter muscle in every day life.

There are several noticeable differences in the evolution of masseter cross-sectional area
when comparing the two biting positions. When biting on the molars with increasing
force, the muscle experiences a consistent pronounced thickening across all transverse
measurements planes (neglecting \( H_5 \) due to measurement errors explained previously).
Especially, the middle sections of the muscle (\( H_2 \) and \( H_3 \)) increase clearly, while the top
and bottom end of the muscle increase noticeably less.

The vertical cross section \( V \) is found to increase upon contraction like all other planes.
However, there is a negative trend for increasing bite force. It is hypothesized that the
masseter shortens along its principle direction while the tendon connecting the masseter
muscle with the skull experiences significant stretching. This view on muscle deforma-
tion is in line with the experimentally observed thickening in the transverse planes but
is fundamentally different from the numerical simulations where the overall length of the
masseter muscle is constrained by the boundary conditions and leads to a different me-
chanical response as shown in Section 8.4.

The positive trend of area change for the incisor biting case is likely to be caused by dis-
tinct differences in the kinematic constraints on the mastication system. When biting on
the incisors the masseter muscle is limited to shorten extensively, but experiences thickening
in the transverse measurement planes as the masseter contracts. Despite the general
increase of cross-sectional area upon bite force generation, the upper part of the masseter
(\( H_1 \) and \( H_2 \)) experiences no significant bite force dependent thickening. In particular,
only the lower part of the masseter (\( H_3 \) and \( H_4 \)) show a positive correlation between bite
force and thickening.

The increased fluctuations of measurement values for the transverse plane \( H_1 \) are observed
for both biting positions and are related to the proximity to the upper end of the masseter
muscle. Most probably, as increasing bite forces lead to a shortening of the masseter in
vertical direction, the initially measured cross section of the muscle will shift downwards
and hence change the part of the muscle that is examined.
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8.4 Discussion

The biting process is analyzed with respect to bite force, internal muscle forces, and a location specific quantification of muscle deformation. The comparison of maximal bite force from experimental measurements and FE simulation reveals remarkable agreement for the molar biting, as shown in Figure 8.7 as well as with data presented by Palinkas et al. (2010) and Paphangkorakit and Osborn (1997). The numerical simulations consider previously presented material parameters, see Chapter 4, and required no additional parameter fitting to provide such realistic predictions. The difference between experiment and simulation for biting on the incisors is attributed to omitting the temporalis muscle in the FE model representation. The numerical underestimation of maximal bite force is related to the missing muscle force exerted on the coronoid process of the mandible which serves as an additional lever arm to generate a larger closing force between the incisors.

A direct comparison of absolute values for the experimentally observed and numerically predicted cross-sectional areas is not possible (Raadsheer et al., 1994; Serra et al., 2008; Van Spronsen et al., 1989). The geometric reconstruction of the mastication system is based on a semi-automatic segmentation of MR images, repeated smoothing of surfaces and the final approximation of the individual objects by sufficiently refined meshes. Similarly, the experimental quantification of muscle deformation relies on a discrete map of cross-sectional areas approximated at specific bite forces and different measurement locations. However, regardless of the differences in the characterization of the masseter geometry, the experimental and numerical results are shown to provide reasonable properties of the masseter and to describe a similar mechanical response.

In order to allow for a comparison of muscle deformations determined in simulations and experiments, the cross-sectional area is normalized by the reference area of the individual measurement planes. This provides means to determine characteristic trends that depend on bite force, measurement location and biting position for both studies.

Analysis of Figure 8.17 reveals similar tendencies in area size change based on the predicted and the experimentally observed muscle behavior within the individual measurement planes. The transverse plane close to the upper and lower end of the muscle experience the smallest area change relative to the reference area while the middle section experiences pronounced deformations for increasing muscle forces which is observed for both data sets. The area change in the vertical cross section, shown in Figure 8.17(a), reveals critical properties of the masseter muscle. While the FE model predicts a decrease in masseter size, the experimental study shows an explicit increase of masseter area for increasing biting force. The kinematic constraint of the masseter model restricting any shortening during the biting phase together with the pronounced thinning in the lower masseter result in an area decrease. It is hypothesized that the FE model is over-constrained with respect to the flexibility of masseter shortening during biting, especially, considering the lack of differentiability of active masseter and passive tendon tissue in the MR images. This results in incorrect assignment of material properties and it is suggested to consider active and passive regions in the geometric representation. The tendinous tissue at the upper end of the masseter behaves passively and should, therefore, be considered separately (Röhrle and Pullan, 2007).
Figure 8.17: Normalized cross-sectional area for each measurement plane. Comparison of numerically predicted and experimentally observed muscle deformation depending on bite force.
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8.5 Conclusions

This chapter presents an extensive experimental and numerical investigation of the mechanics of mastication. An anatomy based FE model of the mastication system was developed. Semi-automatic segmentation of medical images, subsequent mesh generation and the definition of physically motivated kinematic constraints constitute the individual steps in the preparation of a realistic geometric representation of the mastication system, including the muscles of mastication (masseter, temporalis, medial and lateral pterygoid muscle) as well as skull and mandible. Incorporating the numerical implementation of a physically based constitutive model for skeletal muscle tissue, presented in Chapter 4, provides means for a reliable description of active muscle response in mastication and jaw kinematics (Anliker, 2014). The FE model is used for the simulation of incisor and molar biting using a model version including the masseter, mandible and skull. Respective boundary conditions and kinematic constraints were imposed for the muscle and the temporomandibular joint.

The numerical simulations show a significant difference for the two biting positions in terms of muscle and biting forces as well as muscle deformations. The numerically predicted maximum bite forces show considerable agreement with the experimentally observed limit. The relative difference between both values for the incisor biting case are related to the missing temporalis muscle in the numerical simulation. The FE model was validated for sufficient mesh refinement and material parameters from Weickenmeier et al. (2014a) were confirmed by comparison of muscle force of the newly generated FE model. The evaluation scheme for the calculation of bite and muscle forces, the stress in the measurement planes, and the cross-sectional area is confirmed to provide reliable results in comparison to Anliker (2014).

As a simplification of the FE model, uniform fiber orientation was assumed. Investigating inhomogeneous fiber orientation by means of location dependent muscle fiber orientation demonstrated the impact on internal muscle stresses, as well as bite and muscle forces. Based on the preliminary results, it seems relevant to include an anatomically based representation of fiber orientations.

In collaboration with Nestlé Research, a measurement setup was developed that allows for simultaneous bite force measurements and ultrasound based visualization of masseter muscle deformations during biting. All measurement data were analyzed with respect to repeatability and reliability across the experimental campaign. Muscle shape change was observed to heavily depend on biting location and bite force magnitude. Multiple measurement sites were defined in order to reconstruct the overall three-dimensional muscle response during molar and incisor biting.

Comparison of experimentally observed and numerically predicted shape changes revealed qualitative agreement despite the error sources discussed in previous sections. In summary, the FE model represents a reliable predictive tool for the investigation of the mastication system. Accuracy of force and shape change predictions can most certainly be improved through model extensions as proposed in the following section. The experimental campaign provided novel insight into the mechanical properties of masseter muscle.
deformation during active contraction by relating bite force to location dependent muscle deformations for multiple biting positions.

**Outlook**

Based on the results of the experimental campaign it is suggested to continue the investigation of biting location specific muscle involvement and muscle recruitment patterns for individual jaw movements. Electromyography (EMG) is a well established measurement method to quantify activation levels of muscle tissue and would provide substantial insight in the individual muscle recruitment patterns during jaw movements.

In order to incorporate an anatomy based representation of muscle fiber orientation, diffusion tensor MR imaging (DT-MRI) would identify the location specific principal direction of muscle fibers allowing for a one-to-one mapping of the fiber direction field onto the FE mesh presented within this study.

The incorporation of the temporalis muscle is expected have a significant impact on prediction accuracy of biting forces in the incisor biting case.

In view of numerical simulations for medical applications (i.e. cranio-maxillofacial surgery, jaw bone prosthesis due to bone tumor) as well as for simulations of the biting experience of novel food textures for the food industry, the FE model could be extended to include the soft tissues of the face together with the mouth cavity and the tongue, in order to allow for the visualization of the activated full-thickness tissue response.
Part IV

General Conclusions and Appendix
Conclusions and outlook

The work presented in this thesis investigated the mechanical behavior of facial soft tissues by means of integrating theoretical and experimental approaches. The first part engaged in the numerical implementation of two constitutive material models within the finite element (FE) environment. The second approach considered the experimental characterization of facial soft tissue properties. The main achievements are summarized here.

9.1 Contributions of the present work

The numerical implementations of a physically based skeletal muscle model and a generalized elastic-viscoplastic material model suitable for facial soft tissues provided new possibilities for FE simulations of facial tissue behavior. In particular, the implementation of the muscle model revealed that the decoupling of the strain energy function into a distortional and a dilatational part resulted in highly unphysical volume growth in the numerical simulation of a uniaxial tension test with activated muscle tissue, as well as negative eigenvalues of the tangent moduli. This confirmed previous findings that the decoupled approach experiences an artificial numerical error for constitutive models of fiber-reinforced materials. As a consequence, a new constitutive model was proposed which considers muscle as nearly incompressible and provides meaningful numerical results.

In the case of the generalized elastic-viscoplastic soft tissue model, a strongly objective integration scheme and a new mixed FE formulation were developed based on the introduction of the relative deformation gradient. This tensor represents the deformation mapping between the last converged and the current configuration. The specific model formulation presented by Rubin and Bodner was implemented in a user element. Both, the muscle and soft tissue model, were used throughout all of the presented numerical simulations and have proven to be numerically robust, to provide optimal convergence, to ensure material incompressibility across all applicable ranges of stretch, and preserved objectivity under superposed rigid body motion.

In view of the numerical simulation of facial expressions in the forehead as well as the mastication process, two anatomy based FE models were developed. Based on magnetic
resonance images, the multilayered tissue structure of the forehead was reconstructed. Similarly, semi-automatic segmentation of MR images provided the geometric representation of the muscles of mastication and the bone structure of skull and mandible. The simulation of forehead wrinkling included the experimentally observed tissue layer interaction properties. The consideration of glide plane spaces in the forehead model resulted in a realistic representation of the predicted wrinkle pattern upon frontalis muscle contraction.

In an extensive suction based measurement campaign, the mechanical properties of superficial facial soft tissues were characterized. The related development of an experimental setup was optimized for repeatability, reliability, and accuracy for both measurement devices, the Cutometer and the Aspiration device. Measurements in three different regions of the face allowed for the characterization of location specific tissue behavior. Different measurement profiles were defined in order to differentiate between short and long term properties of the superficial tissues, to quantify cyclic tissue response, and to enable a fitting of the individual material model parameters to the experimentally observed response. By means of varying probe opening diameter, skin and subcutaneous tissue were addressed in separate measurement series allowing for the determination of two tissue specific material parameter sets for the Rubin and Bodner model. In an inverse FE optimization, material parameters sets for skin and subcutis were determined such to provide optimal agreement between the experimentally observed and numerically predicted material response for the whole range of measurement protocols. The proposed material parameters were shown to represent the experimental data, especially including the cyclic tissue response, remarkably well. This was considered to verify the considerable predictive capability of the Rubin and Bodner model as well as the newly developed element formulation.

Realistic modeling of tissue layer interaction at the boundary of individual layers was considered to provide a significant improvement of existing FE models of the face. An experimental setup was developed which allowed for ultrasound based imaging of the full-thickness skin deformation field upon external displacement. A tissue motion tracking scheme was implemented which extracted the deformation profile across the individual tissue layers. Experimental data was presented, which indicated a significantly increased deformation gradient across the boundary between muscle and periosteum in comparison to a rather homogeneous decrease in the displacement magnitude within the two most superficial layers, thus visualizing the so called glide plane spaces. The measurement protocol was used to investigate location dependent variations in interaction properties. Quantitative indications suggested a significantly stronger connection between individual tissues in the region of the temporal fusion zone- an observation well described in anatomical literature. These experimental findings were successfully included in the forehead model resulting in the above mentioned realistic wrinkle pattern.

Based on the reliability of the measurement protocol, feasibility of the measurement technique as a clinically relevant examination tool for monitoring pathological alterations in the skin of scleroderma patients was investigated. Direct comparison of young, aged, and sclerotic skin revealed visible trends in changes of superficial tissue and their interactions properties. Pathological skin thickening in scleroderma, the loss of elasticity in aged skin, and the significantly different transmission of externally applied displacement across full-
9.2. Outlook

The achievements of the present thesis contribute to a better understanding of the mechanical behavior of facial soft tissues. However, physically based FE modeling and the experimental characterization of soft biological tissues offer significant potential for future investigations.

Experimental Characterization of Skin  Skin tissue is a multilayered structure of constituents with distinct functions. In particular, skin contains a collagen network which causes a locally varying anisotropic behavior that has been neglected in the numerical simulations in the present thesis. Visualization of the collagen network by way of multiphoton microscopy should be explored in order to establish a measurement technique capable of quantifying skin anisotropy, especially during mechanical loading as in skin extension tests.

The suction based measurement setup provides the opportunity to adapt probe opening shape and size such to account for an anisotropic response. Similar strategies have been proposed in literature, but all lack to combine the experimental data with a physical based constitutive material model. A corresponding three-dimensional inverse FE analysis would allow for the identification of the fiber contributions in the Rubin and Bodner model and represent a valuable extension of the material parameters presented within this thesis.

Such experimental investigations should go hand in hand with the development of a simplified FE model of the face which is compatible with the user element implementation
Chapter 9. Conclusions and outlook

presented in this thesis and which pays particular attention to the superficial tissue layers including epidermis, dermis, and subcutaneous tissue or the superficial musculoaponeurotic system (SMAS), respectively. Such a FE model gives way to simulate time, location, and history dependent behavior of facial soft tissues as it is of significant interest to the cosmetic industry and dermatology.

FE Modeling of the Mastication System  
Realistic simulation of the mastication system is gaining importance in the planning of craniomaxillofacial surgeries as well as the food industry given the possibility to predict surgical outcome and eating experience from a biomechanical stand point. The simulations presented in this thesis can be elaborated in terms of incorporating the other muscles of mastication besides the masseter. As the FE meshes already exist, this step requires the experimental quantification of muscle recruitment patterns through electromyography (EMG) measurements during specific jaw movements and biting. The biting location specific activation of individual muscles has been rarely investigated in literature so far.

A second important key in physical based numerical simulation of muscle response is the concise representation of muscle fiber orientation. Diffusion tensor magnetic resonance imaging (DT-MRI) is a reliable measurement technique to visualize fiber structures which allows to extract the principal directions of the underlying network. In case of muscle tissue, DT-MRI provides the fiber orientations which are directly related to the main direction of force development. The incorporation of location specific fiber data in the FE mastication model would substantially improve numerically predicted muscle shape changes and muscle forces.

Both EMG and DT-MRI measurements would allow for improved calibration and validating of the FE model. In return, numerical simulations could be used to explore the jaw kinematics in eating disorders, the impact of CMF surgery on mastication, and the biocompatibility of implants and prosthesis for mandible reconstruction.

Ultrasound Imaging of Soft Tissue Mechanics  
The visualization of soft tissue mechanics opens up several opportunities for clinical practice. In particular, biomechanics allows to relate pathological tissue changes to alterations in material properties and interactions. Quantitative evaluation of ultrasound image data provides means for diagnosis of tissue diseases and monitoring of etiopathogenesis and the impact of therapy. The investigation of sclerotic skin in the present thesis demonstrated combined ultrasound imaging and skin extension testing as a potential clinical tool. It should be investigated further how a standardized skin loading procedure could improve intra- and inter-subject variability in order to develop a mechanically based skin score system for scleroderma.

In general, the broad range of applicability, availability, and high image resolution promotes ultrasound based mechanical characterization of soft tissue behavior as a reliable source of experimental data for the validation of constitutive modeling and numerical simulations. More specifically, the increasing clinical interest of ultrasound in dermatology represents a new field for a collaboration of medical practice and the field of biomechanics.


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