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# Modeling of the coupled electromechanical activation of the human heart

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**Masterarbeit:**

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# Preface

In my evolving career as young mathematician I have faced many different aspects of applied mathematics, including applications in electrical engineering, thermomechanics and abstract theories on evolution equations. Following this pattern, I should now treat a completely different topic and indeed the present thesis deals with a topic from an evolving science called *biophysics*. To be more precise I am dealing with the topic of modeling the mechanical and electrical activation of the human heart.

With this topic, in my opinion, I have finally touched a group of topics which combines the most interesting aspects of all previous work and adds the extra ingredient of human physiology. I hope that I can stick to this topic for a longer time and be able to contribute to this fascinating field.

I want to thank Prof. Olaf Steinbach for encouraging me to treat this topic. Furthermore I want to thank Prof. Gerhard Holzapfel and Prof. Gernot Plank for their input where my knowledge of electrobiomechanics was limited. The first chapters of my thesis would not look the way they do as it were not for those two. I also want to dearly thank my dear friend and colleague Arno Kimeswenger for the daily discussions and his input and opinion. I think we both helped each other a lot to bring our theses to a good end. Yet more I want to thank Dipl.-Ing. Harald Schmidt for proofreading my thesis.

Last but not least I want to heartily thank my parents for their overall support during my studies. This work is dedicated to them.

# Contents

# Notation

Throughout this thesis we will use the following notation:

- Scalar quantities will be denoted by a letter in normal font, e.g.: $\phi$.
- Vector valued quantities will be denoted by a bold letter in normal font, e.g.: $\boldsymbol{u}$.
- Matrices will be denoted by a normal letter in sans serif font, e.g.: $\mathsf{A}$.
- Tensor valued quantities will be denoted by a bold letter in sans serif font, e.g.: $\mathsf{T}$.

This notation will apply henceforth until otherwise stated.

# Introduction

The human heart has played an important role for understanding the body since antiquity. In the fourth century B. C., the Greek philosopher Aristotle identified the heart as the most important organ of the body, the first to form according to his observations of chick embryos, see [56]. He characterized it as the seat of many human abilities, such as intelligence, motion and sensation. Therefore, in Aristotle's view, it was a very hot organ and all other vital organs[1] in the human body exist merely to cool the heart.

During the last millennium, the pursuit of knowledge of the human heart has gained more importance, not only by a desire to understand the mechanical and electrochemical processes, but also by the increasing clinical importance. According to the World Health Organization (WHO) heart diseases are one of the top ten causes of death in western society (see [84]). Thus, improving the understanding of the function of the human heart may lead to new techniques for the diagnosis and treatment of heart problems.

Over the last decades, the amount of information about the mechanisms of the human heart has rapidly increased. Now we are in the position to observe cellular and even sub-cellular processes. Nevertheless there remain several unanswered questions, for example why does defibrillation really work, and what is happening in the heart at that time.

The most prominent and standard tool in cardiology is the *electrocardiogram*, abbr. ECG. It dates back to Wilhem Einthoven, see [16]. However, in the ECG one deals with the human heart as a black-box and tries to reconstruct some dipole distribution. This is known as the inverse problem of electrocardiography, see [36, 76]. This problem is essentially ill-posed and does not provide satisfying results. Furthermore one has no possibility to study complex arrhythmias in the human heart, by just using an ECG. So nowadays we try to model the human heart more detailed with sub-cellular to macroscopic models as well as their interaction and coupling. This reflects and is based upon the increasing physiological knowledge about the human heart. These days it is known that changes in the macroscopic scale of the heart, for example high blood pressure, acts down to the sub-cellular and the genetic level but also vice versa. This is a quite new research field know as *epigenetics*. For more information about epigenetics one should refer to [54].

The newly developed models give the possibility for *in silico* simulations and enable

[1] e.g.: brain and lungs

studies of heart diseases without harming a human patient. However, very few attention has been payed to a strict mathematical formulation and to a numerical analysis. In this thesis we shall try to give a brief overview of the existing mathematical models for describing the coupled effects of electro-chemical and mechanical processes in the human heart. We will arrive at essentially non-linear coupled systems of partial differential equations and also ordinary differential equations.

Chapter 1 gives a short overview of the physiological functionality, essentially the cardiac cycle, as reference for our purposes. In Chapter 2 we will model the electric activation of the human heart which will lead us to the well-known *Bi-Domain* model of L. Tung presented in [79]. In Chapter 3 we will describe the purely mechanic model of the human heart. For this purposes we shall present a material law developed by G. Holzapfel in [32]. In Chapter 4 we will try to couple the independent models of the electric and mechanic activation of the human heart by incorporating the most recent literature. Finally in Chapter 5 we will account for the analysis and solvability of each model separately. The analysis of the fully coupled problem is postponed to further work.

While Chapter 1 describes the human heart as a whole, the subsequent chapters focus on the ventricles, a distinct part of the human heart playing a key-role in its functioning: the ventricles are indispensable to life, whereas the atria, which form the other part of the human heart are not. Furthermore these two parts are, except for one passage which will also be described in Chapter 1, completely electrically insulated. Hence, from a physiological insight it is sufficient to focus on the ventricular electromechanics for which almost all literature is about.

# 1 Physiological Background

This introductory chapter is inspired by and excerpted from [36, 71] and [32].

The most studied organ in human physiology appears to be the heart, although its function seems quite simple: it pumps blood through our body by contracting and expanding about 2.5 billion times during a normal lifetime of a human being. As a fact, heart failure, either electrical or mechanical, is one of the most common causes of death in the Western world, see [84].

The human heart is a muscular organ, weighing about 250 to 350 grams with a size comparable to a fist, which, as denoted above, pumps the blood through the blood vessels, delivering nutrients and removing waste from each organ, by repeated, rhythmic contractions. This process, where the oxygen rich blood is delivered to the organs is called the *systemic circulation*. Furthermore the human heart drives deoxygenated blood through our lungs for re-oxygenation (the so called *pulmonary circulation*). Figure 1.1 shows a schematic view of the heart. The coordination of the

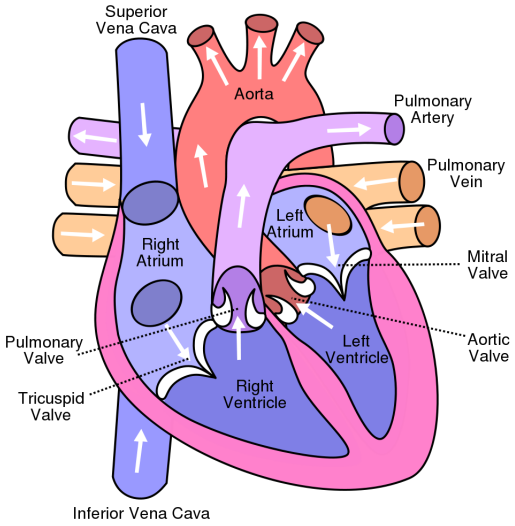


**Figure 1.1** – Schematic view of the human heart.[1]

mechanical activity of the human heart is closely related to the signal transportation in it. Its mathematical modeling will be the main topic of this thesis. In order to develop the models we need to understand the basic underlying physiological

[1] taken from `http://en.wikipedia.org/wiki/Right_ventricle`

principles. That is the goal of this chapter. As a start we will establish some basic mechanic facts about the heart.

## 1.1 Facts & Figures

The location of the human heart is anterior to the vertebral column, i.e. the spine, and posterior to the sternum, i.e. the chest. As one can see in Figure 1.1, the human heart consists of four chambers: the right and left *atria*, which receive the blood from the body acting as a large-volume low-pressure reservoir, and the left and right *ventricles*, which actually do the predominant pumping of the blood through our body.

The mantle of the human heart consists of three layers. The outermost is referred to as *epicardium*, which mainly consists of collagen fibers and serves as a protective layer. The middle one is called the *myocardium*, consisting of muscle cells, called *myocytes*, which do the actual contraction of the heart[2], and innermost the *endocardium*, like the epicardium consisting of mainly collagen which serves as an interface between the heart wall and the human blood.

The thickness of the epicardium, about 100 $\mu$m, and of the endocardium, about 100 $\mu$m, is much less than the one of the myocardium. Although it is not uniform but it is always many magnitudes thicker than the epi and endocardium. Epi- and endocardium being considered as mere protective respectively interfacing layers it is justified to restrict our attention and model to the myocardium itself. Following Holzapfel in [32] we adopt the assumption, that the myocardium can be described as a continuum composed of laminar sheets[3] of parallel myocytes arranged in fibers. Figure 1.2 shows the basic structure of the left ventricle. It was extracted from [32]. As one can see the fiber direction of these muscles rotates, in a mathematical positive sense, throughout the wall thickness from 50° to 70° near the epicardium to $-50°$ to $-70°$ near the endocardium. The organization of the myocardial layers is characterized best by a right-handed orthonormal set of basis vectors $(\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0)$, denoted *fiber direction*, *sheet direction* and *sheet normal direction* respectively. This will be discussed in more detail in Sections 2.4 and 3.4.1. According to [32] we shall use the local index set $\{f, s, n\}$ for referring to fiber, sheet and normal direction. The idea behind this will be explained in Section 2.2.4. Furthermore we will use the pairs $fs, fn$ and $sn$ when talking about the fiber-sheet, fiber-normal and sheet-normal planes respectively. For a detailed overview on the structure of the myocardium

[2] Although it is of great physiological interest we will skip the description on how cells can actually contract, as this would lead us to far away from the main topic, we will assume that they just *do* contract. The interested reader may refer to [36, Chap. 15] or [71, p. 60ff].

[3] There is an discussion about the justifiability of this assumption, see [22].

[4] This figure is taken from [32, p. 3448 Fig. 1.].

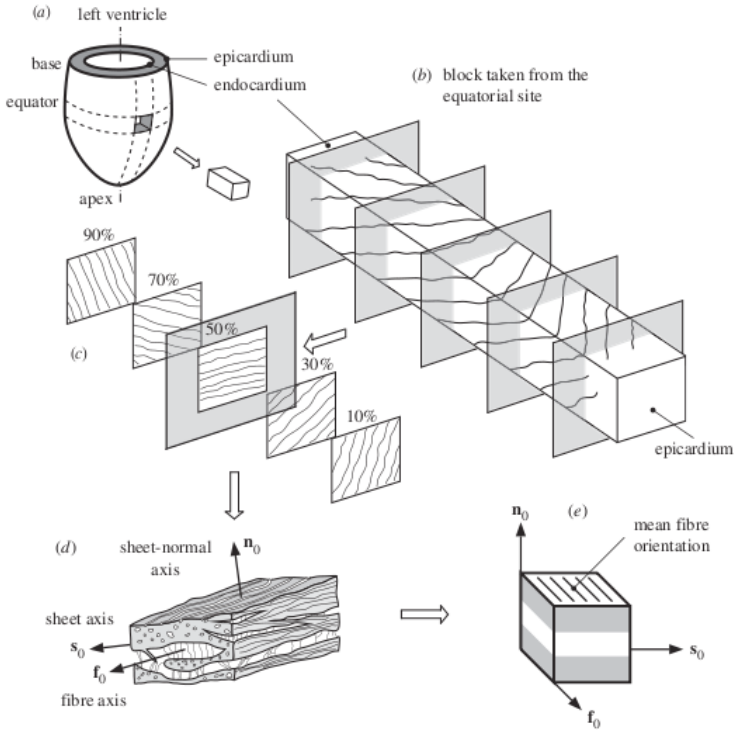


**Figure 1.2** – Schematic view of the muscle structure in the human heart[4].

($a$) shows an schematic view of the left ventricle where a small block of myocardial tissue has been cut out.

($b$) shows the structure of the muscle from the endocardium to the epicardium.

($c$) shows five special longitudinal-circumferential layers at varying thickness of the myocardium, from 10 to 90 per cent of the wall thickness.

($d$) shows the make-up of myocytes, with embedded collagen fibers and the local right-handed orthonormal fiber coordinate system with the fiber axis $\boldsymbol{f}_0$, sheet axis $\boldsymbol{s}_0$ and sheet-normal axis $\boldsymbol{n}_0$.

Finally in ($e$) one sees a cube of layered tissue with local coordinates $(X_1, X_2, X_3)$ which is used to develop the mechanical models in [32].

refer to [17, 32, 39–41, 70] as a starting point. The detailed pure mechanical model of the myocardium is presented in Chapter 3.

The mechanic response of the human heart relies on a very complex electro-chemical signal conduction system which will be discussed in the next section.

## 1.2 Signal Conduction & Overview of the Cardiac Cycle

For a more detailed description about the signal conduction of the human heart the reader is referred to [43, 71].

Cardiac tissue is called a *functional syncytium* of myocytes. This means that cells are separated morphologically but connected through so-called *gap junctions*. Gap junctions enable the cells to exchange different ions and molecules (like e.g. $Na^+$ or ATP[5]) with each other. This transfer between cells is one of the reasons why the heart muscle can contract so fast. For more details on gap junctions refer to [71, p. 16ff].

Myocytes have two very important abilities, namely they are excitable and contractile. The first means, that they can transport electric potentials and these potentials cause the cells to actually contract.[6] The excitability of the myocytes is fundamental for understanding the functionality of the human heart and will be addressed in Section 2.2.4. However, to ensure correctness of the complex process of pumping blood through our body, there is an intense communication and synchronization between the cells, which is controlled by the *signal conduction system* of the heart as depicted in Figure 1.3. The electrical activity of the human heart starts in a bunch of cells known as the *sinoatrial node*, short SA node, which is found just below the superior vena cava of the right atrium. The cells in the SA node are very special cells, as they work as autonomous oscillators, meaning that they can alter their electric potential without effects from outside. This change of electric potential (known as *action potential*) is then mitigated through the heart, starting by the atria. The atria and the ventricles are sperated by a wall which consists of non-excitable cells. Thus the action potential cannot pass directly this barrier. However there exists one pathway through this barrier: another bunch of specialized cells, known as the *atrioventricular node*, or short AV node, located at the bottom of the atria. An

[5] ATP stands for *adenosine triphosphate* and is one of the most important source of energy in the human body. Therefore one also calls ATP the "currency" in our body, see [38].

[6] We will not discuss the details of how muscle cells actually contract, as this will lead us to far away, we will rather assume that they just *do* contract. For a detailed physiological overview the interested reader may refer to [71, p. 60ff] and also [20, 26, 33] and for a detailed mathematical modeling overview one should refer to [36, Chap. 15].

[7] taken from `http://en.wikipedia.org/wiki/Electrical_conduction_system_of_the_heart`

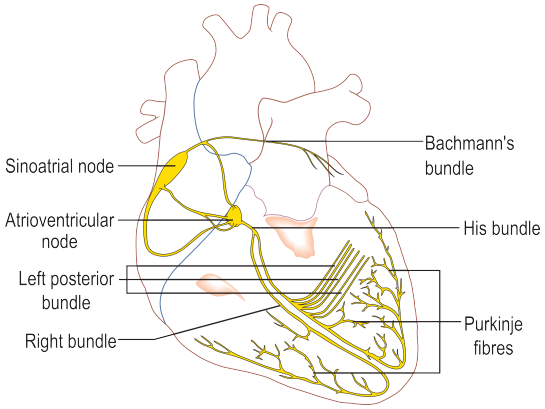


**Figure 1.3** – Schematic view of the signal conduction system of the human heart.[7]

important property of the AV node is, that its conductivity is much smaller than in usual heart cells, so these action potentials travel quite slow through this cells. This happens not without ulterior motive. If the signal would pass the AV node as fast as it travels through other cells, the ventricles would start to contract before the atria have ejected all of the stored blood into the ventricles. After the signal has passed the AV node it branches out through a specialized collection of cells known as the *bundle of His*, which is composed of *Purkinje fibers*. This Purkinje fiber network spreads out in a tree-like way into the left and right *bundle branches* all over the inside of the ventricles. The Purkinje fibers are connected to the ventricular muscle cells through junctions. When an action potential reaches a muscle cell from a Purkinje fiber it causes it to contract, and so the whole ventricle starts to contract. The end of the propagation of the action potential lies in the epicardial surface. After the signal has reached this point, the whole contraction is reversed and starts again from the SA node. Due to the mentioned insulation of the ventricles and the atria and also due to the fact that the ventricles are of greater physiological interest, as aforementioned in the Introduction, the modeling is limited to the ventricular activity of the human heart.

## 1.3 Summary

This was a very brief, and by no means complete, overview of the cardiac cycle in a human heart. It should be evident from the above paragraph, that there is a multitude of features of the myocardium to study. First of all one needs to know how the electric potentials of cells can be altered and how the "communication" of cells works, the latter leading to the so-called *ionic currents*. Bearing in mind the goal, of describing the myocardium as a whole (supposed it can be modeled as a continuum), it is also of great interest how we can describe the propagation of action potentials in the whole human heart without focusing on the cellular structure. This will lead to

the well-known *Bi-Domain* model. Apart from the electric propagation in the human heart we also want to take a glance at the mechanic contraction of the heart. As said before, we will not describe the contractile properties of myocytes here, as this leads too far away. We will stick to a pure formulation of the mechanical models from a continuum mechanical point of view. However, the mechanical and the electrical activities are not self-contained. They depend on each other, thus we need to account for that too, which will lead to coupled multi-field problems.

# 2 Modeling the Electric Activation of the Myocardium

In this chapter we will focus on the electric activation of the human heart. As mentioned in Chapter 1 the electric activation of the human heart is a very complex procedure and relies on various different aspects. This chapter is by no means complete and many of the physiological and physical topics will just be touched on. A very good and detailed physiological overview of the electric activation in the human heart is found in [71]. We will develop the mathematical modeling in this chapter which results are largely taken from [36]. To be able to understand the processes of the electrical activation we need to start at the cellular level. Nevertheless, it occured many times in history of science that a simple approach used to describe the electrical activity of the human heart, was very succeccsive. This was the *electrocardiogram*, abbrv. *ECG*, dating back to 1877. This shall serve us as a motivation for the time being.

## 2.1 Modelling the Human Heart as a Dipole

This part is derived from [36, Chap. 12]. One of the oldest attempts to model the myocardial activity dates back to 1877, when the first electrocardiogram was recorded by Einthoven[1]. It has been known since than that the *action potential* — this is the potential difference across the cardiac cell membrane and it is the actual signal in the human heart which is transported — of the human heart generates an electrical potential field that could be measured on the body surface. In a first approach, the human body was modeled as a volume conductor. This means, when there is a current source somewhere in the body, currents will spread out throughout the body. With those currents flowing, one can measure the potential differences between any two points of the body's surface, given a voltmeter which is sensitive enough. Potential differences are observed whenever the current sources are sufficiently strong. There are three of such occurrences. When the action potential is spreading across the atria, there is a measurable signal, called the *P wave*. When the action potential is propagating through the wall of the ventricles, there is the largest of all deflections, called the *QRS complex*. A schematic view of a single ECG recording is depicted in Figure 2.1. Finally, the recovery of ventricular tissue is seen on the ECG as the $T$

[1] For a more detailed view on the historical background refer to [8, 16].
[2] Taken from `http://en.wikipedia.org/wiki/Sinus_rhythm`.

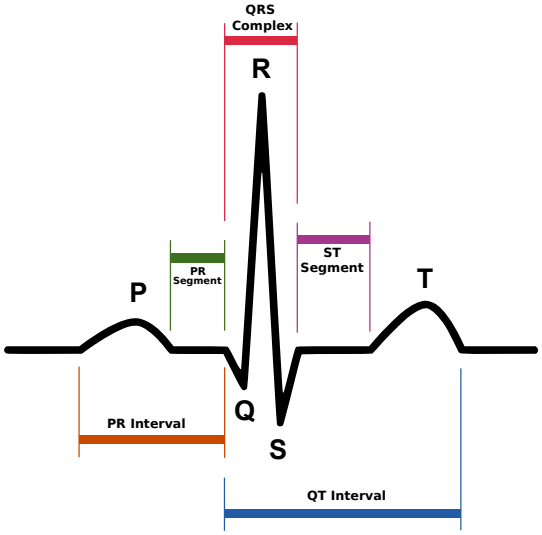


**Figure 2.1** – Schematic view of the sinus rhythm of the heart[2].

*wave*. The recovery of the atria is too weak to be detected on the ECG. Similarly, SA nodal firing, AV nodal conduction, and Purkinje network propagation are not detected on the normal body surface ECG because they do not involve sufficient tissue mass or generate enough extracellular currents. In hospitals, ECG recordings are made routinely using oscilloscopes. We will not turn our attention to the details of the ECG. For a more detailed view about the technical belongings refer to [36]. We will now turn our attention to the mathematical background of the ECG the *volume conductor model*.

**Governing Equations.** In the volume conductor model, we view the human heart as a three-dimensional conducting medium $\Omega$ with a given dipole-like charge $\rho$[3]. The governing equations for a volume conductor are the *Maxwell Equations* which read,

$$\frac{\partial}{\partial t}\boldsymbol{B}(\boldsymbol{x},t) + \operatorname{curl}\boldsymbol{E}(\boldsymbol{x},t) = \boldsymbol{0}, \tag{2.1}$$

$$\operatorname{div}\boldsymbol{B}(\boldsymbol{x},t) = 0, \tag{2.2}$$

$$\frac{\partial}{\partial t}\boldsymbol{D}(\boldsymbol{x},t) - \operatorname{curl}\boldsymbol{H}(\boldsymbol{x},t) = -\boldsymbol{j}(\boldsymbol{x},t), \tag{2.3}$$

$$\operatorname{div}\boldsymbol{D}(\boldsymbol{x},t) = \rho(\boldsymbol{x},t), \tag{2.4}$$

with $\boldsymbol{H}(\boldsymbol{x},t)$ being the magnetic field, $\boldsymbol{B}(\boldsymbol{x},t)$ denoting the magnetic flux, $\boldsymbol{D}(\boldsymbol{x},t)$ describing the electric displacement, $\boldsymbol{E}(\boldsymbol{x},t)$ indicating the electric field and $\boldsymbol{j}(\boldsymbol{x},t)$ terming a given current density. These equations describe the relation between the electric and the magnetic fields in conducting media. By taking the divergence of

[3]This idea goes back to the Einthoven, see [76].

(2.3) we obtain the *continuity equation*

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) + \operatorname{div}\boldsymbol{j}(\boldsymbol{x},t) = 0. \tag{2.5}$$

For giving a full description of the relation between electric and magnetic fields in conducting media, one needs to establish constitutive equations, which read for $\boldsymbol{D}(\boldsymbol{x},t)$ and $\boldsymbol{B}(\boldsymbol{x},t)$

$$\boldsymbol{D}(\boldsymbol{x},t) = \boldsymbol{\varepsilon}(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x},t), \tag{2.6}$$
$$\boldsymbol{B}(\boldsymbol{x},t) = \boldsymbol{\mu}(\boldsymbol{x})\boldsymbol{H}(\boldsymbol{x},t), \tag{2.7}$$

with $\boldsymbol{\varepsilon}(\boldsymbol{x})$ being the electric permittivity, $\boldsymbol{\mu}(\boldsymbol{x})$ being the magnetic permeability. Furthermore in conducting media *Ohm's law* applies, which states that

$$\boldsymbol{j}(\boldsymbol{x},t) = \mathbf{M}(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x},t), \tag{2.8}$$

with $\mathbf{M}(\boldsymbol{x})$[4] being the electric conductivity. As one can see, the constitutive quantities $\boldsymbol{\varepsilon}, \boldsymbol{\mu}, \mathbf{M}$ are assumed to be not time-dependent, which may not be the most general case. For a detailed description of electromagnetism we refer to [35]. It should be mentioned that, especially for human tissue, all those quantities are in fact tensor-valued functions and will be discussed in more detail in Section 2.4.

From biophysics it is known that the electrical activation of the heart is a very fast process, while the variations in the electric and magnetic fields are rather small, see [63], thus we can neglect $\frac{\partial}{\partial t}\boldsymbol{B}$ in (2.1) and obtain

$$\operatorname{curl}\boldsymbol{E}(\boldsymbol{x},t) = \mathbf{0}. \tag{2.9}$$

From that it follows, that there exists a scalar potential $u(\boldsymbol{x})$ such that

$$\boldsymbol{E}(\boldsymbol{x}) = -\operatorname{grad} u(\boldsymbol{x}).$$

Hence, equation (2.9) is fulfilled. Inserting this potential into Ohm's law we obtain

$$\boldsymbol{j}(\boldsymbol{x}) = -\mathbf{M}(\boldsymbol{x})\operatorname{grad} u(\boldsymbol{x}).$$

In accordance to [36, Section 14] we denote $-\frac{\partial}{\partial t}\rho(\boldsymbol{x},t)$ by $f$, being the lumped sum of all current sources in the heart $\Omega$. Then, the continuity equation (2.5) becomes

$$-\operatorname{div}\left(\mathbf{M}(\boldsymbol{x})\operatorname{grad} u(\boldsymbol{x})\right) = f(\boldsymbol{x},t). \tag{2.10}$$

This is a quasi-static Poisson equation. To complete this partial differential equation we still need to incorporate boundary conditions. A very obvious assumption is, that there is no current flux outwards of the heart. This means

$$\boldsymbol{j}\cdot\boldsymbol{n} = 0 \qquad \text{on } \Gamma = \partial\Omega,$$

[4] It is common to use $\boldsymbol{\sigma}$ for the conductivity, however this special letter is reserved for the Cauchy stress tensor which will be introduced in Chapter 3.

where $\boldsymbol{n}$ denotes the outer unit normal vector of $\Omega$. Using this and Ohm's law (2.8), we end up with the Neumann boundary condition

$$(\mathbf{M} \operatorname{grad} u) \cdot \boldsymbol{n} = 0 \qquad \text{on } \Gamma.$$

We may note a few points at this stage. For the boundary value problem to be solvable we need to enforce the condition

$$\int_{\Omega} f \; d\boldsymbol{x} = 0$$

as follows easily by applying Gauss' theorem to the integral of equation (2.10). Next, from calculus we know, that the scalar potential $u$ is unique up to a constant. Thus one usually introduces a scaling condition in the form

$$\int_{\Omega} u(\boldsymbol{x}) \; \mathrm{d}\boldsymbol{x} = 0$$

to fix the constant term of $u$, see [75] for details.

## 2.2 Cardiac Cells, Action Potentials and Ionic Currents

The volume conductor model, although very simple, is still the basis for the electrocardiography in modern medicine. However, to get a more profound understanding of the electric activation of the human heart, and because of the evolving knowledge about epigenetics, as mentioned in the introduction, we need to take account of some physiological details. First of all we need to understand how cardiac cells can transport electric signals.

### 2.2.1 The Cell Membrane

From an electrical point of view, the most important part of a cell is its membrane. Therefore we will not discuss details about the structure of a human cell. The interested reader may refer to [71]. For our end it is sufficient to know, that a human cell consists of a cell membrane and the interior. The inside of the cell, the *intracellular space* is a very complex structure, Both the intracellular and *extracellular space* consist of, among many other things, a dilute aqueous solution of dissolved salts, primarily NaCl and KCl, which dissociate into $Na^+$, $K^+$ and $Cl^-$ ions. Outside the cell in the extracellular space we also find ions in a different concentration. Thus there is an electric imbalance and so cells possess an electric potential, whose idle state is referred to as *resting potential*.

The cell membrane acts as a boundary separating the interior of the cell from its exterior. More important, it is selectively permeable, meaning that it allows some materials, among also ions, to pass into and out the cell. It is composed of a double layer, or *bi-layer*, of phospho-lipid — where *lipid* is specified by a category of water-insoluble, energy rich macromolecules, like fats, waxes, and oils — molecules about 7.5 nm thick. Figure 2.2 shows a schematic view of a cell membrane.

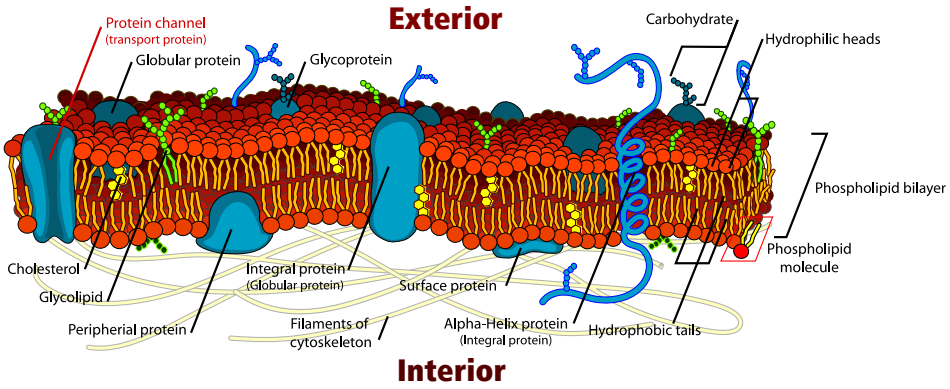


**Figure 2.2** – Schematic view of the cell membrane[5]. For the thesis, the most important part of the cell membrane are the channel proteins which have been marked red.

The cell membrane itself is a very complicated structure and we might dedicate a whole thesis to this, but we will focus on a specific part of the cell membrane: the *channel proteins*, marked red in Figure 2.2. These are protein-lined pores which actual regulate the passage of ions through the cell membrane, thus maintaining concentration differences between the interior and the exterior of a cell.

There are two possibilities to transport molecules through the cell membrane. The first one is the so-called *passive transport*, by which we mean a passive process which is solely driven by concentration gradients[6] . The second possibility to transport molecules through the cell membrane is by a so-called *active transport*. An active transportation process involves the transportation of ions against their concentration gradient and thus is an energy consuming action. The whole maintenance of the concentration differences are set up by the active mechanisms of the cell. Also much of the metabolism of our body works due to such transports. In literature it is also quite common to refer to those active processes as *pumps*.

The most important of those pumps is the $Na^+$–$K^+$ ATPase, see [71], which uses the energy stored in ATP molecules to pump $Na^+$ out of the cell and $K^+$ in. There are

[5]Taken from `http://en.wikipedia.org/wiki/Cell_membrane`.
[6]The diffusion of water in and outside the cell, the *Osmosis*, falls in that category but is not of interest for our models.

much more of these pumps, many of them use Calcium $Ca^{2+}$. However, we will not discuss either of these processes here in detail as this would go beyond the scope of this thesis, the interested reader may refer to [71] for the physiological details and [36] for the modeling details. We will stick to the fact, that the active transport together with the passive transport are essential for the health of a cell itself and for the regulation of the concentration differences.

### 2.2.2 Electric Circuit Model of the Cell Membrane

Since the cell membrane separates charges, it can be viewed as a capacitor, see [35] for details. The capacitance of any insulator is defined as the ratio of the charge across the capacitor to the voltage potential necessary to hold that charge, and it is denoted by

$$C_m = \frac{Q}{V}. \tag{2.11}$$

From standard electrostatics, e.g. Coulomb's law, see [35], we can derive the fact that for two parallel conducting plates separated by an insulator of thickness $d$, the capacitance is found to be

$$C_m = \frac{k\varepsilon_0}{d},$$

where $k$ is the dielectric constant for the insulator and $\varepsilon_0$ is the permittivity of free space. The capacitance of the cell membrane is typically 1.0 $\mu$F/cm$^2$. Taking that $\varepsilon_0 = \frac{10^{-9}}{36\pi}$F/m we calculate the dielectric constant of the cell membrane to be about 8.5.

We can think of the cell membrane as an electric circuit, as shown in Figure 2.3.

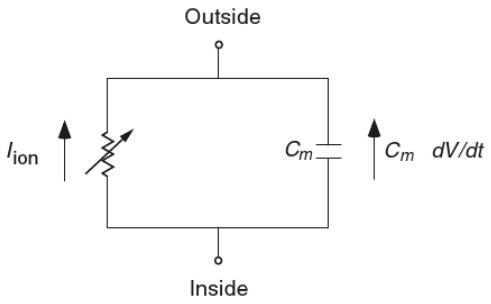


**Figure 2.3** – A very simple circuit model of the cell membrane[7]. Please note that in this reference the trans-membrane potential is denoted by $V$ rather than $u_{\mathrm{tm}}$.

It is assumed that the membrane acts like a capacitor in parallel with a, not necessarily ohmic, resistor. We know that the current is $\frac{\mathrm{d}}{\mathrm{d}t}Q$, thus from (2.11) it follows that the current flowing over the capacitor is given by $C_m \frac{\mathrm{d}}{\mathrm{d}t} u_{\mathrm{tm}}$, provided that $C_m$ is constant. Finally we use Kirchoff's law and obtain

$$C_m \frac{\mathrm{d}}{\mathrm{d}t} u_{\mathrm{tm}} + I_{\mathrm{ion}} = 0. \tag{2.12}$$

Equation (2.12) is a very fundamental statement and will be often used throughout this thesis. The function $I_{\mathrm{ion}}$, called the *ionic current*, describes the current flowing through the resistor depicted in Figure 2.3. Further, we assume some external current sources to be applied either on the inside, which we then call $s_i$, or on the outside of a cell which then are named $s_e$. So we obtain the following two equations which will be used in Chapter 5:

$$C_m \frac{\mathrm{d}}{\mathrm{d}t} u_{\mathrm{tm}} + I_{\mathrm{ion}} = s_e, \tag{2.13}$$

$$C_m \frac{\mathrm{d}}{\mathrm{d}t} u_{\mathrm{tm}} + I_{\mathrm{ion}} = -s_i. \tag{2.14}$$

### 2.2.3 Functional Dependence of $I_{\mathrm{ion}}$

As written above the differences in ionic concentrations between the inside and outside of a cell create a potential difference along the cell membrane, called the *trans-membrane potential* $u_{\mathrm{tm}}$. This trans-membrane potential in particular drives a current flux between the interior and the exterior of a cell which we denoted above as ionic current $I_{\mathrm{ion}}$. We will not discuss the physical details of the ionic currents. The interested reader may refer to [36, Chapt. 2, 3 and 5]. The most important aspect for modeling is that the ionic current has a functional dependence on the action potential $u_{\mathrm{tm}}$, i.e. $I_{\mathrm{ion}} = I_{\mathrm{ion}}(u_{\mathrm{tm}})$. The difficulties arise, when one tries to figure out how this dependence may look like. In [36] we find two possibilities how to describe the functional dependence of the ionic current, a quasi-linear one reading

$$I_{\mathrm{ion}}(u_{\mathrm{tm}}) = \sum_{\mathrm{ions}} g_{\mathrm{ions}}(u_{\mathrm{tm}} - u_{\mathrm{ions}}),$$

where ions stands for a list of ions of interest (like $\mathrm{Na}^+$, $\mathrm{K}^+$ and so on). The values $g_{\mathrm{ions}}$ represent not necessarily constant conductivities. For each ion, $u_{\mathrm{ions}}$ denotes the *Nernst potential*, see [36, Chapt. 3] for details. This model is quite popular, as one can divide the dependence of the ionic current up to different ionic currents for each ion and then lump all together to a so-called *leakage current*. The second possibility is to use a similar decomposition of the ionic current into a current for each ion using

[7] Taken from [36, p.87, Figure 2.13].

the Goldman-Hodgkin-Katz current equation reading

$$I_{\mathrm{S}} = P_S \frac{z^2 F^2}{RT} u_{\mathrm{tm}} \frac{c_i - c_e \exp\left(-\frac{zFu_{\mathrm{tm}}}{RT}\right)}{1 - \exp\left(-\frac{zFu_{\mathrm{tm}}}{RT}\right)},$$

where $S$ stands for the type of ion, $z$ is the valence of the ion $S$, $c_i$ and $c_e$ are the respective concentrations in the intra and extra cellular regions, $R$ is the universal gas constant, $T$ is the absolute temperature, $P_S$ is the permeability of the cell membrane to the specific ion $S$ and $F$ is Faraday's constant. In the next section we will see how we can describe the evolution of the ionic current.

### 2.2.4 Excitability of Myocytes

In Section 2.2.3 we have seen how the trans-membrane potential $u_{\mathrm{tm}}$ causes ionic currents $I_{\mathrm{ion}}$ to flow through the membrane. Regulation of this membrane potential by control of the ionic channels is one of the most important cellular functions. Myocytes, especially, use this membrane potential, as discussed in Chapter 1 as a signal to control the contraction of the myocardium. Thus, the contraction is dependent on the generation of electric signals. As aforementioned, heart cells belong to a class of very special cells: they are excitable. This means, that if we apply a current which is sufficiently strong, the membrane potential performs a pronounced oscillation before eventually returning to the resting potential value. Figure 2.4 shows a schematic view of an action potential typical for ventricular heart cells. We need to mention at this

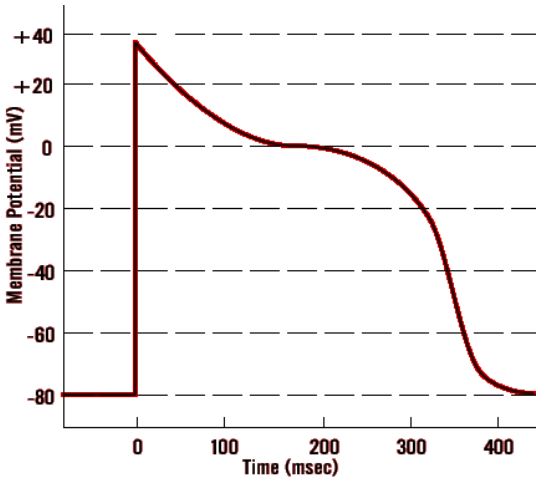


**Figure 2.4** – Typical curve of an ventricular cell action potential[8].

[8] Taken from `http://library.thinkquest.org/C003758/Function/The%20Cardiac%20Action%20Potential.htm`.

point that the shape of the action potentials differs from cell to cell in the heart. This means, the models for the SA node will not be adequate for describing the potential of the AV node and the other cell types in the myocardium respectively.

In Chapter 1 we referred to this change of potential as action potential. The most obvious advantage of excitability is that an excitable cell either responds in full to a stimulus or not at all, and thus a stimulus of sufficient amplitude may be reliably distinguished from background noise. In this way, noise is filtered out, and a signal is reliably transmitted.

The studies on the generation and propagation of those signals have been made for nearly a hundred years. Although the generation and propagation of signals have been extensively studied by physiologists for at least the past hundred years, the most important landmark in these studies is the work of Alan Hodgkin and Andrew Huxley, see [30], who developed the first quantitative model for the propagation of an electrical signal along a squid giant axon. Their model was originally used to explain the action potential in the long giant axon of a squid nerve cell, but the ideas have since been extended and applied to a wide variety of excitable cells.

In the spirit of Hodgkin and Huxley many models have been developed. All those models do share a common structure, see [46]. They are called *Hodgkin-Huxley-type models*, since they are all based, mathematically, on the original model from Hodgkin and Huxley [30]. In [46] we find a very good summary of the various models for ionic currents. The models are based on viewing the cell membrane as an electrical circuit and applying Kirchoff's law to it. This means that the membrane current model consists of a capacitive current term and a variety of ionic current terms appropriate for a specific type of cell. The general form of the spatially-independent model with $n$ ionic currents is

$$C_m \frac{\mathrm{d}}{\mathrm{d}t} u_{\mathrm{tm}} = -\sum_{i=1}^{n} \bar{g}_i a_i^p b_i^q (u_{\mathrm{tm}} - V_i) + I_{\mathrm{app}}(t), \tag{2.15}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} a_i = \frac{a_i^\infty(u_{\mathrm{tm}}) - a_i}{\tau_{a_i}(u_{\mathrm{tm}})}, \qquad i = 1, 2, \ldots, n, \tag{2.16}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} b_i = \frac{b_i^\infty(u_{\mathrm{tm}}) - b_i}{\tau_{b_i}(u_{\mathrm{tm}})}, \qquad i = 1, 2, \ldots, n, \tag{2.17}$$

where $C_m$ is the capacitance of the cell membrane, $u_{\mathrm{tm}}$ is the trans-membrane potential, $\bar{g}_i$ is the maximal conductance of the channel for ion $i$, $a_i$ and $b_i$ are the gating variables taking values between 0 and 1, $V_i$ is the Nernst potential for the $i^{\mathrm{th}}$ ion, $I_{\mathrm{appl}}$ is the applied stimulus current. The latter may consist of a signal coming from an adjacent cell or from an external applied current. Further, $a_i^\infty$ and $b_i^\infty$ are the steady state values of the gating variables at potential $u_{\mathrm{tm}}$, $\tau_{a_i}$ and $\tau_{b_i}$ are the relaxation time constants at potential $u_{\mathrm{tm}}$ and finally $p, q$ denote some arbitrary real exponents. Many of the excitability models known throughout literature can be

written in this form. There is a huge collection of those models available for simulation through the *CellML*-Project[9]. Taking note, we write the evolution equation for the ionic current $I_{\text{ion}}$ in the following abstract way as a system of nonlinear ordinary differential equations:

$$I_{\text{ion}} = g(t, u_{\text{tm}}, \boldsymbol{v}),$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v} = \boldsymbol{f}(t, u_{\text{tm}}, \boldsymbol{v}), \tag{2.18}$$
$$\boldsymbol{v}(t=0) = \boldsymbol{v}_0. \tag{2.19}$$

With this notation we can cover almost any possible shape of the ionic current appearing in the literature. We will now turn our attention to the mathematical modeling of macroscopic signal propagation in the human heart.

## 2.3 The Bi-Domain Model

We will now turn our focus to the macroscopic propagation of electric signals in the myocardium. It would be possible to model the whole human heart on a cellular basis, however, this would be computational very expensive. Furthermore we would need to develop a very detailed cell model which would have to bee applied to each cell and then coupled among each other. The latter is for being able to describe the propagation of signals through the cells. This coupling is complicated by the fact, that the signal which is transported is in fact the trans-membrane potential $u_{\text{tm}}$, and thus the intra and extra cellular spaces have to be continuously connected and intertwined, so that we can move continuously between any two points within one space without traversing through the complementary space. This is only possible in a three-dimensional domain[10]. As aforementioned, it is yet not possible to write and solve equations that account for the cellular structure and the details of the geometry of the human heart. In a first step, see Section 2.1, we saw that modeling the human heart in a macroscopic sense as a dipole suffices for some medical application but is not adequate for a complete description of the electrical activation of the human heart. A more accurate description will be obtained by the *Bi-Domain model* developed by L. Tung, see [79] as well as [29, 43] for details.

For deriving an accurate model for the electric activation of the myocardium we apply a procedure from continuum mechanics, known as *homogenization*. With this we

[9] `http://www.cellml.org` This is a open-source project, where cell models are described using the XML Markup Language for a platform independent description of different models. The CellML model repository is updated regularly with the most recent advances in cell physiology. There are, of course, models which cannot be covered by this. One of them would be the Aliev-Panfilov model [3].

[10] In fact, as we mentioned in the Introduction in Chapter 1 the myocardium is a syncytium, thus we can assure that traversing the intracellular space in a continuously way is possible.

can write equations in an averaged, or smoothed, sense which is adequate for the most computational situations. In continuum mechanics, it is quite common to study averaged quantities, to avoid modeling the molecular structure of solids and fluids, see e.g. [18, 34] but also [61] and [36, Chap. 7,12] for mathematical details and a justification.

In homogeneous idealization, we can look at the myocardium as a two-phase medium. This means that every point $\boldsymbol{x} \in \Omega$ is composed of a certain fraction of intracellular space as well as extracellular space. Apparently, for each point $\boldsymbol{x}$ in space we can define an electric potential for the intracellular space, $u_i$ and for the extracellular space, $u_e$, respectively. Thus also the trans-membrane potential can be defined in the whole space as $u_{\text{tm}} = u_i - u_e$. We shall use the subscripts $e, i$ for denoting extra and intra cellular space from now on until otherwise stated. As in the volume conductor model in Section 2.1 , we can also assume that the quasi-stationary Maxwell equations hold, and that way, by using Ohm's law (2.8) in both domains we obtain

$$\boldsymbol{j}_i = -\mathbf{M}_i \operatorname{grad} u_i, \tag{2.20}$$

$$\boldsymbol{j}_e = -\mathbf{M}_e \operatorname{grad} u_e, \tag{2.21}$$

where $\boldsymbol{j}_k$ and $\mathbf{M}_k$ for $k \in \{e, i\}$ are the respective currents and conductivity tensors in each domain. It should be mentioned that the tensors may also depend on the deformation of the heart as well as on the change of the ionic current $I_{\text{ion}}$. This will be discussed in Chapter 4.

We closed Section 2.2.2 with the equations (2.13)–(2.14), describing a very simplified cable model of the cell membrane. Their, the quantities were only time-dependent. However, in reality this is not true. Thus, the quantities $u_{\text{tm}}, s_i, s_e$ will depend on the position $\boldsymbol{x}$. Nevertheless, we may assume that there exist some kind of density functions $\tilde{u}_{\text{tm}}, \tilde{s}_e, \tilde{s}_i$ such that

$$\bullet = \int_A \tilde{\bullet} \ \mathrm{d}\boldsymbol{x},$$

where $\bullet$ may be replaced by any of the above mentioned quantities and the region $A$ being a small test volume either in $\Omega_e$ or $\Omega_i$. For the time being we shall pick a small test volume in $\Omega_e$. Having that we can now formulate a simple balance principle for the current in each region reading as

$$-\int_{\partial A} (\boldsymbol{j}_e, \boldsymbol{n}) \ ds_{\boldsymbol{x}} = -\frac{\mathrm{d}}{\mathrm{d}t} \int_A \chi C_m \tilde{u}_{\text{tm}}(\boldsymbol{x}, t) \ \mathrm{d}\boldsymbol{x} - \int_A \chi \tilde{I}_{\text{ion}} \ \mathrm{d}\boldsymbol{x} + \int_A \tilde{s}_e \ \mathrm{d}\boldsymbol{x}\,. \tag{2.22}$$

The signs account for the direction of the currents *from* the extracellular *into* the intracellular region. The constant $\chi$ represents the area of the cell membrane per unit volume, and needs to be introduced, because the ionic current $\tilde{I}_{\text{ion}}$ and also the trans-membrane current $C_m \frac{\mathrm{d}u_{\text{tm}}}{\mathrm{d}t}$ are measured per unit cell membrane. Its value is

shown in Table 2.1. For the current $\boldsymbol{j}_i$ holds an analogous balance principle. We will now interchange the use of the "$\sim$" symbol for reasons of readability. Next, we use Gauss' theorem on the left side of equation (2.22) and obtain

$$-\int_A \operatorname{div} \boldsymbol{j}_e(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x} = -\frac{\mathrm{d}}{\mathrm{d}t}\int_A \chi C_m u_{\mathrm{tm}}(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x} - \int_A \chi I_{\mathrm{ion}}\ \mathrm{d}\boldsymbol{x} + \int_A s_e(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x}\,.$$

Next, interchanging integration and derivation with respect to time in the above equation we obtain

$$-\int_A \operatorname{div} \boldsymbol{j}_e(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x} = -\int_A \chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}}(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x} - \int_A \chi I_{\mathrm{ion}}\ \mathrm{d}\boldsymbol{x} + \int_A s_e(\boldsymbol{x},t)\ \mathrm{d}\boldsymbol{x}\,.$$

This needs to hold for every test volume $A \subset \Omega_e$. Assuming continuous integrands and using Ohm's law (2.8) we arrive at the point-wise equation

$$\chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}} + \chi I_{\mathrm{ion}}(u_{\mathrm{tm}}) + \operatorname{div}(\mathbf{M}_e \operatorname{grad} u_e) = -s_e. \tag{2.23}$$

Similar we obtain

$$\chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}} + \chi I_{\mathrm{ion}}(u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_i) = s_i. \tag{2.24}$$

when formulating the balance principle in $\Omega_i$.

From (2.23)–(2.24) we see, that we have two equations for three variables $u_i, u_e, u_{\mathrm{tm}}$, thus we may eliminate one of those variables. In the literature it is common to eliminate the intracellular potential $u_i$. Recalling the definition of $u_{\mathrm{tm}} := u_i - u_e$ we can eliminate the intracellular potential by subtracting (2.24) from (2.23). We obtain the equations

$$\chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}} + \chi I_{\mathrm{ion}}(u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_e) = s_i, \tag{2.25}$$

$$\operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) + \operatorname{div}((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e) = -(s_i + s_e). \tag{2.26}$$

To complete the model we need to impose boundary conditions for $u_e$ and $u_{\mathrm{tm}}$. Assuming that the heart is surrounded by a non-conductive medium we can impose boundary conditions of Neumann type

$$\begin{aligned} \boldsymbol{n} \cdot \boldsymbol{j}_i &= 0, \\ \boldsymbol{n} \cdot \boldsymbol{j}_e &= 0, \end{aligned}$$

with $\boldsymbol{n}$ being the outer unit normal vector of the boundary $\Gamma := \partial\Omega$.

Substituting Ohm's law (2.8) in the definitions of $\boldsymbol{j}_i$ and $\boldsymbol{j}_e$ we finally obtain the complete model as

$$\chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}} + \chi I_{\mathrm{ion}}(u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_e) = s_i, \tag{2.27}$$

$$\operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) + \operatorname{div}((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e) = -(s_i + s_e), \tag{2.28}$$

in $\Omega \times (0,T]$ with the imposed boundary conditions of Neumann type

$$\boldsymbol{n} \cdot (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} + \mathbf{M}_i \operatorname{grad} u_e) = 0 \qquad \text{on } \Gamma \times (0,T], \tag{2.29}$$

$$\boldsymbol{n} \cdot (\mathbf{M}_e \operatorname{grad} u_e) = 0 \qquad \text{on } \Gamma \times (0,T]. \tag{2.30}$$

This is the *bi-domain model* as it was introduced by L. Tung in [79]. However, as aforementioned, this modeling of the human heart is restricted to the ventricles. Therefore we may not assume homogeneous boundary conditions and should replace them by the conditions

$$\boldsymbol{n} \cdot (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} + \mathbf{M}_i \operatorname{grad} u_e) = g_{N,i} \qquad \text{on } \Gamma \times (0,T],$$

$$\boldsymbol{n} \cdot (\mathbf{M}_e \operatorname{grad} u_e) = g_{N,e} \qquad \text{on } \Gamma \times (0,T].$$

Anyway, for the well-posedness of the equations (2.27)–(2.28) we must assume the solvability condition

$$\int_\Gamma (g_{N,i} + g_{N_e}) \, \mathrm{d}s_{\boldsymbol{x}} + \int_\Omega (s_i + s_e) \, \mathrm{d}\boldsymbol{x} = 0, \tag{2.31}$$

which is obtained easily by integrating (2.28) and using Gauss' theorem together with the boundary conditions.

It is noted that Dirichlet boundary conditions can be imposed to avoid solving a pure Neumann problem[11], however we will not discuss this in further details. The Neumann problem will be addressed in Chapter 5.

The ionic current still needs to be accounted for and we also need to describe the conductivity tensors $\mathbf{M}_i$ and $\mathbf{M}_e$. We have seen in Section 2.2.4 that we can write many of the models for the ionic current as a system of ordinary differential equations

$$I_{\mathrm{ion}} = g(t, u_{\mathrm{tm}}, \boldsymbol{v}),$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v} = \boldsymbol{f}(\boldsymbol{v}, u_{\mathrm{tm}}, t).$$

In this system $\boldsymbol{v}$ describes the vector of dependent variables (gating, conductions, and so on) and $\boldsymbol{f}, g$ denote (non)linear functions, as suggested in [59]. Later on we will extend the dependence of $I_{\mathrm{ion}}$ to the mechanical behavior as well. Next we will establish some basic facts about the conductivity tensors $\mathbf{M}_i$ and $\mathbf{M}_e$.

## 2.4 Accounting for the Fiber Orientation

It is known, that the myocardium is the most important part, when describing the pumping process of the human heart. For the electrochemical modeling we have

[11] This has a physiological reason. When measuring the heart activity one usually uses electrodes, and by them one fixes the value of the potentials at a region.

derived the Bi-Domain model (2.27)–(2.30). Now we need to establish the conductive properties of the myocardium. One important fact is, that the conduction in the human heart is highly anisotropic, and as said above, the quantities $\mathbf{M}_i$ and $\mathbf{M}_e$ are tensor-valued functions.

This specific anisotropy comes from the structure of the myocardium as discussed in Chapter 1. There we introduced a local coordinate system spanned by $\boldsymbol{f}_0, \boldsymbol{s}_0$ and $\boldsymbol{n}_0$. From the definition of a tensor, see [55, Chap. 1], we know that the components of a tensor depend on the chosen basis. However we can write the components of each conductivity tensor as

$$\mathsf{M}(\boldsymbol{x}) := \{m_{ij}(\boldsymbol{x}\}_{i,j=1}^{3},$$

but we need to bear in mind, that the components of the tensor depend on the chosen basis via

$$m_{ij} = (\boldsymbol{e}_i, \mathbf{M}\boldsymbol{e}_j)$$

for a given orthonormal basis $\{\boldsymbol{e}_i\}$. We can do this also for more general non-orthogonal basis vectors, but this lies beyond the scope of this thesis. The reader is referred to [31, Section 1.6] for details. In practice it is common not to distinguish between second-order tensors and their representing matrices and denote them with the same symbol. We will henceforth use this with a tacit understanding until otherwise stated.

Since we model the heart as a continuous medium the local coordinate systems will vary throughout the heart. So in fact there is no preferred right-hand coordinate system. At each point of the tissue, the first axis is in the direction of the fiber, the second axis is in the plane of the fiber sheet and perpendicular to the first axis, and the third axis is perpendicular to the sheet of the fiber. Thus we have $\boldsymbol{f}_0 = \boldsymbol{f}_0(\boldsymbol{X})$ and in analogy for $s$ and $n$. Furthermore as we look at the myocardium as being composed of parallel laminar sheets, these functions need to be also continuous. To account for this varying coordinate system we will introduce a rotation of the fixed Cartesian axes that will give us a set of axes aligned with the fiber and the fiber sheet as suggested in [83]. To this end we consider a point $\boldsymbol{X}$. We can express this point in terms of the local coordinate system as

$$\boldsymbol{X} = X_f \boldsymbol{f}_0 + X_s \boldsymbol{s}_0 + X_n \boldsymbol{n}_0,$$

where $X_f, X_s, X_n$ are the components of $\boldsymbol{X}$ with respect to the basis $\boldsymbol{f}_0, \boldsymbol{s}_0$ and $\boldsymbol{n}_0$. The orthogonal matrix that rotates axes aligned with the fiber and fiber sheet onto the original axes can now be defined as

$$(\mathsf{P})_{ij} := \frac{\partial X_i}{\partial X_j} \qquad \text{for } i = 1, 2, 3 \text{ and } j = f, s, n. \tag{2.32}$$

We know, from standard linear algebra, that this defines a proper rotation matrix and thus we know that $\mathsf{P}^{-1} = \mathsf{P}^\top$. This allows us to interchange between tensors in the original frame and tensors in the fiber and fiber sheet oriented frame as follows

$$\mathbf{M}^*(\boldsymbol{x}) = \mathsf{P}^\top \mathbf{M}(\boldsymbol{x})\mathsf{P}, \tag{2.33}$$

$$\mathbf{M}(\boldsymbol{x}) = \mathsf{P}\mathbf{M}^*(\boldsymbol{x})\mathsf{P}^\top, \tag{2.34}$$

where the superscript "*" means, that we work in the local basis. Focusing on the local coordinate system it becomes obvious, that the matrix $\mathsf{M}$ associated to conductivity tensor $\mathbf{M}$ has to be diagonal with respect to the local basis $\{\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0\}$ that means

$$\mathbf{M}^* = m_f \boldsymbol{f}_0 \otimes \boldsymbol{f}_0 + m_s \boldsymbol{s}_0 \otimes \boldsymbol{s}_0 + m_n \boldsymbol{n}_0 \otimes \boldsymbol{n}_0,$$

or

$$\mathsf{M}^* = \operatorname{diag}(m_f, m_s, m_n).$$

This characterizes the myocardium as an *orthotropic material*. More details on orthotropic materials will be discussed in Section 3.4.1. Thus we can interpret the values $m_f, m_s, m_n$ as eigenvalues and $\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0$ as eigenvectors of $\mathsf{M}^*$, respectively $\mathbf{M}^*$. Applying the transformation rules (2.33) to Ohm's law we can now express the global conductivity tensors $\mathbf{M}_i$ and $\mathbf{M}_e$ through

$$\mathbf{M}_i := \mathsf{P}\mathbf{M}_i^*\mathsf{P}^\top$$

$$\mathbf{M}_e := \mathsf{P}\mathbf{M}_e^*\mathsf{P}^\top.$$

Summarizing, we have seen that for given local conductivity tensors we can completely specify the parameters of the bi-domain model. The values are given in Table 2.1.

| Parameter | Value |
|---|---|
| $C_m$ | 0.01 $\mathrm{F/m^2}$ |
| $\chi$ | $2 \cdot 10^5$ $\mathrm{1/m}$ |
| $m_f^i$ | 0.3 $\mathrm{S/m}$ |
| $m_s^i$ | 0.1 $\mathrm{S/m}$ |
| $m_n^i$ | 0.031525 $\mathrm{S/m}$ |
| $m_f^e$ | 0.2 $\mathrm{S/m}$ |
| $m_s^e$ | 0.165 $\mathrm{S/m}$ |
| $m_n^e$ | 0.13514 $\mathrm{S/m}$ |

**Table 2.1** – Values of the parameters used in the bi-domain model: the conductivity values, the value for $\chi$ and the value for $C_m$ are taken from [37],[28] and [64].

## 2.5 The Final Electric Model

In this chapter we have developed the basic models for the electric part of the cardiac cycle and eventually derived the bi-domain model. Furthermore we described the conductive properties of the human heart with tensor-valued functions and we took account of the ionic currents, by modeling it in the most abstract way. Summarizing the complete electronic model of the human heart in dimensional form reads as find $(u_{\mathrm{tm}}, u_e) \in [\mathcal{C}^2(\Omega)]^2 \cap [\mathcal{C}^1(\partial\Omega)]^2 \times (0,T]$ and $\boldsymbol{v} \in [C^1((0,T])]^n$ such that:

$$\chi C_m \frac{\partial u_{\mathrm{tm}}}{\partial t} + \chi g(u_{\mathrm{tm}}, \boldsymbol{v}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_e) = s_i, \tag{2.35}$$

$$\operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) + \operatorname{div}((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e) = -(s_i + s_e), \tag{2.36}$$

in $\Omega \times (0,T]$ and

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \boldsymbol{f}(t, u_{\mathrm{tm}}, \boldsymbol{v}) \tag{2.37}$$

in $(0,T]$, completed by the boundary and initial conditions

$$\boldsymbol{n} \cdot (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} + \mathbf{M}_i \operatorname{grad} u_e) = g_{N.i} \qquad \text{on } \partial\Omega \times (0,T], \tag{2.38}$$

$$\boldsymbol{n} \cdot (\mathbf{M}_e \operatorname{grad} u_e) = g_{N,e} \qquad \text{on } \partial\Omega \times (0,T], \tag{2.39}$$

$$u_{\mathrm{tm}}(\boldsymbol{x}, 0) = u_{\mathrm{tm}}^0 \qquad \text{in } \Omega, \tag{2.40}$$

$$u_{\mathrm{e}}(\boldsymbol{x}, 0) = u_{\mathrm{e}}^0 \qquad \text{in } \Omega, \tag{2.41}$$

$$\boldsymbol{v}(0) = \boldsymbol{v}_0. \tag{2.42}$$

The value $n$ stands for the complexity of the model for the ionic current $I_{\mathrm{ion}}$.

# 3 Modeling the Mechanical Processes of the Human Heart

In this chapter we present the models covering the pure mechanic deformation of the human heart. In contrast to the modeling of the electric activation of the human heart, the mechanic models are already established and we can describe the deformation of the human heart with the standard equations from continuum mechanics.

We presume some basic knowledge about tensor algebra, see for example [55, Chap. 1, 2] and non-linear elasticity, see for example [31, 55]. However, we will recite some of the basic facts of tensor algebra, as well as the governing equations of continuum mechanics.

## 3.1 Essentials from Continuum Mechanics

Before starting with the derivation of the governing equations of non-linear continuum mechanics we will briefly recite the most important notations and definitions from solid mechanics. This part is mostly taken from [55].

### 3.1.1 Bodies, Configurations and Motions

We start with the general definition of a body $\mathcal{B}$ and its configuration $B$.

**Definition 3.1.** *A* body $\mathcal{B}$ *is a set whose elements can be put into a one-to-one correspondence with points of a region* $B$ *in a three-dimensional Euclidean point space. The elements of* $\mathcal{B}$ *are called* particles*, or* material points*, and* $B$ *is called a* configuration *of* $\mathcal{B}$[1]*.*

As a body moves the configuration $B$ will change in time.

**Definition 3.2.** *Let* $t \in I \subset \mathbb{R}^+$ *denote the time. The family* $\{B_t : t \in I\}$ *of unique configurations of* $\mathcal{B}$ *at time time* $t$ *is called the* motion *of* $\mathcal{B}$*.*

We assume, that as $\mathcal{B}$ moves continuously also $B_t$ changes continuously.

[1] The distinction between body and occupation in space makes sense, see [78] for details.

Further, it is quite convenient to identify a so-called *reference configuration*, $B_r$ say, which is an arbitrarily chosen fixed configuration. Then any particle $P$ of $\mathcal{B}$ may be labeled by its position vector $\boldsymbol{X} \in B_r$[2], relative to a chosen origin $\boldsymbol{O}$. Let further $\boldsymbol{x}$ be the position vector of $P$ in the configuration $B_t$ at time $t$ relative to another chosen origin $\boldsymbol{o}$. However we will simplify things a bit and chose $\boldsymbol{O} = \boldsymbol{o}$. Similar to that we say that $\mathcal{B}$ occupies the configuration $B_t$ at time $t$ and call $B_t$ the *current configuration*. Since $B_r$ and $B_t$ are configurations of $\mathcal{B}$ there exists a bijective mapping $\boldsymbol{\chi}\colon B_r \to B_t$ such that

$$\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t) \qquad \text{for all } \boldsymbol{X} \in B_r, \qquad\qquad \boldsymbol{X} = \boldsymbol{\chi}^{-1}(\boldsymbol{x}, t) \qquad \text{for all } \boldsymbol{x} \in B_t. \tag{3.1}$$

We see from (3.1), that we can characterize either of the coordinates with its counterpart. Figure 3.1 shows a schematic summary.

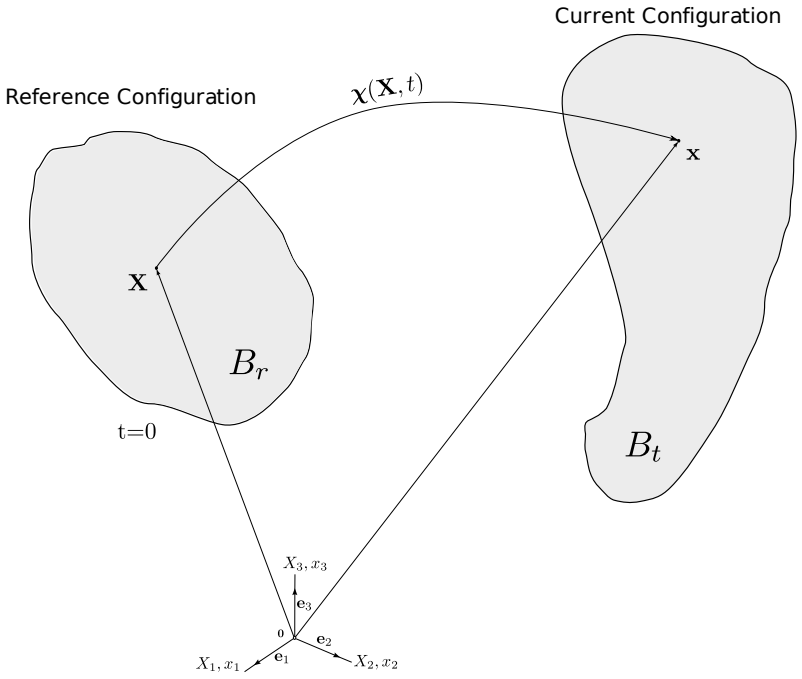


**Figure 3.1** – Reference configuration $B_r$ and current configuration $B_t$ with the position vectors $\boldsymbol{X}$ and $\boldsymbol{x}$ of a material point $P$ and the motion $\boldsymbol{\chi}(\boldsymbol{X}, t)$. The coordinate system is spanned by an orthonormal basis $\{\boldsymbol{e}_i\}_{i=1}^3$

.

For each particle $P$ (with label $\boldsymbol{X}$) $\boldsymbol{\chi}$ describes the motion of $P$ with $t$ as parameter, and hence also the motion of $\mathcal{B}$. In continuum mechanics it is usual to assume that $\boldsymbol{\chi}(\boldsymbol{X}, t)$ is twice continuously differentiable with respect to position and time.

[2]The configuration $B_r$ needs not be a configuration which is actually occupied by $\mathcal{B}$ during the motion, however in most of the literature it is assumed so.

### 3.1.2 Material and Spatial Descriptions

In the development of the basic principles of continuum mechanics a body $\mathcal{B}$ is assigned to various physical properties which are represented by scalar, vector and tensor fields defined on *either* $B_r$ *or* $B_t$[3]. In case of $B_r$ both the position vector $\boldsymbol{X}$ and the time $t$ serve as independent variables, the fields are said to be defined in *referential, material or Lagrangian* description then. Alternatively, in the case of $B_t$, $\boldsymbol{x}$ and $t$ serve as independent variables. Here, we refer to the *spatial or Eulerian* description. The distinction between these two descriptions is crucial. To make things more clear: In material description attention is paid to a particle, and we observe what happens to the particle as it moves. Spatial description puts attention to a specific point in space, and we study what happens at the point as time changes. For example, in fluid mechanics it is very common to work in the spatial description in which all relevant quantities are referred to the position in space and time. It is not useful to relate them to material points $\boldsymbol{X}$ which are in general not known. In solid mechanics there is the advantage that one can use both descriptions.

For convenience, the consistency relation $\boldsymbol{X} = \boldsymbol{x}$ must hold for $t = 0$. Every point $\boldsymbol{X}$ and $\boldsymbol{x}$ can be represented by the orthonormal basis vectors $\{\boldsymbol{e}_i\}_{i=1}^3$ reading

$$\boldsymbol{X} = X_i \boldsymbol{e}_i, \qquad \boldsymbol{x} = x_i \boldsymbol{e}_i, \tag{3.2}$$

where $X_i$ are the *material coordinates* and $x_i$ are the *spatial coordinates*. We could also choose two different bases for the representation, but this shall be omitted here. The case of general bases is discussed in [31, 55]. In (3.2) Einstein's sum convention applies. We will also use it henceforth except where stated otherwise. Furthermore, to distinct between material and spatial description we shall denote quantities which are in material description always by capital letters and use small letters for the spatial description.

### 3.1.3 Material and Spatial Derivatives

In this section we apply Einstein's summation convention. it will henceforth apply until otherwise stated. We will now introduce various differential operators in material and spatial description.

**Definition 3.3** (Material Gradient, Spatial Gradient)**.** *The* material gradient *of a sufficiently*

[3]Examples for such quantities are: density, temperature, shape of surface, velocity, stress, strain. This distinction between reference and current configuration often leads to delicate modeling problems, when one tries to combine two models which are defined on different configurations, like fluid structure interaction see [10].

*smooth material field* $\Phi(\boldsymbol{X},t)$ *is defined by*

$$\operatorname{Grad}\Phi(\boldsymbol{X},t) := \frac{\partial}{\partial X_i}\Phi(\boldsymbol{X},t)\boldsymbol{e}_i.$$

*The* spatial gradient *of a sufficiently smooth spatial field* $\phi(\boldsymbol{x},t)$ *is defined as*

$$\operatorname{grad}\phi(\boldsymbol{x},t) := \frac{\partial}{\partial x_i}\phi(\boldsymbol{x},t)\boldsymbol{e}_i.$$

*In case of a vector-valued function* $\boldsymbol{u}$ *we define the material or spatial gradient as*

$$\operatorname{grad}\boldsymbol{u}(\boldsymbol{x},t) := \nabla_{\boldsymbol{x}} \otimes \boldsymbol{u} = \frac{\partial}{\partial x_q}\boldsymbol{u} \otimes \boldsymbol{e}_q = \frac{\partial}{\partial x_q}u_p\boldsymbol{e}_p \otimes \boldsymbol{e}_q,$$
$$\operatorname{Grad}\boldsymbol{U}(\boldsymbol{X},t) := \nabla_{\boldsymbol{X}} \otimes \boldsymbol{U} = \frac{\partial}{\partial X_q}\boldsymbol{U} \otimes \boldsymbol{e}_q = \frac{\partial}{\partial X_q}U_p\boldsymbol{e}_p \otimes \boldsymbol{e}_q.$$

*In case of a tensor-valued function* $\mathbf{t}$ *we define the material or spatial gradient as*

$$\operatorname{grad}\mathbf{t}(\boldsymbol{x},t) := \nabla_{\boldsymbol{x}} \otimes \mathbf{t} = \frac{\partial}{\partial x_i}\mathbf{t} \otimes \boldsymbol{e}_i = \frac{\partial}{\partial x_i}t_{pq}\boldsymbol{e}_p \otimes \boldsymbol{e}_q \otimes \boldsymbol{e}_i,$$
$$\operatorname{Grad}\mathbf{T}(\boldsymbol{X},t) := \nabla_{\boldsymbol{X}} \otimes \mathbf{T} = \frac{\partial}{\partial X_i}\mathbf{T} \otimes \boldsymbol{e}_i = \frac{\partial}{\partial X_i}T_{pq}\boldsymbol{e}_p \otimes \boldsymbol{e}_q \otimes \boldsymbol{e}_i.$$

**Definition 3.4** (Material Divergence, Spatial Divergence)**.** *The* material divergence *of a sufficiently smooth material field* $\boldsymbol{\Phi}(\boldsymbol{X},t)$ *is defined as*

$$\operatorname{Div}\boldsymbol{\Phi}(\boldsymbol{X},t) := \frac{\partial}{\partial X_i}\Phi_i(\boldsymbol{X},t).$$

*The* spatial divergence *of a sufficiently smooth spatial field* $\boldsymbol{\phi}(\boldsymbol{x},t)$ *is defined as*

$$\operatorname{div}\boldsymbol{\phi}(\boldsymbol{x},t) := \frac{\partial}{\partial x_i}\phi_i(\boldsymbol{x},t).$$

*In case of tensor-valued functions* $\mathbf{t},\mathbf{T}$ *we define the spatial and material divergence as*

$$\operatorname{div}\mathbf{t}(\boldsymbol{x},t) := \frac{\partial}{\partial x_p}t_{pq}(\boldsymbol{x},t)\boldsymbol{e}_q,$$
$$\operatorname{Div}\mathbf{T}(\boldsymbol{X},t) := \frac{\partial}{\partial X_p}T_{pq}(\boldsymbol{x},t)\boldsymbol{e}_q.$$

**Definition 3.5** (Material Time Derivative of a Material Field)**.** *The* material time derivative *of a material field* $\Phi(\boldsymbol{X},t)$*, either scalar or vector-valued, is defined as*

$$\dot{\Phi}(\boldsymbol{X},t) = \frac{\partial}{\partial t}\Phi(\boldsymbol{X},t) := \left(\frac{\partial}{\partial t}\Phi(\boldsymbol{Y},t)\right)\Big|_{\boldsymbol{Y}=\boldsymbol{X}}.$$

**Definition 3.6** (Velocity, Acceleration)**.** *The* velocity $\boldsymbol{V}$ *of a particle* $P$ *is defined as*

$$\boldsymbol{V}(\boldsymbol{X},t) := \frac{\partial}{\partial t}\boldsymbol{\chi}(\boldsymbol{X},t),$$

*meaning the rate of change in Position of* $P$*. The* acceleration $\boldsymbol{A}$ *of* $P$ *is defined as*

$$\boldsymbol{A}(\boldsymbol{X},t) := \frac{\partial^2}{\partial t^2}\boldsymbol{\chi}(\boldsymbol{X},t).$$

**Remark 3.1.** *Due to the identification of material and spatial coordinates we can define the velocity and the acceleration in spatial coordinates as*

$$\begin{aligned}\boldsymbol{v}(\boldsymbol{x},t) &:= \boldsymbol{V}(\boldsymbol{\chi}^{-1}(\boldsymbol{x},t),t) = \boldsymbol{V}(\boldsymbol{X},t),\\ \boldsymbol{a}(\boldsymbol{x},t) &:= \boldsymbol{A}(\boldsymbol{\chi}^{-1}(\boldsymbol{x},t),t) = \boldsymbol{A}(\boldsymbol{X},t).\end{aligned}$$

When dealing with multi-physics problems we will often need to switch between the Eulerian and the Lagrangian description of a function. For example: Let $\phi$ be a scalar spatial field, this means $\phi = \phi(\boldsymbol{x},t)$. Since $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X},t)$ we may define $\Phi(\boldsymbol{X},t) := \phi(\boldsymbol{\chi}(\boldsymbol{X},t),t)$ and thus we can switch between the two descriptions, provided $\boldsymbol{\chi}$ is known. When we want to calculate the material time derivative of a spatial field we need to be cautious. The connection of the two descriptions is given by

**Lemma 3.1.** *Let* $\phi(\boldsymbol{x},t)$ *be a given sufficiently smooth function in spatial coordiantes and* $\Phi(\boldsymbol{X},t) := \phi(\boldsymbol{\chi}^{-1}(\boldsymbol{x},t),t)$*. Then it holds:*

$$\frac{\partial}{\partial t}\Phi(\boldsymbol{X},t) = \frac{d}{dt}\phi(\boldsymbol{x},t) = \frac{\partial}{\partial t}\phi(\boldsymbol{x},t) + (\operatorname{grad}\phi(\boldsymbol{x},t),\boldsymbol{v}(\boldsymbol{x},t)).$$

*Proof.* The proof follows by taking the total derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ of the equation $\Phi(\boldsymbol{X},t) = \phi(\boldsymbol{\chi}^{-1}(\boldsymbol{x},t),t) = \phi(\boldsymbol{x},t)$. □

**Remark 3.2.** *An analogous result holds for vector-valued functions* $\boldsymbol{\phi}(\boldsymbol{x},t)$*:*

$$\frac{\partial}{\partial t}\boldsymbol{\Phi}(\boldsymbol{X},t) = \frac{d}{dt}\boldsymbol{\phi}(\boldsymbol{x},t) = \frac{\partial}{\partial t}\boldsymbol{\phi}(\boldsymbol{x},t) + \operatorname{grad}(\boldsymbol{\phi}(\boldsymbol{x},t))\boldsymbol{v}(\boldsymbol{x},t).$$

**Remark 3.3.** *With this we can write the acceleration* $\boldsymbol{a}$ *as*

$$\frac{\partial^2}{\partial t^2}\boldsymbol{\chi}(\boldsymbol{X},t) = \boldsymbol{a}(\boldsymbol{x},t) = \frac{\partial}{\partial t}\boldsymbol{v}(\boldsymbol{x},t) + (\operatorname{grad}\boldsymbol{v}(\boldsymbol{x},t))\boldsymbol{v}(\boldsymbol{x},t).$$

**Remark 3.4.** *For the sake of brevity we abbreviarte the total derivative with a superimposed dot, i.e.* $\dot{u}$*.*

### 3.1.4 The Deformation Gradient F

We define the *deformation gradient* $\mathbf{F}$ as

$$\mathbf{F}(\boldsymbol{X}, t) := \operatorname{Grad} \boldsymbol{x}(\boldsymbol{X}, t) = \operatorname{Grad} \boldsymbol{\chi}(\boldsymbol{X}, t).$$

This special gradient is a Cartesian tensor of order two and can be expressed as

$$\mathbf{F} = \frac{\partial}{\partial X_A} x_b \boldsymbol{e}_b \otimes \boldsymbol{e}_A,$$

or in component form as

$$F_{bA} = \frac{\partial}{\partial X_A} x_b$$

with $x_b = \chi_b(\boldsymbol{X}, t)$. It should be mentioned that the basis vectors for $\boldsymbol{X}$ and $\boldsymbol{x}$ need not to coincide, we assumed it here just for simplicity. The deformation gradient is an example of a so-called *two-point tensor*, which means it involves points from two different descriptions. In literature it is quite common to express this fact by means of indices used for the components of the tensor. An uppercase index stands for the material description and a lowercase one for the spatial description. We also define the *Jacobian* $J$ as

$$J(\boldsymbol{X}, t) := \det \mathbf{F}(\boldsymbol{X}, t).$$

From a physical point of view it is reasonable to assume that $J \neq 0$ which is justified by the following: Consider the equation $\mathbf{F}\Delta\boldsymbol{X} = \mathbf{0}$ for a small line element $\Delta\boldsymbol{X}$. Provided $\Delta\boldsymbol{X} \neq \mathbf{0}$ $J = 0$ would imply that there is at least one line element whose length is reduced to zero by the deformation, in other words, annihilated. This is physically unrealistic and so we can exclude this from our consideration. Having that we can ensure that $\mathbf{F}$ is nonsingular and so there exists the inverse $\mathbf{F}^{-1}$ given by

$$\mathbf{F}^{-1}(\boldsymbol{x}, t) = \operatorname{grad} \boldsymbol{X}(\boldsymbol{x}, t),$$

with the components

$$(\mathbf{F}^{-1})_{Ba} = \frac{\partial X_B}{\partial x_a}.$$

This is a direct consequence of the implicit function theorem (see [82] for details).

**Connection between** Grad **and** grad**.** For our purposes it is useful to have some transformation rules for the gradients with respect to the material and spatial descriptions. They are summarized in the following lemma.

**Lemma 3.2.** *Let $\phi, \boldsymbol{u}, \mathbf{T}$ respectively be scalar, vector and second-order tensor fields associated with a moving body $\mathcal{B}$. Then it holds:*

$$\begin{aligned}\operatorname{Grad}\phi &= \mathbf{F}^{\top}\operatorname{grad}\phi,\\ \operatorname{Grad}\boldsymbol{u} &= (\operatorname{grad}\boldsymbol{u})\mathbf{F},\\ \operatorname{Div}\boldsymbol{u} &= J\operatorname{div}(J^{-1}\mathbf{F}\boldsymbol{u}),\\ \operatorname{Div}\mathbf{T} &= J\operatorname{div}(J^{-1}\mathbf{F}\mathbf{T}).\end{aligned}$$

*Proof.* See [55]. □

**Deformation of Area and Volume Elements.** In continuum mechanics it is very important to know how to transform domains of integration. Consider the surface $S_r = \partial B_r$ which is deformed into the surface $S_t = \partial B_t$. Let $ds_{\boldsymbol{X}}$ and $ds_{\boldsymbol{x}}$ be the respective surface elements. Then the relation of the two is given by *Nanson's formula* reading

$$\boldsymbol{n}ds_{\boldsymbol{x}} = J\mathbf{F}^{-\top}\boldsymbol{N}ds_{\boldsymbol{X}}. \tag{3.3}$$

A proof of formula (3.3) can be found in [55]. A rather easier result holds for the transformation of volume elements. If $\mathrm{d}\boldsymbol{x}$ and $\mathrm{d}\boldsymbol{X}$ describe the respective volume elements in $B_t$ and $B_r$ it holds

$$\mathrm{d}\boldsymbol{x} = J\,\mathrm{d}\boldsymbol{X}\,.$$

This is just an application of the transformation theorem for integrals, see [82] for details. Concerning the Jacobian $J$ it is assumed that $J > 0$. With this assumption one can interpret $J$ as a measure for volume change.

**Some Important Results from Tensor Algebra.** In this paragraph we summarize the most important facts about the deformation gradient $\mathbf{F}$. These results are taken from [55].

**Theorem 3.3** (The square root theorem)**.** *If $\mathbf{S}$ is a positive definite, symmetric second-order tensor then there exists a unique, positive definite, symmetric second order tensor $\mathbf{U}$ such that*

$$\mathbf{U}^2 = \mathbf{S}.$$

*Proof.* See [55]. □

**Theorem 3.4** (The polar decomposition theorem)**.** *Let* $\mathbf{F}$ *be a second-order Cartesian tensor such that* $\det \mathbf{F} > 0$*. Then there exist unique, positive definite, symmetric tensors* $\mathbf{U}$ *and* $\mathbf{v}$ *and a unique proper orthogonal tensor* $\mathbf{R}$ *such that*

$$\mathbf{F} = \mathbf{RU} = \mathbf{vR}.$$

*Proof.* See [55]. □

We shall mention some important tensors which will be used hereafter. We define the *Green strain tensor*[4] $\mathbf{E}$ by

$$\mathbf{E} := \frac{1}{2}\left(\mathbf{F}^\top \mathbf{F} - \mathbf{I}\right).$$

Similarly, we define tensors $\mathbf{C}$ and $\mathbf{b}$ by

$$\mathbf{C} := \mathbf{F}^\top \mathbf{F} = \mathbf{U}^2$$
$$\mathbf{b} := \mathbf{F}\mathbf{F}^\top = \mathbf{v}^2.$$

We refer to $\mathbf{C}$ and $\mathbf{b}$ as the *right* and *left Cauchy-Green deformation tensor*. The terms left and right refer to that $\mathbf{C}$ works solely on the material description and $\mathbf{b}$ works on the spatial description. These two tensors are by definition symmetric and positive definite and can be decomposed into

$$\mathbf{U} = \sum_{i=1}^{3} \lambda_i \boldsymbol{\nu}^i \otimes \boldsymbol{\nu}^i,$$
$$\mathbf{v} = \sum_{i=1}^{3} \mu_i \boldsymbol{v}^i \otimes \boldsymbol{v}^i,$$

where $\lambda_i, \mu_i$ are the eigenvalues and $\boldsymbol{\nu}^i, \boldsymbol{v}^i$ are the eigenvectors of $\mathbf{U}$ and $\mathbf{v}$. Eventually it is useful to note that we can define the *displacement* $\boldsymbol{U}$ of a particle by

$$\boldsymbol{U}(\boldsymbol{X}, t) := \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X}.$$

This field relates the position $\boldsymbol{X}$ of a particle $P$ in the undeformed configuration to its position $\boldsymbol{x}$ in the deformed configuration at time $t$. The displacement $\boldsymbol{U}$ is a function of the material coordinates $\boldsymbol{X}$. We can also define the displacement field in spatial coordinates as

$$\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{x} - \boldsymbol{X}(\boldsymbol{x}, t).$$

Here the position $\boldsymbol{x}$ of a particle $P$ at time $t$ is specified by its position $\boldsymbol{X}(\boldsymbol{x}, t)$ in the reference configuration $B_r$ plus its displacement $\boldsymbol{u}(\boldsymbol{x}, t)$ from that position. Due to the

[4] The motivation for defining this special tensor is a pure mathematical one. It follows from standard linear algebra $\|d\boldsymbol{x}\|^2 - \|d\boldsymbol{X}\|^2 = (d\boldsymbol{X}, 2\mathbf{E}d\boldsymbol{X})$. And thus $\mathbf{E}$ can be seen as a measure for strain.

correspondance between the reference and current configuration the two descriptions $\boldsymbol{U}$ and $\boldsymbol{u}$ are related by

$$\boldsymbol{u}(\boldsymbol{x},t) := \boldsymbol{U}(\boldsymbol{\chi}^{-1}(\boldsymbol{x},t),t).$$

It shall be noted that $\boldsymbol{U}$ and $\boldsymbol{u}$ need to have the same values. Further, when choosing the reference configuration $B_r$ to coincide with the initial configuration $B_t|_{t=0}$ we see that the displacement has to vanish in the reference configuration. This can be expressed as

$$\boldsymbol{U}(\boldsymbol{X},t=0) = \boldsymbol{u}(\boldsymbol{x},t=0) = \boldsymbol{0}.$$

This new variable will emerge as the independent one when considering boundary value problems in non-linear elasticity. Having defined the displacement $\boldsymbol{U}$ we immediatealy see that

$$\boldsymbol{\chi}(\boldsymbol{X},t) = \boldsymbol{x}(\boldsymbol{X},t) = \boldsymbol{X} + \boldsymbol{U}(\boldsymbol{X},t)$$

and

$$\mathbf{F}(\boldsymbol{X},t) = \mathbf{I} + \operatorname{Grad}\boldsymbol{U}(\boldsymbol{X},t),$$

where $\operatorname{Grad}\boldsymbol{u}$ is the *displacement gradient*. Similarly we obtain in spatial coordinates that

$$\operatorname{grad}\boldsymbol{u}(\boldsymbol{x},t) = \mathbf{I} - \mathbf{F}^{-1}(\boldsymbol{x},t).$$

### 3.1.5 Analysis of Motion

Recalling the velocity $\boldsymbol{v}$, we can define the *velocity gradient tensor* by

$$\mathbf{L} = \operatorname{grad}\boldsymbol{v}, \tag{3.4}$$

which has components $L_{ij} = \frac{\partial v_i}{\partial x_j}$ with respect to the basis $\{\boldsymbol{e}_i\}$. Using the identity $\operatorname{Grad}\boldsymbol{u} = (\operatorname{grad}\boldsymbol{u})\mathbf{F}$ it follows that

$$\operatorname{Grad}\boldsymbol{v} = \mathbf{L}\mathbf{F}.$$

Assuming $\boldsymbol{x} = \chi(\boldsymbol{X},t)$ to be smooth enough we see that further

$$\operatorname{Grad}\boldsymbol{v} = \operatorname{Grad}\dot{\boldsymbol{x}} = \frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Grad}\boldsymbol{x} = \dot{\mathbf{F}}.$$

Using this with the identity $\frac{\partial}{\partial t}\det\mathbf{F} = \det\mathbf{F}\operatorname{tr}(\mathbf{F}^{-1}\dot{\mathbf{F}})$ we obtain the important result

$$\dot{J} = J\operatorname{tr}\mathbf{L} = J\operatorname{div}\boldsymbol{v}.$$

In this thesis we will assume that $\dot{J} = 0$, which is the case for an *isochoric* process, and this leads to the *incompressibility condition*

$$\operatorname{div}\boldsymbol{v} = 0. \tag{3.5}$$

**Integration of tensors** There is also an analog to the Gaussian theorem for tensors. Recall that for a vector-valued function $\boldsymbol{v}$ we have that

$$\int_{B_t} \operatorname{div} \boldsymbol{v} \ \mathrm{d}\boldsymbol{x} = \int_{\partial B_t} (\boldsymbol{v}, \boldsymbol{n}) \ ds_{\boldsymbol{x}}.$$

For tensors we need a slight different form of the Gauss' theorem reading

$$\int_{B_t} \operatorname{grad} \phi \ \mathrm{d}\boldsymbol{x} = \int_{B_t} \phi \boldsymbol{n} \ ds_{\boldsymbol{x}},$$

which becomes

$$\int_{B_t} \frac{\partial \phi}{\partial x_i} \ \mathrm{d}\boldsymbol{x} = \int_{\partial B_t} \phi n_i \ ds_{\boldsymbol{x}} \tag{3.6}$$

in components. Similar for a tensor $\mathbf{T}$ it holds

$$\int_{B_t} \operatorname{grad} \mathbf{T} \ \mathrm{d}\boldsymbol{x} = \int_{\partial B_t} \mathbf{T} \otimes \boldsymbol{n} \ ds_{\boldsymbol{x}}. \tag{3.7}$$

Finally recalling the definition of the divergence of a tensor $\mathbf{T}$ we obtain

$$\int_{B_t} \operatorname{div} \mathbf{T} \ \mathrm{d}\boldsymbol{x} = \int_{\partial B_t} \mathbf{T}^{\top} \boldsymbol{n} \ ds_{\boldsymbol{x}}. \tag{3.8}$$

## 3.2 Equilibrium Laws and Equations of Motion

The mechanics of continuous media are described by equations which express the balance of mass, linear momentum, angular momentum and energy in a moving body. These balance equations apply to all bodies, solid or fluid, and all of them give rise to field equations for sufficiently smooth motions. We will give a brief overview of the balance equations leaving out their derivation. For additional information one should refer to [31, 55].

### 3.2.1 Mass Conservation

We shall hereafter define $R_t \subset B_t$ and $R_r \subset B_r$ arbitrary. As $R_t$ moves it always consists of the same material, so its mass does not change, which means

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{R_t} \rho(\boldsymbol{x}, t) \ \mathrm{d}\boldsymbol{x} = 0.$$

By using Reynold's transport theorem, see [81, Theorem 11.60], and using the fact that $R_t$ was arbitrary we obtain the equation of *mass conservation*

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)\,\mathrm{div}\,\boldsymbol{v} = 0. \tag{3.9}$$

Recall that $\dot{J} = J\,\mathrm{div}\,\boldsymbol{v}$. With that we obtain that

$$\frac{\partial}{\partial t}(\rho J) = 0,$$

thus $\rho J$ must be constant over time and so we obtain the more compact formulation

$$\frac{\rho_r}{\rho} = J$$

with $\rho_r$ being the mass density in the reference configuration. For an incompressible material this simply becomes $\rho = \rho_r$.

### 3.2.2 Euler's Laws of Motion

The main two balance equations are given by the balance of *linear* and *angular* momentum $\boldsymbol{m}(\boldsymbol{x},t) := \int_{R_t} \rho\boldsymbol{v}\ \mathrm{d}\boldsymbol{x}$ and $\boldsymbol{h}(\boldsymbol{x},t) := \int_{R_t} \boldsymbol{x}\times\rho\boldsymbol{v}\ \mathrm{d}\boldsymbol{x}$ respectively and read as

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{m} = \int_{R_t} \rho\boldsymbol{b}\ \mathrm{d}\boldsymbol{x} + \int_{\partial R_t} \boldsymbol{t}(\boldsymbol{n})\ ds_{\boldsymbol{x}}, \tag{3.10}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{h} = \int_{R_t} \rho\boldsymbol{x}\times\boldsymbol{b}\ \mathrm{d}\boldsymbol{x} + \int_{R_t} \boldsymbol{x}\times\boldsymbol{t}(\boldsymbol{n})\ ds_{\boldsymbol{x}}. \tag{3.11}$$

with $\boldsymbol{b}$ being the body's *volume forces*, $\boldsymbol{t}(\boldsymbol{n})$ being the *stress vector*[5] and $\boldsymbol{n}$ being the outer unit normal.

We have to mention that these equations do depend on the choice of the particular basis $\{\boldsymbol{e}_i\}$. They resemble Newton's laws for particles and rigid bodies. The main difference in continuum mechanics is that the first equation above does not imply the second one i.e. the equations are independent. For obtaining a local (point-wise) description of these equations we need to know about the dependence of $\boldsymbol{t}$ on $\boldsymbol{n}$. This is governed by the well known theorem of Cauchy:

[5] This is called *Cauchy's stress principle* and is regarded as an axiom. It gives a mathematical description of the surface forces of an body. It states

> "The action of the material occupying the part of $B_t$ exterior to a closed surface $S$ on the material occupying the interior part is represented by a vector field, denoted $\boldsymbol{t}(\boldsymbol{n})$, defined on $S$ and with physical dimensions of force per unit area."

See [55] for details.

**Theorem 3.5.** *Let* $(\boldsymbol{t}(\boldsymbol{n}), \boldsymbol{b})$ *be a system of surface and body forces for* $\mathcal{B}$ *during a motion. The Euler equations of motion* (3.10)–(3.11) *hold if and only if*

1. *There exists a second-order Cartesian tensor* $\boldsymbol{\sigma}$*, the* Cauchy stress tensor *such that* $\boldsymbol{t}(\boldsymbol{n}) = \boldsymbol{\sigma}^\top \boldsymbol{n}$*.*

2. *The stress tensor* $\boldsymbol{\sigma}$ *is symmetric, i.e.* $\boldsymbol{\sigma} = \boldsymbol{\sigma}^\top$*.*

*Proof.* A proof for this theorem can be found either in [55] or in [31]. □

With this theorem we can formulate the point-wise equations of motion which are also called *Cauchy's equation of motion* reading

$$0 = \dot{\rho} + \rho \operatorname{div} \boldsymbol{v}, \tag{3.12}$$

$$\rho \boldsymbol{a} = \rho \boldsymbol{b} + \operatorname{div} \boldsymbol{\sigma}, \tag{3.13}$$

$$\boldsymbol{\sigma}^\top = \boldsymbol{\sigma}. \tag{3.14}$$

The divergence in (3.13) comes from an application of the divergence theorem (3.8). These equations are not yet complete, they provide seven equations for thirteen scalar fields. To close the gap we need to find more equations which will lead to *constitutive equations* for $\boldsymbol{\sigma}$. However, we will postpone this to Section 3.3.

For a more convenient mathematical analysis we will transform the above equations of motion to the reference configuration $B_r$. This is achieved by using Nanson's formula (3.3). For the stress vector $\boldsymbol{t}(\boldsymbol{n})$ we get

$$\int_{\partial B_t} \boldsymbol{t}(\boldsymbol{n}) \, ds_{\boldsymbol{x}} = \int_{\partial B_t} \boldsymbol{\sigma}\boldsymbol{n} \, ds_{\boldsymbol{x}} = \int_{\partial B_r} J\boldsymbol{\sigma}\mathbf{F}^{-\top}\boldsymbol{N} \, ds_{\boldsymbol{X}} = \int_{\partial B_r} \mathbf{S}^\top \boldsymbol{N} \, ds_{\boldsymbol{X}},$$

where we have defined the *nominal stress tensor*, or *engineering stress*, by $\mathbf{S} := J\mathbf{F}^{-1}\sigma$. The tensor $\mathbf{S}^\top$ is referred to as *first Piola-Kirchhoff stress tensor*. The nominal stress tensor $\mathbf{S}$ measures force per unit reference area while $\boldsymbol{\sigma}$ measures force per unit deformed area. Further, $\mathbf{S}$ is in general not symmetric but satisfies the relation $\mathbf{FS} = \mathbf{S}^\top \mathbf{F}^\top$ arising from the symmetry of $\boldsymbol{\sigma}$. With this we rewrite the equations of motion (3.13) in terms of $\mathbf{S}$. To do so we look at the integral form of (3.13) reading

$$\int_{R_t} \rho \boldsymbol{b} \; \mathrm{d}\boldsymbol{x} + \int_{\partial R_t} \boldsymbol{\sigma}\boldsymbol{n} \, ds_{\boldsymbol{x}} = \int_{R_t} \rho \boldsymbol{a} \; \mathrm{d}\boldsymbol{x}\,.$$

Using Nanson's formula (3.3) and $\rho \; \mathrm{d}\boldsymbol{x} = \rho_r \; \mathrm{d}\boldsymbol{X}$ we obtain

$$\int_{R_r} \rho_r \boldsymbol{B} \; \mathrm{d}\boldsymbol{X} + \int_{\partial R_r} \mathbf{S}^\top \boldsymbol{N} \, ds_{\boldsymbol{X}} = \int_{R_r} \rho_r \boldsymbol{A} \; \mathrm{d}\boldsymbol{X},$$

where $B(\boldsymbol{X}, t) := \boldsymbol{b}(\boldsymbol{\chi}^{-1}(\boldsymbol{x}, t), t)$ and eventually taking the divergence theorem for Cartesian tensors we arrive at the equation of motion in the reference configuration

$$\operatorname{Div} \mathbf{S} + \rho_r \boldsymbol{B} = \rho_r \boldsymbol{A}. \tag{3.15}$$

The transformed equations of motion (3.15) is the basis for further analysis.

### 3.2.3 Boundary and Initial Conditions

We shall make a few notes on boundary and initial conditions for the equations of motion. In Chapter 4 we will focus mainly on the quasi-equilibrium equations

$$\operatorname{div} \boldsymbol{\sigma} = 0$$

or

$$\operatorname{Div} \mathbf{S} = 0$$

rather than the full equations of motion. Therefore we would not need to impose any kind of initial conditions. However, for the time being we are to discuss the initial conditions. We also need to formulate appropriate boundary conditions in order to formulate a boundary-value problem. From a physical point of view it is convenient to formulate boundary conditions in Eulerian description. Typical boundary conditions in problems of non-linear elasticity are those in which we specify either $\boldsymbol{\chi}(\boldsymbol{x}, t)$ or $\boldsymbol{u}(\boldsymbol{x}, t)$ for one part of the boundary $\Gamma_D \subset \partial B_t$ say, and the stress vector $\boldsymbol{t}$ on the remainder, $\Gamma_N$, so that $\bar{\Gamma}_D \cup \bar{\Gamma}_N = \partial B_t$. In applied mathematics these boundary conditions are called Dirichlet and Neumann boundary conditions and read as

$$\boldsymbol{\chi} = \boldsymbol{X}(\boldsymbol{x}, t) + \boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{g}_{D,1}(\boldsymbol{x}, t) \quad \text{on } \Gamma_D, \tag{3.16}$$

$$\boldsymbol{u} = \boldsymbol{g}_{D,2}(\boldsymbol{x}, t) \quad \text{on } \Gamma_D, \tag{3.17}$$

and

$$\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n} = \boldsymbol{g}_N(\boldsymbol{x}, t) \quad \text{on } \Gamma_N. \tag{3.18}$$

From (3.16)–(3.17) we see that we can focus on Dirichlet boundary conditions purely in $\boldsymbol{u}$.

However, for the mathematical analysis of the equations of non-linear elasticity it is more useful to work on the reference configuration. In contrast to linear elasticity, where we may neglect the difference between the reference configuration and the deformed configuration, we have to consider these differences in case of non-linear elasticity. An example shall illustrate the main differences when dealing with non-linear elasticity. Consider a body $B_t$ where a constant hydrostatic pressure $p_0$ acts

on the Neumann boundary $\Gamma_N$, which means $\boldsymbol{\sigma}\boldsymbol{n} = -p_0\boldsymbol{n}$. In non-linear elasticity we may push-back this boundary condition to the reference configuration. This is done by Nanson's formula and thus we obtain for a simple hydrostatic pressure the non-linear boundary condition $\mathbf{S}^\top \boldsymbol{N} = -Jp_0\mathbf{F}^{-\top}\boldsymbol{N}$ on $\Gamma_{N,r}$, where $\Gamma_{N,r}$ denotes the Neumann boundary in the reference configuration $B_r$. This means, that for seemingly simple Neumann boundary conditions we may obtain essential non-linear boundary conditions in the reference configuration. As for the Dirichlet boundary conditions, they remain the same as we can write $\boldsymbol{g}_D(\boldsymbol{x},t) = \boldsymbol{g}_D(\boldsymbol{\chi}(\boldsymbol{X},t),t) =: \tilde{\boldsymbol{g}}_D(\boldsymbol{X},t)$. For a more detailed discussion on boundary conditions in non-linear elasticity we refer to [55, Chap. 5]. Summarizing, we obtain the following boundary conditions in the reference configuration:

$$\boldsymbol{U} = \tilde{\boldsymbol{g}}_D(\boldsymbol{X},t) \qquad \text{on } \Gamma_{D,r}, \tag{3.19}$$

$$\boldsymbol{t} = \mathbf{S}^\top \boldsymbol{N} = \tilde{\boldsymbol{g}}_N(\mathbf{F},\boldsymbol{X},t) \qquad \text{on } \Gamma_{N,r}, \tag{3.20}$$

where we indicate the possible non-linearity in the Neumann boundary condition. For mathematical reasons we may also rewrite the boundary conditions in a more abstract way as

$$\begin{aligned} \gamma_0^{\text{int}}\boldsymbol{u} &= \boldsymbol{g}_D \qquad && \text{on } \Gamma_D, \\ \gamma_1^{\text{int}}\boldsymbol{u} &= \boldsymbol{g}_N && \text{on } \Gamma_N, \end{aligned}$$

with the trace operators $\gamma_{\{0,1\}}^{\text{int}}(\cdot)$ which will be defined in Chapter 5. When dealing with time-dependent problems one also needs to impose initial conditions of the form

$$\boldsymbol{U}(t=0,\boldsymbol{X}) = \boldsymbol{u}(t=0,\boldsymbol{x}) = \boldsymbol{0}, \tag{3.21}$$

$$\boldsymbol{V}(t=0,\boldsymbol{X}) = \boldsymbol{V}_0(\boldsymbol{X}) = \boldsymbol{v}_0(\boldsymbol{x}) = \boldsymbol{v}(t=0,\boldsymbol{x}). \tag{3.22}$$

The equations of motion together with the boundary and initial conditions form a system of highly non-linear second-order partial differential equations to obtain either $\boldsymbol{U}$ or $\boldsymbol{u}$. So far our system reads, in spatial coordinates, as

$$\begin{aligned} \operatorname{div}\boldsymbol{\sigma}(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)\boldsymbol{b}(\boldsymbol{x},t) &= \rho(\boldsymbol{x},t)\boldsymbol{a}(\boldsymbol{x},t), \\ \frac{\partial}{\partial t}\rho(\boldsymbol{x},t) + \operatorname{div}\boldsymbol{v}(\boldsymbol{x},t) &= 0, \\ \boldsymbol{\sigma}(\boldsymbol{x},t) &= (\boldsymbol{\sigma}(\boldsymbol{x},t))^\top, \end{aligned}$$

in $B_t$ and $t > 0$ with the boundary and initial conditions

$$\begin{aligned} \boldsymbol{u}(\boldsymbol{x},t) &= \boldsymbol{g}_D(\boldsymbol{x},t) \qquad && \text{on } \Gamma_D, \\ \boldsymbol{\sigma}(\boldsymbol{x},t)\boldsymbol{n} &= \boldsymbol{g}_N(\boldsymbol{x},t) && \text{on } \Gamma_N, \\ \boldsymbol{u}(\boldsymbol{x},0) &= \boldsymbol{0}, \\ \boldsymbol{v}(\boldsymbol{x},0) &= \boldsymbol{v}_0. \end{aligned}$$

In material coordinates we have

$$\begin{aligned} \operatorname{Div} \mathbf{S}(\boldsymbol{X},t) + \rho_r(\boldsymbol{X})\boldsymbol{b}(\boldsymbol{X},t) &= \rho_r(\boldsymbol{X})\boldsymbol{A}(\boldsymbol{X},t), \\ \rho_r(\boldsymbol{X}) &= \rho(\chi(\boldsymbol{X},t),t)J(\boldsymbol{X},t), \\ \mathbf{F}(\boldsymbol{X},t)\mathbf{S}(\boldsymbol{X},t) &= (\mathbf{F}(\boldsymbol{X},t)\mathbf{S}(\boldsymbol{X},t))^{\top} \end{aligned}$$

in $B_r$ and $t > 0$ with the boundary and initial conditions

$$\begin{aligned} \boldsymbol{U}(\boldsymbol{X},t) &= \tilde{\boldsymbol{g}}_D(\boldsymbol{X},t) && \text{on } \Gamma_{D,r}, \\ \mathbf{S}^{\top}(\boldsymbol{X},t)\boldsymbol{N} &= \tilde{\boldsymbol{g}}_N(\mathbf{F},\boldsymbol{X},t) && \text{on } \Gamma_{N,r}, \\ \boldsymbol{U}(\boldsymbol{X},0) &= \mathbf{0}, \\ \boldsymbol{V}(\boldsymbol{X},0) &= \boldsymbol{v}_0. \end{aligned}$$

Taking all the boundary and initial conditions together the system is not complete yet. This can easily be checked by counting the independent equations, seven equations for thirteen scalar fields. Therefore we need to find more equations to complete the system. This can be achieved by constitutive laws.

## 3.3 Constitutive Equations

This part is taken and adapted from [31] and [55].

We have seen that the equations of motion are not complete. Hence we must establish additional equations in the form of appropriate *constitutive laws* which are furnished to specify the ideal material in question. A constitutive law should approximate the observable physical behavior of a real material under specific conditions of interest. Generally speaking, a constitutive law establishes a functional relationship between the Cauchy stress $\boldsymbol{\sigma}$ and some quantities like position, deformation, temperature and so on. Our aim here is to give an overview on the theory for constitutive equations, however we can not go too much into detail as this is far beyond the scope of this thesis. For a more detailed overview we refer to [31, 77].

### 3.3.1 Hyper-elastic Materials

Before starting with the definition of *hyper-elastic materials* we briefly summarize the most important facts about elastic materials.

The constitutive relation for an elastic material is written in the form

$$\boldsymbol{\sigma} = \mathbf{g}(\mathbf{F}),$$

where $\mathbf{g}$ is a symmetric tensor-valued function on the space of deformation gradients. For simplicity we assume that the material under consideration is homogeneous, i.e. $\mathbf{g}$ does not depend on the position $\boldsymbol{x}$, an assumption which may be softened. We also assume that $\mathbf{g}$ neither depends on the velocity $\boldsymbol{v}$ nor on higher order derivatives in time and $\mathbf{L}$. We also assume that $\mathbf{g}(\mathbf{I}) = 0$ which means that there is no stress when there is no deformation. Otherwise we refer to the material as *residually stressed*, which will be discussed in more detail afterwards. One of the most important assumptions on the function $\mathbf{g}$ is that it is *objective*, which means that the material properties are independent of superimposed rigid-body motions. In terms of tensors this is summarized in the following definition:

**Definition 3.7.** *Let $\phi$, $\boldsymbol{u}$, $\mathbf{T}$ be scalar, vector and second-order tensor-valued functions defined on $B_t$. Let $\phi', \boldsymbol{u}', \mathbf{T}'$ be the corresponding fields on $B_t'$, where $B_t'$ is obtained from $B_t$ by a rigid body motion $\boldsymbol{x}' = \mathbf{Q}\boldsymbol{x} + \boldsymbol{c}$ with $\mathbf{Q}$ being a proper orthogonal tensor and $\boldsymbol{c}$ denoting an arbitrary vector in $\mathbb{R}^3$. The fields are said to be* objective *if, for all such motions,*

$$\begin{aligned} \phi' &= \phi, \\ \boldsymbol{u}' &= \mathbf{Q}\boldsymbol{u}, \\ \mathbf{T}' &= \mathbf{Q}\mathbf{T}\mathbf{Q}^\top, \end{aligned}$$

*holds.*

There are of course examples of functions which are not objective, like the velocity $\boldsymbol{v}$. For more details about elastic materials, especially isotropic ones, we refer to [31, 55]. We now turn our attention to a special class of elastic materials, the so-called hyper-elastic materials. For this we take a look at the energy balance equation of continuum mechanics reading

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{R_t} \frac{1}{2}\rho(\boldsymbol{v},\boldsymbol{v})\ \mathrm{d}\boldsymbol{x} + \int_{R_t} \mathrm{tr}(\boldsymbol{\sigma}\mathbf{D})\ \mathrm{d}\boldsymbol{x} = \int_{R_t} \rho(\boldsymbol{b},\boldsymbol{v})\ \mathrm{d}\boldsymbol{x} + \int_{\partial R_t} (\boldsymbol{t},\boldsymbol{v})\ ds_{\boldsymbol{x}}$$

where $\mathbf{D} := \frac{1}{2}(\mathbf{L} + \mathbf{L}^\top)$. For a derivation of this energy balance equation see [55]. We introduce the following physical quantities:

- The *kinetic energy*

$$K(R_t) := \int_{R_t} \frac{1}{2}\rho(\boldsymbol{v},\boldsymbol{v})\ \mathrm{d}\boldsymbol{x}\,.$$

- The *rate of working*, or *power* of the forces acting on $R_t$,

$$P(R_t) := \int_{R_t} \rho(\boldsymbol{b},\boldsymbol{v})\ \mathrm{d}\boldsymbol{x} + \int_{\partial R_t} (\boldsymbol{t},\boldsymbol{v})\ ds_{\boldsymbol{x}}.$$

- The quantity

$$S(R_t) := \int_{R_t} \operatorname{tr}(\boldsymbol{\sigma}\mathbf{D}) \ \mathrm{d}\boldsymbol{x},$$

  which is a measure for the stored energy or the amount of work dissipated in the form of heat or a mixture of both.

Now we can rewrite the energy balance equation as

$$P(R_t) = \frac{\mathrm{d}}{\mathrm{d}t} K(R_t) + S(R_t).$$

Next we focus on the term $S(R_t)$. For an elastic material we assume a functional dependence of $\boldsymbol{\sigma}$ on the deformation gradient $\mathbf{F}$. By recalling the definition of the nominal stress tensor $\mathbf{S} = J\mathbf{F}^{-1}\boldsymbol{\sigma}$ we obtain

$$\mathbf{S} = J\mathbf{F}^{-1}\boldsymbol{\sigma} = (\det \mathbf{F})\mathbf{F}^{-1}\mathbf{g}(\mathbf{F}) =: \mathbf{h}(\mathbf{F}),$$

where $\mathbf{h}$ is the so-called *response function*. By looking at the definition of $S(R_t)$ we get

$$\int_{R_t} \operatorname{tr}(\boldsymbol{\sigma}\mathbf{D}) \ \mathrm{d}\boldsymbol{x} = \int_{R_r} J \operatorname{tr}(\boldsymbol{\sigma}\mathbf{D}) \ \mathrm{d}\boldsymbol{X}\,.$$

The integrand on the right hand side can be interpreted as working-rate of the stresses per unit reference volume or more simple the stress power density. With that we establish the following relation by using the definitions of $\boldsymbol{\sigma}, \mathbf{S}, \mathbf{L}$

$$J \operatorname{tr}(\boldsymbol{\sigma}\mathbf{D}) = J \operatorname{tr}(\boldsymbol{\sigma}\mathbf{L}) = \operatorname{tr}(\mathbf{FSL}) = \operatorname{tr}(\mathbf{SLF}) = \operatorname{tr}(\mathbf{S}\dot{\mathbf{F}}) = \operatorname{tr}(\mathbf{h}(\mathbf{F})\dot{\mathbf{F}}).$$

With this result we can give a definition for a hyper-elastic material:

**Definition 3.8.** *A material is said to be a* hyper-elastic *or* Green elastic material *if there exists a function $W(\mathbf{F})$, called the* strain energy function*, such that*

$$\dot{W}(\mathbf{F}) = \operatorname{tr}(\mathbf{h}(\mathbf{F})\dot{\mathbf{F}}).$$

In literature one also finds the notation *Helmholtz free energy*, although this particular name is most used in case the function $W$ depends on more than just the deformation $\mathbf{F}$, e.g. temperature, electric field and so on. With that we can rewrite the term $S(R_t)$

$$S(R_t) = \int_{R_t} \operatorname{tr}(\boldsymbol{\sigma}\mathbf{L}) \ \mathrm{d}\boldsymbol{x} = \int_{R_r} \frac{\partial}{\partial t} W(\mathbf{F}) \ \mathrm{d}\boldsymbol{X} = \frac{\mathrm{d}}{\mathrm{d}t} \int_{R_r} W(\mathbf{F}) \ \mathrm{d}\boldsymbol{X},$$

with the term $\int_{R_r} W(\mathbf{F})\ \mathrm{d}\boldsymbol{X}$ being the elastic strain energy in the region $R_r$. Taking a closer look at the strain energy function we see that

$$\frac{\partial}{\partial t} W(\mathbf{F}) = \frac{\partial W}{\partial F_{ij}} \frac{\partial F_{ij}}{\partial t} = \mathrm{tr}(\frac{\partial W}{\partial \mathbf{F}} \dot{\mathbf{F}}).$$

Here we need to interpret the term $\frac{\partial W}{\partial \mathbf{F}}$. It is a second-order tensor with components defined by the convention (see [55])

$$\left(\frac{\partial W}{\partial \mathbf{F}}\right)_{ij} := \frac{\partial W}{\partial F_{ji}}. \tag{3.23}$$

Due to $\dot{\mathbf{F}} = \mathbf{L}\mathbf{F}$ we obtain

$$\frac{\partial W}{\partial t} = \mathrm{tr}\left(\frac{\partial W}{\partial \mathbf{F}} \mathbf{L}\mathbf{F}\right) = \mathrm{tr}\left(\mathbf{F}\frac{\partial W}{\partial \mathbf{F}} \mathbf{L}\right).$$

On the other hand, we know that

$$\frac{\partial W}{\partial t} = J\,\mathrm{tr}\,(\boldsymbol{\sigma}\mathbf{L})$$

and by comparison we arrive at the fundamental relation

$$\boldsymbol{\sigma} = J^{-1}\mathbf{F}\frac{\partial W}{\partial \mathbf{F}} =: \mathbf{g}(\mathbf{F})$$

or in more simpler form, taking the definition of the nominal stress $\mathbf{S}$, we obtain the relation

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{F}} =: \mathbf{h}(\mathbf{F}).$$

We will stick to the formulation in the reference configuration, i.e. we will work in terms of $\mathbf{h}(\mathbf{F})$.

**Assumptions on the response function $h(F)$.** We have seen that $\mathbf{S} = J^{-1}\mathbf{F}^{-1}\mathbf{g}(\mathbf{F}) = \mathbf{h}(\mathbf{F})$. We now require the response function $\mathbf{h}(\mathbf{F})$ to be objective. By a simple calculation it can be shown that the relation

$$\mathbf{h}(\mathbf{Q}\mathbf{F}) = \mathbf{h}(\mathbf{F})\mathbf{Q}^\top \tag{3.24}$$

needs to hold for arbitrary proper rotations $\mathbf{Q}$. This poses a restriction on the shape of the strain energy function. Let us recall the polar decomposition theorem (Theorem 3.4) which gives a partition of $\mathbf{F}$ into $\mathbf{R}$ and $\mathbf{U}$. Since (3.24) needs to hold for arbitrary rotations we may choose $\mathbf{Q} = \mathbf{R}^\top$. Thus we obtain

$$\mathbf{h}(\mathbf{F})\mathbf{R} = \mathbf{h}(\mathbf{R}^\top\mathbf{F}) = \mathbf{h}(\mathbf{R}^\top\mathbf{R}\mathbf{U}) = \mathbf{h}(\mathbf{U}),$$

which means, that for $\mathbf{h}$ to be objective it is necessary that it depends on $\mathbf{F}$ through $\mathbf{U}$. In literature this is usually accomplished by choosing $\mathbf{h}$ to depend either on $\mathbf{C}$ or $\mathbf{E}$, because $\mathbf{C} = \mathbf{U}^2$ and $\mathbf{E} = \frac{1}{2}(\mathbf{U}^2 - \mathbf{I})$. Furthermore, we adopt some basic assumptions from non-linear elasticity. To specify the behavior of $W(\mathbf{F})$ for small and large deformations we require that:

- $W(\mathbf{F}) \to \infty$ as $\|\mathbf{F}\| \to \infty$. This means, that the energy increases as we increase the deformation. This property is also called *coercivity*.
- $\det \mathbf{F} \to 0$ implies that $W(\mathbf{F}) \to \infty$. This means, it requires "infinite" energy to compress the body $\mathcal{B}$ to a point.
- $W(\mathbf{F}) = \infty$ if $\det \mathbf{F} < 0$.

In the next paragraph we will restrict deformations to the special class of *isochoric* ones.

**Incompressibility.** Let us focus on incompressible materials which means $\det \mathbf{F} = J = 1$ or $\operatorname{div} \boldsymbol{v} = 0$. In this case we need to adapt the formulation of the strain energy function by introducing the Lagrangian multiplier $p$ to enforce incompressibility (We skip the derivation. The reader may refer to [55] for details.). For an incompressible material the relation between the stress tensor and the strain energy function becomes

$$\boldsymbol{\sigma} = \mathbf{F}\frac{\partial W}{\partial \mathbf{F}} - p\mathbf{I}.$$

In the spatial coordinates we can link the incompressibility condition with the displacement $\boldsymbol{u}$. We know that for an incompressible material

$$\operatorname{div} \boldsymbol{v}(\boldsymbol{x}, t) = 0$$

needs to hold. Assuming that $\boldsymbol{v}$ is smooth enough we can rewrite the equation as

$$\operatorname{div} \boldsymbol{v}(\boldsymbol{x}, t) = \operatorname{div} \dot{\boldsymbol{u}}(\boldsymbol{x}, t) = \frac{\mathrm{d}}{\mathrm{d}t} \operatorname{div} \boldsymbol{u}(\boldsymbol{x}, t) = 0.$$

This together with the inital condition $\boldsymbol{u}(\boldsymbol{x}, 0) = \mathbf{0}$ leads to

$$\operatorname{div} \boldsymbol{u}(\boldsymbol{x}, t) = 0. \tag{3.25}$$

For the material description we obtain for the nominal stress

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{F}} - p\mathbf{F}^{-1}.$$

The incompressibility condition in this case reads as

$$\det \mathbf{F} = 1.$$

Furthermore we assume that the strain energy function $W(\mathbf{F})$ vanishes in the absence of deformations, this means $W(\mathbf{I}) = 0$. So far we have assumed that the strain energy function $W(\mathbf{F})$ vanishes for $\mathbf{F} = \mathbf{I}$. However, this does not exclude the possibility of an *in situ* stress. This will be briefly discussed in the next section.

### 3.3.2 Residual Stress

We have assumed that the reference configuration $B_r$ is stress *free*. However, for the application of non-linear elasticity to model biological tissue there are many situations in which a stress free reference configuration does not exist and there are so-called *residual stresses* not associated with a deformation and not given by a constitutive law[6]. For biological tissues, those stresses are generated by growth, remodeling or adoption, see [68] for details. We do not intend to discuss residual stress in detail nor will we include it in our models, we just want to emphasize that in most of the literature it is forgotten to mention residual stresses and their importance in bio-mechanics.

We assume that the strain energy function $W(\mathbf{F})$ vanishes in the reference configuration. However, we have not specified the behavior of the derivative $\frac{\partial W}{\partial \mathbf{F}}$ yet. Recalling the definition of the nominal stress $\mathbf{S}$ we define the residual stress as

$$\mathbf{S}^{(r)} := \left.\frac{\partial W}{\partial \mathbf{F}}\right|_{\mathbf{F}=\mathbf{I}}. \tag{3.26}$$

In the literature we can also find the notation $\boldsymbol{\tau}$ for the residual stress. Furthermore as the residual stress is defined in the reference configuration we need not to distinguish between nominal stress and Cauchy stress as they coincide. It is assumed in [55] that the residual stress must satisfy the equilibrium equation

$$\operatorname{Div} \mathbf{S}^{(r)} = 0 \qquad \text{in } B_r. \tag{3.27}$$

If the boundary $\partial B_r$ is traction free (unloaded) then, additionally, the residual stress must satisfy the boundary condition

$$\mathbf{S}^{(r)^\top} \boldsymbol{N} = \mathbf{S}^{(r)} \boldsymbol{N} = \mathbf{0} \qquad \text{on } \partial B_r. \tag{3.28}$$

[6] The term residual stress is not clearly specified. There are different notions which do all slightly differ in their definition. The oldest definition dates back to Biot in 1965 and he called it *initial stress*. Another definition goes back to Hoger in 1985. He actually called it residual stress. However, we will go with the definition by Ogden. To illustrate the principle of residual stress we refer to an experiment, which is often cited by Prof. Ogden in his lectures. When one takes a small tube of arterial tissue and cuts it open one would usually expect that nothing will happen. However, the arterial tissue opens up with a great velocity and stretches itself. This is due to the residual stress which is released when cutting the tissue.

Now we want to establish some basic facts about the residual stress. For that we use the identity

$$\mathrm{Div}(\mathbf{S}^{(r)} \otimes \boldsymbol{X}) = (\mathrm{Div}\, \mathbf{S}^{(r)}) \otimes \boldsymbol{X} + \mathbf{S}^{(r)}. \tag{3.29}$$

By using this identity together with Gauss' theorem and (3.27), (3.28) we obtain

$$\int_{B_r} \mathbf{S}^{(r)} \ \mathrm{d}\boldsymbol{X} = 0.$$

Its immediate consequence is that the residual stress must not be uniform. In other words, if, in a residually stressed configuration, the boundary $\partial B_r$ is load free, then the residual stress distribution is necessarily inhomogeneous and is therefore geometry dependent. A further consequence is that the material response of a residually stressed body relative to the residually stressed configuration, and hence the constitutive law, is geometry dependent and inhomogeneous. For a more detailed treatment of residual stresses in the context of modeling the myocardium refer to [2],[58] ,[24] and [14].

## 3.4 Constitutive Model for the Myocardium

After having established the basic facts on non-linear elasticity, we continue to specify the constitutive model for the myocardium. We focus on a specific model, introduced by Holzapfel in [32]. Of course, there are many other models around and in [32] one finds a good summary of those. However, before introducing the Holzapfel model we need to state a restriction on the model. To the best of our knowledge there is no model of the passive myocardium which accounts for the whole structure of the myocardium. All models concentrate on the ventricular activity. Thus, the Holzapfel model may only validated for the ventricles of the human heart. For a detailed overview of the experiments leading to the subsequent model we refer to [32] and the bibliography there. At this point we will specify the reference configuration occupied by the myocardium as $\Omega_r \subset \mathbb{R}^3$ and the deformed configuration with $\Omega_t \subset \mathbb{R}^3$.

### 3.4.1 Orthotropic Materials

The Holzapfel model is a constitutive model for a special kind of anisotropic materials, so-called *orthotropic* materials. For explaining the idea of an orthotropic material we recall the definition of the local coordinate system $\{\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0\}$ as introduced in Chapter 1. This coordinate system represents a natural orthonormal coordinate system spanned by the fibers in $\Omega_r$[7]. To be more precise, as discussed in Section 2.4,

[7] In fact, the fibers need not be exactly orthogonal but for simplicity we assume it here.

this coordinate system is in fact $\boldsymbol{X}$-dependent as can easily be seen in the Figure 1.2. An orthotropic material is defined as a material which exhibits two or three axis of symmetry, which means that the material properties change along these directions. If there is just one axis of symmetry the material is referred to as being *transversely isotropic*, see [31] for details. Examples for orthotropic materials are wood, fiber reinforced polymers and in particular the myocardium. Orthotropic materials allow the strain energy function to obtain a very special form, similar to the one of an isotropic material. For an isotropic material the most general form of the strain energy function is described by the Rivlin-Eriksen representation theorem, see [31, 55]. It states that the strain energy function, say $\Psi$, can be written as

$$\Psi(\mathbf{C}) = \Psi(I_1(\mathbf{C}), I_2(\mathbf{C}), I_3(\mathbf{C}))$$

with

$$\begin{aligned} I_1(\mathbf{C}) &:= \operatorname{tr}\mathbf{C}, \\ I_2(\mathbf{C}) &:= \frac{1}{2}\left(I_1^2 - \operatorname{tr}(\mathbf{C}^2)\right), \\ I_3(\mathbf{C}) &:= \det\mathbf{C}. \end{aligned}$$

The quantities $I_1, I_2, I_3$ are called the *isotropic invariants*. The Rivlin-Eriksen theorem is a very general statement as it does not need any phenomenological assumptions and is not based on experimental data. For a general introduction into invariant based constitutive models we refer to [74]. The general idea for handling anisotropic materials is to split up the strain energy function $W$ into an isotropic part $W_{\text{iso}}$ and an anisotropic part $W_{\text{aniso}}$, this means

$$W(\mathbf{F}) = W_{\text{iso}}(\mathbf{C}) + W_{\text{aniso}}(\mathbf{C}),$$

where we explicitly require the dependence of $W$ on $\mathbf{F}$ through $\mathbf{C} = \mathbf{F}^\top\mathbf{F}$ to automatically have an objective strain energy function as mentioned in Section 3.3.1. For a transversely isotropic material we know from [31, 55] that we can introduce new invariants $I_4, I_5$. Suppose we have a transversely isotropic material with the preferred direction $\boldsymbol{v}$. Then we may introduce the new invariants

$$\begin{aligned} I_4(\mathbf{C}) &:= (\boldsymbol{v}, \mathbf{C}\boldsymbol{v}), \\ I_5(\mathbf{C}) &:= \left(\boldsymbol{v}, \mathbf{C}^2\boldsymbol{v}\right). \end{aligned} \tag{3.30}$$

These invariants account for the direction $\boldsymbol{v}$. Similar, if we have two preferred directions, say $\boldsymbol{v}, \boldsymbol{w}$, we may add the invariants

$$\begin{aligned} I_6(\mathbf{C}) &:= (\boldsymbol{w}, \mathbf{C}\boldsymbol{w}), \\ I_7(\mathbf{C}) &:= \left(\boldsymbol{w}, \mathbf{C}^2\boldsymbol{w}\right), \end{aligned}$$

as well as a coupling invariant

$$I_8(\mathbf{C}) := (\boldsymbol{v}, \mathbf{C}\boldsymbol{w}) = (\boldsymbol{w}, \mathbf{C}\boldsymbol{v}).$$

We need to mention that the invariant $I_8$ is not an invariant at all because it changes the sign when the direction of either $\boldsymbol{v}$ or $\boldsymbol{w}$ is reversed. To overcome this one may change the dependence of $I_8$ to $I_8^2$ as suggested in [32]. In case of orthotropic materials, which means that $\boldsymbol{v}$ and $\boldsymbol{w}$ are orthogonal, it has been shown in [45] that the invariant $I_8$ can be expressed in terms of the other invariants by

$$I_8^2 = I_2 + I_4 I_6 + I_5 + I_7 - I_1(I_4 + I_6).$$

For the shape of the strain energy function it is quite common to use an exponential ansatz in an additive way. This has two major reasons. First, exponentials automatically fulfil the mathematical assumptions needed for guaranteeing existence of solutions, like poly-convexity. This will be briefly addressed in Chapter 5. Secondly, the idea of using exponentials dates back to phenomenological studies of Fung, see [19]. Therefore one also refers to those models as *Fung-type models*.

### 3.4.2 The Holzapfel Model

Bearing in mind the local coordinate system as depicted in Figure 1.2 and the definition of the invariant $I_4$ as given in equation (3.30), we now consider the invariant $I_4$ associated with each of the directions defined by the local coordinate system $\{\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0\}$. The notation

$$I_{4f} := (\boldsymbol{f}_0, \mathbf{C}\boldsymbol{f}_0) = \|\mathbf{F}\boldsymbol{f}_0\|, \tag{3.31}$$
$$I_{4s} := (\boldsymbol{s}_0, \mathbf{C}\boldsymbol{s}_0) = \|\mathbf{F}\boldsymbol{s}_0\|, \tag{3.32}$$
$$I_{4n} := (\boldsymbol{n}_0, \mathbf{C}\boldsymbol{n}_0) = \|\mathbf{F}\boldsymbol{n}_0\| \tag{3.33}$$

shall be used here. From the assumption that the basis $\{\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0\}$ is orthonormal, we conclude that

$$\sum_{i\in\{f,s,n\}} I_{4i} = \mathbf{C} : (\boldsymbol{f}_0 \otimes \boldsymbol{f}_0 + \boldsymbol{s}_0 \otimes \boldsymbol{s}_0 + \boldsymbol{n}_0 \otimes \boldsymbol{n}_0) = \mathbf{C} : \mathbf{I} = I_1.$$

Thus, only three of the invariants $I_1, I_{4f}, I_{4s}, I_{4n}$ are independent and we can eliminate one. In [32], the invariant $I_{4n}$ is chosen to be eliminated. We might also introduce the invariants associated with $\mathbf{C}^2$ as indicated above, however, following [32, 45], we cancel these invariants and just introduce the orthotropic invariants

$$I_{8,fs} = I_{8,sf} := (\boldsymbol{f}_0, \mathbf{C}\boldsymbol{s}_0),$$
$$I_{8,fn} = I_{8,nf} := (\boldsymbol{f}_0, \mathbf{C}\boldsymbol{n}_0),$$
$$I_{8,sn} = I_{8,ns} := (\boldsymbol{s}_0, \mathbf{C}\boldsymbol{n}_0).$$

The symmetry of the above defined invariants follows from the symmetry of $\mathbf{C}$. Again, following [32], it can be shown from experimental results that one may omit the dependence on the invariants $I_2$, $I_{8sn}$ and $I_{8fn}$. Furthermore, we assume the material to be incompressible, thus the dependence on $I_3$ cancels out too. Therefore we now assume that the strain energy function is of the form

$$W(\mathbf{C}) = W_{\text{iso}}(I_1(\mathbf{C})) + W_{\text{aniso}}(I_{4f}(\mathbf{C}), I_{4s}(\mathbf{C}), I_{8,fs}(\mathbf{C})).$$

From this we determine the abstract structure of the Cauchy stress $\boldsymbol{\sigma}$ and the nominal stress $\mathbf{S}$. Before doing so we need to have some information about the derivatives with respect to $\mathbf{F}$. By using the chain rule and bearing in mind that we need to account for the incompressibility we obtain

$$\mathbf{S} = W_1 \frac{\partial}{\partial \mathbf{F}} I_1 - p\mathbf{F}^{-1} + W_{4f} \frac{\partial}{\partial \mathbf{F}} I_{4f} + W_{4s} \frac{\partial}{\partial \mathbf{F}} I_{4s} + W_{8fs} \frac{\partial}{\partial \mathbf{F}} I_{8fs},$$

with the notation $W_\alpha = \frac{\partial}{\partial I_\alpha} W$, the partial derivative with respect to the invariant $I_\alpha$. At this point we carry out the differentiations $\frac{\partial}{\partial \mathbf{F}} I_\alpha$. However, the exact differentiation is not of interest for this thesis and we just state the results. The proofs may be found in [31, 55]. It holds

$$\begin{aligned}
&\frac{\partial}{\partial \mathbf{F}} I_1(\mathbf{C}) = 2\mathbf{F}^\top, \\
&\frac{\partial}{\partial \mathbf{F}} I_{4\kappa}(\mathbf{C}) = 2\boldsymbol{\kappa}_0 \otimes \boldsymbol{\kappa}_0, && \kappa \in \{f, s\}, \\
&\frac{\partial}{\partial \mathbf{F}} I_{8fs}(\mathbf{C}) = \boldsymbol{f}_0 \otimes \boldsymbol{s}_0 + \boldsymbol{s}_0 \otimes \boldsymbol{f}_0.
\end{aligned}$$

It follows that

$$\mathbf{S} = 2W_1\mathbf{F}^\top - p\mathbf{F}^{-1} + 2W_{4f}\boldsymbol{f}_0 \otimes \boldsymbol{f}_0 + 2W_{4s}\boldsymbol{s}_0 \otimes \boldsymbol{s}_0 + W_{8fs}\left(\boldsymbol{f}_0 \otimes \boldsymbol{s}_0 + \boldsymbol{s}_0 \otimes \boldsymbol{f}_0\right).$$

For the Cauchy stress we multiply from left with $\mathbf{F}$ and use the fact that $\mathbf{F}(\boldsymbol{a} \otimes \boldsymbol{b}) = \mathbf{F}\boldsymbol{a} \otimes \mathbf{F}\boldsymbol{b}$, see [31, p. 267]. Then we obtain for the Cauchy stress

$$\boldsymbol{\sigma} = 2W_1\mathbf{b} - p\mathbf{I} + 2W_{4f}\boldsymbol{f} \otimes \boldsymbol{f} + 2W_{4s}\boldsymbol{s} \otimes \boldsymbol{s} + W_{8fs}\left(\boldsymbol{f} \otimes \boldsymbol{s} + \boldsymbol{s} \otimes \boldsymbol{f}\right),$$

with $\boldsymbol{f} = \mathbf{F}\boldsymbol{f}_0, \boldsymbol{s} = \mathbf{F}\boldsymbol{s}_0$. As indicated in Section 3.4.1, the invariant $I_{8fs}$ changes its sign if either one of the vectors $\boldsymbol{f}_0, \boldsymbol{s}_0$ is reversed by the deformation tensor $\mathbf{F}$. To overcome this inconvenience, we change the dependence from $I_8$ to $I_8^2$. Further, we need some restrictions on the strain energy function $W$. To this end we consider the reference configuration where $\mathbf{F} = \mathbf{I}$. When assuming no residual stresses to be present we obtain

$$\mathbf{0} = 2(W_1 - p_0)\mathbf{I} + 2W_{4f}\boldsymbol{f}_0 \otimes \boldsymbol{f}_0 + 2W_{4s}\boldsymbol{s}_0 \otimes \boldsymbol{s}_0 + W_{8fs}\left(\boldsymbol{f}_0 \otimes \boldsymbol{s}_0 + \boldsymbol{s}_0 \otimes \boldsymbol{f}_0\right),$$

where $p_0$ is the value of the hydrostatic pressure in the reference configuration. This requires

$$\begin{aligned} W_1 - p_0 &= 0, \\ W_{4f} = W_{4s} = W_{8fs} &= 0 \end{aligned}$$

in the reference configuration. These results together with the information taken from [19] motivates the introduction of the following exponential ansatz for $W$:

$$\begin{aligned} W(\mathbf{C}) := \frac{a}{2b}\exp\left(b(I_1(\mathbf{C})-3)\right) + \sum_{i=f,s}\frac{a_i}{2b_i}\left(\exp\left(b_i(I_{4i}(\mathbf{C})-1)^2\right)-1\right) \\ + \frac{a_{fs}}{2b_{fs}}\left(\exp\left(b_{fs}I_{8fs}(\mathbf{C})^2\right)-1\right). \end{aligned} \tag{3.34}$$

The values for the parameters $a, a_f, a_s, a_{fs}, b, b_f, b_s, b_{fs}$ are found in Table 3.1.

| Parameter | Value |
|---|---|
| $a$ | 0.059 kPa |
| $a_f$ | 18.472 kPa |
| $a_s$ | 2.481 kPa |
| $a_{fs}$ | 0.216 kPa |
| $b$ | 8.023 |
| $b_f$ | 16.026 |
| $b_s$ | 11.120 |
| $b_{fs}$ | 11.436 |

**Table 3.1** – Values of the parameters $a, a_f, a_s, a_{fs}, b, b_f, b_s, b_{fs}$ as used for the Holzapfel model. The values are taken from [32].

It remains to give the representation for the nominal stress $\mathbf{S}$ and the Cauchy stress $\boldsymbol{\sigma}$. Bearing in mind that the dependence of the invariant $I_{8fs}$ has been changed to $I_{8fs}^2$ and carrying out the differentiation we obtain for the nominal stress

$$\begin{aligned} \mathbf{S} = a\exp(b(I_1-3))\mathbf{F}^\top - p\mathbf{F}^{-1} + 2a_f(I_{4f}-1)\exp(b_f(I_{4f}-1)^2)\boldsymbol{f}_0\otimes\boldsymbol{f}_0 \\ + 2a_s(I_{4s}-1)\exp(b_s(I_{4s}-1)^2)\boldsymbol{s}_0\otimes\boldsymbol{s}_0 \\ + a_{fs}I_{8fs}\exp(b_{fs}I_{8fs}^2)(\boldsymbol{f}_0\otimes\boldsymbol{s}_0 + \boldsymbol{s}_0\otimes\boldsymbol{f}_0) \end{aligned} \tag{3.35}$$

and similar, as indicated above, for the Cauchy stress

$$\begin{aligned} \boldsymbol{\sigma} = a\exp(b(I_1-3))\mathbf{b} - p\mathbf{I} + 2a_f(I_{4f}-1)\exp(b_f(I_{4f}-1)^2)\boldsymbol{f}\otimes\boldsymbol{f} \\ + 2a_s(I_{4s}-1)\exp(b_s(I_{4s}-1)^2)\boldsymbol{s}\otimes\boldsymbol{s} \\ + a_{fs}I_{8fs}\exp(b_{fs}I_{8fs}^2)(\boldsymbol{f}\otimes\boldsymbol{s} + \boldsymbol{s}\otimes\boldsymbol{f}). \end{aligned} \tag{3.36}$$

## 3.5 Summary

Summarizing we have arrived giving a full description of the activities of the passive myocardium. The governing equations are set by Euler's equations of motion with suitable boundary and initial conditions and read, in material coordinates: Find $(\boldsymbol{U}(\boldsymbol{X},t), p(\boldsymbol{X},t))$ such that

$$\begin{aligned}
\operatorname{Div}\mathbf{S}(\boldsymbol{U}) - \operatorname{Div}(p\mathbf{F}^{-\top}) + \rho_r \boldsymbol{b} &= \rho_r \frac{\partial^2}{\partial t^2}\boldsymbol{U} && \text{in } \Omega_r \times (0,T), && (3.37)\\
\det \mathbf{F} &= 1 && \text{in } \Omega_r \times (0,T), && (3.38)\\
\boldsymbol{U} &= \tilde{\boldsymbol{g}}_D(\boldsymbol{X},t) && \text{on } \Gamma_{D,r} \times (0,T), && (3.39)\\
\mathbf{S}^{\top}\boldsymbol{N} &= \tilde{\boldsymbol{g}}_N(\boldsymbol{X},t) && \text{on } \Gamma_{N,r} \times (0,T), && (3.40)\\
\boldsymbol{U}(\boldsymbol{X},0) &= \mathbf{0} && \text{in } \Omega_r, && (3.41)\\
\boldsymbol{V}(\boldsymbol{X},0) &= \boldsymbol{V}_0 && \text{in } \Omega_r, && (3.42)
\end{aligned}$$

for a given time interval $(0,T)$. Similarly we can state the equations in Eulerian coordinates reading: Find $\boldsymbol{u}(\boldsymbol{x},t), p(\boldsymbol{x},t)$ such that

$$\begin{aligned}
\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{u}) - \operatorname{grad} p + \rho\boldsymbol{b} &= \rho\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{u} && \text{in } \Omega_t \times (0,T),\\
\operatorname{div}\boldsymbol{u} &= 0 && \text{in } \Omega_t \times (0,T),\\
\boldsymbol{u} &= \boldsymbol{g}_D(\boldsymbol{x},t) && \text{on } \Gamma_D \times (0,T),\\
\boldsymbol{\sigma}\boldsymbol{n} &= \boldsymbol{g}_N(\boldsymbol{x},t) && \text{on } \Gamma_N \times (0,T),\\
\boldsymbol{u}(\boldsymbol{x},0) &= 0 && \text{in } \Omega_t\big|_{t=0} = \Omega_r,\\
\boldsymbol{v}(\boldsymbol{x},0) &= \boldsymbol{v}_0 && \text{in } \Omega_t\big|_{t=0} = \Omega_r
\end{aligned}$$

holds, where we need to enforce incompressibility by setting $J = \det\mathbf{F} = 1$ or $\operatorname{div}\boldsymbol{u} = 0$ as shown in (3.25), and furthermore, the shape of the nominal stress tensor is characterized by the Holzapfel model (3.35).

# 4 Coupling of the Electro–Chemical and Mechanical Models

In this chapter we will merge the presented models for the electric and mechanic response of the human heart. This leads us to a coupled multi-physics problem. There are different approaches to couple the electric and mechanic response in the human heart, hence we try to give a summary on the models known in literature, see [23, 52, 59, 83] and the bibliography found in these articles for more details.

## 4.1 Coupling of the Bi-Domain Model with the Deformation

We start with deriving the coupled bi-domain equations. To this end, recall the respective equations in (2.35)–(2.37). As a matter of fact, we have a moving body in the coupled setting. Thus we first need to specify the material and spatial description of these equations. We consider the time derivative $\frac{\partial}{\partial t} u_{\mathrm{tm}}$ as material time derivative. Let us turn our attention to the divergence terms. We will demonstrate the results for one specific integral so the other terms can be treated in analogy. The divergence in the bi-domain model is to be understood in spatial description, thus we may integrate it over the current configuration $\Omega_t$. Doing so we obtain

$$\int_{\Omega_t} \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) \; \mathrm{d}\boldsymbol{x} \,.$$

By applying Gauss' theorem we conclude

$$\int_{\Omega_t} \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) \; \mathrm{d}\boldsymbol{x} = \int_{\partial\Omega_t} (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}, \boldsymbol{n}) \; ds_{\boldsymbol{x}}.$$

The integral on the right hand side can now be transformed into the reference configuration by using Nanson's formula (3.3), hence we arrive at

$$\int_{\partial\Omega_t} (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}, \boldsymbol{n}) \; ds_{\boldsymbol{x}} = \int_{\partial\Omega_r} \left(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}, J\mathbf{F}^{-\top}\boldsymbol{N}\right) \; ds_{\boldsymbol{X}}.$$

Next, by using the transformation rules from Lemma 3.2 we get

$$\int_{\partial\Omega_r} \left(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}, J\mathbf{F}^{-\top}\boldsymbol{N}\right) \; ds_{\boldsymbol{X}} = \int_{\partial\Omega_r} \left(\mathbf{M}_i\mathbf{F}^{-\top} \operatorname{Grad} u_{\mathrm{tm}}, J\mathbf{F}^{-\top}\boldsymbol{N}\right) \; ds_{\boldsymbol{X}},$$

which can be rewritten as

$$\int_{\partial\Omega_r} J\Big(\mathbf{F}^{-1}\mathbf{M}_i\mathbf{F}^{-\top}\operatorname{Grad} u_{\mathrm{tm}}, \boldsymbol{N}\Big)\, ds_{\boldsymbol{X}}. \tag{4.1}$$

In literature, see [49, 59], the term $\mathbf{F}^{-1}\mathbf{M}_i\mathbf{F}^{-\top}$ is replaced by $\mathbf{M}_i\mathbf{C}^{-1}$ or just replaced by $\mathbf{M}_i$. This may not be justified mathematically unless one assumes that $\boldsymbol{n}$ is an eigenvector of $\mathbf{M}_{\{i,e\}}$. However, there is a quite vivid way to argue this procedure, following [71]. Let us assume a regular heart activity, without any fluttering. Then we can argue as follows: A myocyte will contract *after* the action potential has passed. From the shape of the action potential of ventricular cells we know that the gradients of $u_{\mathrm{tm}}$ and $u_e$ are very steep in the moment of activating the cell, but nearly vanishing afterwards, when the cell contracts. Thus, the mechanic reaction of the cell does not change much during the development of the transmembrane or extracellular potential. However, with the period of the action potential being smaller than the time the heart cell needs to contract and relax, the deformation *does* affect the electric signal processing, as it has been shown numerically in [59]. Summarizing we can say that, physiologically speaking, we need to consider time delays in the coupling of the mechanical and electrical behavior. At this point we will not go into details any further, and leave this point open. We now go back to (4.1). Due to the lack of a mathematical proof we may not use the formulations found in literature but better stick to the original term $\mathbf{F}^{-1}\mathbf{M}_i\mathbf{F}^{-\top}$. Following [31, p.82ff], we define this operation as *pull-pack operation*, denoted by $\boldsymbol{\chi}_*^{-1}(\mathbf{M}_i)$. This special operation transforms quantities defined in the current configuration to the reference configuration. Thus we obtain

$$\int_{\partial\Omega_r} J\Big(\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_{\mathrm{tm}}, \boldsymbol{N}\Big)\, ds_{\boldsymbol{X}} = \int_{\Omega_r} \operatorname{Div}(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_{\mathrm{tm}})\ \mathrm{d}\boldsymbol{X}\,.$$

The procedure shown above can be carried out for all divergence terms occurring in the bi-domain model. Assuming continuous integrands we arrive at the strong formulation of the coupled bi-domain model which reads:

$$\begin{aligned}\chi C_m\frac{\partial}{\partial t}u_{\mathrm{tm}} + \chi I_{\mathrm{ion}} - J^{-1}\operatorname{Div}(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_{\mathrm{tm}}) \\ - J^{-1}\operatorname{Div}(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_e) = S_i,\end{aligned}$$

$$J^{-1}\operatorname{Div}(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_{\mathrm{tm}}) + J^{-1}\operatorname{Div}(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}+\mathbf{M_e}\right)\operatorname{Grad} u_e) = -(S_i+S_e),$$

in $\Omega_r\times(0,T]$ where $S_k := s_k(\boldsymbol{\chi}(\boldsymbol{X},t),t)$ and $k=i,e$. To complete the set of equations we need to transform the boundary conditions into material coordinates. That means,

$$\begin{aligned}\Big(J\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_e}\right)\operatorname{Grad} u_e, \boldsymbol{N}\Big) &= G_{N,e},\\ \Big(J(\boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_{\mathrm{tm}} + \boldsymbol{\chi}_*^{-1}\left(\mathbf{M_i}\right)\operatorname{Grad} u_e), \boldsymbol{N}\Big) &= G_{N,i},\end{aligned}$$

where $G_{N,e}, G_{N,i}$ are appropriate functions in the reference configuration, defined as $G_{N,k} := g_{N,k}(\boldsymbol{\chi}(\boldsymbol{X}, t), t)$ and $k = i, e$ with the Neumann data from (2.38)–(2.39). In combination with the incompressibility assumption $J = 1$ we get the final coupled model

$$\chi C_m \frac{\partial}{\partial t} u_{\mathrm{tm}} + \chi I_{\mathrm{ion}} - \mathrm{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \,\mathrm{Grad}\, u_{\mathrm{tm}}) - \mathrm{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \,\mathrm{Grad}\, u_e) = S_i, \quad (4.2)$$

$$\mathrm{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \,\mathrm{Grad}\, u_{\mathrm{tm}}) + \mathrm{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i} + \mathbf{M_e}) \,\mathrm{Grad}\, u_e) = -(S_i + S_e), \quad (4.3)$$

in $\Omega_r \times (0, T]$ and the boundary conditions

$$\left(\boldsymbol{\chi}_*^{-1}(\mathbf{M_e}) \,\mathrm{Grad}\, u_e, \boldsymbol{N}\right) = G_{N,e} \qquad \text{on } \partial\Omega_r \times (0, T], \quad (4.4)$$

$$\left(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \,\mathrm{Grad}\, u_{\mathrm{tm}} + \boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \,\mathrm{Grad}\, u_e, \boldsymbol{N}\right) = G_{N,i} \qquad \text{on } \partial\Omega_r \times (0, T]. \quad (4.5)$$

Finally, we need to impose a solvability condition reading as

$$\int_{\Omega_r} (S_i + S_e) \; \mathrm{d}\boldsymbol{X} + \int_{\partial\Omega_r} (G_{N,e} + G_{N,i}) \; ds_{\boldsymbol{X}} = 0. \quad (4.6)$$

There is another coupling procedure, involving the deformation, in the model of ionic currents. However, we postpone this discussion for after describing the coupling with the mechanic field.

## 4.2 Coupling the Equations of Motion

In this part of the thesis we describe how the electric activation of the human heart influences its mechanical behavior. The incorporation of the human heart's electric activation is done by adjusting the strain energy function in a suitable way. In the literature, see [48, 53, 72], we find two ways of doing this, known as the *active strain formulation* and the *active stress formulation*. The latter appearing to be a special case of the first one, as we will see.

### 4.2.1 The Active Stress and the Active Strain Formulation

As discussed in Chapter 1, myocytes have the ability to contract and relax at rather high frequencies following the beat of the human heart. The contraction and relaxation of smooth muscles influence the distribution of stress and strain in the vascular wall, see [20, 26, 33] for details. In Chapter 3 we introduced the constitutive model by Holzapfel. However, this model is a pure *passive* one. That means, it covers just the

passive mechanic response of the human heart due to its stretching, but does not account for induced changes in the electrical behavior and vice versa. This second response is referred to as *active response* because the muscle fibers do *actively* respond to changes in the electric behavior.

The excitation-contraction coupling, short ECC, in cardiac muscular fibers is a complex mechanism involving many variables such as the trans-membrane potential, ionic conductance, intracellular calcium concentration, membrane strain and stress, and changes in the rest length of muscle fibers due to the interaction of actin and myosin. The specification of a realistic comprehensive model able to account for the principal mechanisms involved in ECC, yet simple enough to be practical, is an arduous task. However, this lies far beyond the scope of this thesis and we may refer to [71] for details. Thus we need to combine the macroscopic constitutive passive mechanical models with the microscopic active ones. The aforementioned microscopic models are referenced in [11, 50, 57, 60].

To cut things short, the key concept found in literature is the following: at the macroscopic level, the presence of muscle fibers enters the model as tension generated by the fibers themselves, which is then called the *active stress*. In addition, this tension has a preferred direction, which is defined by the orientation of the fiber. In case that excitable soft tissues, or the ventricular myocardium, are considered as a whole, the overall tension state is described by adding up the passive and the active stress. This essentially means that we can split up the strain energy function used in the equations of motion into an active and an passive part, i.e. $W(\mathbf{C}) = W_{\text{pass}}(\mathbf{C}) + W_{\text{act}}(\mathbf{C}, \boldsymbol{w})$, with $\boldsymbol{w}$ being a vector of other physiologically relevant dependent variables to be defined later on. This formulation is broadly accepted and widely used in [23, 52, 59, 83].

Contrasting to that, there is the idea of the active strain formulation introduced in [48] where one rather uses a multiplicative decomposition of the deformation gradient $\mathbf{F}$ into a visible elastic part $\mathbf{F}_e$ and an active part $\mathbf{F}_a$. The active part is then again assumed to be of the form $\mathbf{F}_a = \gamma_f \boldsymbol{f}_0 \otimes \boldsymbol{f}_0 + \gamma_s \boldsymbol{s}_0 \otimes \boldsymbol{s}_0 + \gamma_n \boldsymbol{n}_0 \otimes \boldsymbol{n}_0$, where $\gamma_f, \gamma_s, \gamma_n$ are scalar fields which account for the electro-physiology and therefore we need to state evolution equations for each of those fields similar to the models for the ionic current $I_{\text{ion}}$ as described in Section 2.2.4.

In [48] it is further shown that the active stress formulation is a special case of the active strain formulation, when assuming small deformations of the myocytes. Therefore, we keep with the majority of authors and use henceforth the active stress formulation. For a deeper discussion the reader may again refer to [48].

According to results shown in [83], the term $\rho\ddot{\boldsymbol{x}}$ in the equations of motion is of practically negligible order, so we use the so-called *quasi-static* equations of motion

which read as

$$\mathrm{Div}\left(\mathbf{T}\mathbf{F}^{\top}\right) = 0 \qquad \text{in } \Omega_r$$

where we have rewritten the equation using the so-called *second Piola-Kirchhoff stress tensor* $\mathbf{T}$ defined by $\mathbf{T} := J\boldsymbol{\chi}_*^{-1}(\boldsymbol{\sigma})$, see [55] for more details. This formulation responds to the convenient notation used in literature about the electromechanical coupling. One should, however, bear in mind, that the tensor $\mathbf{T}$ does not admit a physical interpretation, see [55]. In this setting we can write the stress-strain relation, see [31], as

$$\mathbf{T} = 2\frac{\partial W(\mathbf{C})}{\partial \mathbf{C}} - p\mathbf{C}^{-1}$$

with the term $p\mathbf{C}^{-1}$ to enforce incompressibility. Unlike in Chapter 3 we do not specify a shape of the strain energy function to be able to cover the more general case of other strain energy functions than the Holzapfel model. Following [83] we adjust the strain tensor by

$$(\mathbf{T}^*)_{MN} = 2\frac{\partial W(\mathbf{C}*)}{\partial C^*_{MN}} - pC^{*^{-1}}_{MN} + T_a\delta_{Mf}\delta_{Nf}C^{*^{-1}}_{MN},$$

where we have used the "*"-notation introduced in Section 2.2.4 to express the tensors with respect to the basis $\{\boldsymbol{f}_0, \boldsymbol{s}_0, \boldsymbol{n}_0\}$. The term $T_a$ is a scalar function which generates the active tension and will be discussed in more detail later. The term $\delta_{Mf}\delta_{Nf}$ is added to enforce the active tension to work only in the direction of the muscle fibers. This has turned out to be a quite useful assumption, see [66, 73, 80] for details. The question remains of how to model the active tension term $T_a$. From physiology it is known, that the active tension depends on the stretch in the direction of the fiber $\lambda_f$ which is defined by $\lambda_f := \sqrt{C^*_{ff}}$. Furthermore, the active tension highly depends on the inner calcium concentration, $[\mathrm{Ca}^{2+}]_i$, in the muscle cells. The authors of [59] propose the following abstract structure to model the active tension $T_a$:

$$\begin{aligned}\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} &= \boldsymbol{g}\left(\boldsymbol{w}, \lambda_f, \dot{\lambda}_f, [\mathrm{Ca}^{2+}]_i\right),\\ T_a &= h(\boldsymbol{w}),\end{aligned}$$

with $\boldsymbol{g}, h$ being some given non-linear functions. We will not focus on specific models in this thesis, however, we cite two possibilities to model the active tension. The first one can be found in [49] and an updated version in [23]. There, a purely phenomenological model is used to describe the evolution of the active tension. The second one is a high level physiological model developed in [51] and used for example in [59]. The second approach couples the models for the Ionic current $I_{\mathrm{ion}}$ with the deformation model by introducing a new set of dependent variables collected in the vector $\boldsymbol{a}$ which stands for various length-dependent biochemical quantities. Thus we obtain the following

new abstract model for the ionic current $I_{\text{ion}}$:

$$I_{\text{ion}} = g(t, u_{\text{tm}}, \boldsymbol{v}, \boldsymbol{a}),$$
$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{v}, u_{\text{tm}}, \boldsymbol{a}, t).$$

We will use this formulation because it covers even the most general case. For a collection of various models for the generation of active tension one can look up in the CellML repository mentioned in Section 2.2.4.

## 4.3 Summary of the Fully Coupled Electromechanical Model

In this chapter we have merged the two different models for the electrical activation and the mechanical reaction of the human heart. As a result we obtain a fully coupled system of partial differential equations under the incompressibility assumption which reads as: Find $(u_{\text{tm}}, u_e, \boldsymbol{U}, \boldsymbol{v}, \boldsymbol{w}, p)$ such that

$$\chi C_m \frac{\partial}{\partial t} u_{\text{tm}} + \chi I_{\text{ion}} - \operatorname{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \operatorname{Grad} u_{\text{tm}}) - \operatorname{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \operatorname{Grad} u_e) = -S_i, \quad (4.7)$$
$$\operatorname{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \operatorname{Grad} u_{\text{tm}}) + \operatorname{Div}(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i} + \mathbf{M_e}) \operatorname{Grad} u_e) = -(S_i + S_e), \quad (4.8)$$
$$\operatorname{Div}\left(\mathbf{T}\mathbf{F}^{\top}\right) - \operatorname{Div}(p\mathbf{F}^{-\top}) = 0, \quad (4.9)$$
$$\det \mathbf{F} = 1, \quad (4.10)$$

in $\Omega_r \times (0, T]$, with boundary conditions

$$\left(\boldsymbol{\chi}_*^{-1}(\mathbf{M_e}) \operatorname{Grad} u_e, \boldsymbol{N}\right) = G_{N,e} \quad \text{on } \partial\Omega_r \times (0, T], \quad (4.11)$$
$$\left(\boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \operatorname{Grad} u_{\text{tm}} + \boldsymbol{\chi}_*^{-1}(\mathbf{M_i}) \operatorname{Grad} u_e, \boldsymbol{N}\right) = G_{N.i} \quad \text{on } \partial\Omega_r \times (0, T], \quad (4.12)$$
$$\boldsymbol{U} = \boldsymbol{g}_D \quad \text{on } \Gamma_{D,r} \times (0, T], \quad (4.13)$$
$$\mathbf{F}\mathbf{T}\boldsymbol{N} = \boldsymbol{g}_N \quad \text{on } \Gamma_{N,r} \times (0, T], \quad (4.14)$$
$$u_{\text{tm}}(\boldsymbol{X}, 0) = u_{\text{tm},0}(\boldsymbol{X}), \quad (4.15)$$
$$u_e(\boldsymbol{X}, 0) = u_{e,0}(\boldsymbol{X}), \quad (4.16)$$

completed by the constitutive equations reading as

$$(\mathbf{T}^*)_{MN} = 2\frac{\partial W(\mathbf{C}^*)}{\partial C^*_{MN}} - pC^{*^{-1}}_{MN} + T_a\delta_{Mf}\delta_{Nf}C^{*^{-1}}_{MN}, \tag{4.17}$$

$$I_{\text{ion}} = g(t, u_{\text{tm}}, \boldsymbol{v}, \boldsymbol{a}), \tag{4.18}$$

$$T_a = h(\boldsymbol{w}), \tag{4.19}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{w} = \boldsymbol{g}\left(\boldsymbol{w}, \lambda_f, \dot{\lambda}_f, [\mathrm{Ca}^{2+}]_i\right), \tag{4.20}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{v} = \boldsymbol{f}(\boldsymbol{v}, u_{\text{tm}}, \boldsymbol{a}, t), \tag{4.21}$$

$$\boldsymbol{v}(t=0) = \boldsymbol{v}_0, \tag{4.22}$$

$$\boldsymbol{w}(t=0) = \boldsymbol{w}_0, \tag{4.23}$$

and the values for $\mathbf{M}_i, \mathbf{M}_e, \chi, C_m$ to be found in Table 2.1.

# 5 Analysis

In this final chapter we will discuss the possibilities of a mathematical analysis, in terms of weak solutions. As mentioned in the introduction, we will focus on the analysis of the uncoupled problems and discuss their solvability. It is assumed that the reader is familiar with functional analysis and some basic concepts of measure theory. For more details on functional analysis one should refer to [21, 75, 82, 85–90].

## 5.1 Notation and Definitions

Before starting with the mathematical analysis we need to introduce the standard notations.

### Elliptic, Compact and Self-Adjoint Operators

**Definition 5.1** (Duality Pairing)**.** *Let $X$ be a Banach space and denote by $X^*$ its dual. Let further $l \in X^*$. We define the* duality pairing *of $l$ with $x \in X$ as*

$$\langle l, x \rangle_{X^* \times X} := l(x).$$

**Remark 5.1.** *To avoid confusion we will use $\langle \cdot, \cdot \rangle_{X^* \times X}$ for the duality pairing and $\langle \cdot, \cdot \rangle_H$ for the inner product provided $H$ is a Hilbert space.*

**Theorem 5.1** (Riesz Representation Theorem)**.** *Let $\mathcal{H}$ be a Hilbert space. A linear functional $f$ on $\mathcal{H}$ belongs to $\mathcal{H}^*$ if and only if there exists a $x \in \mathcal{H}$ such that for every $y \in \mathcal{H}$ we have*

$$f(y) = \langle y, x \rangle_{\mathcal{H}^* \times \mathcal{H}},$$

*and in this case $\|f\|_{\mathcal{H}^*} = \|x\|_{\mathcal{H}}$. Moreover, $x$ is uniquely determined by $f \in \mathcal{H}^*$.*

*Proof.* See [1, Theorem 1.12]. □

**Remark 5.2.** *The previous theorem guarantees the existence of the* Riesz-isomorphism *$\mathcal{J} \colon \mathcal{H}^* \to \mathcal{H}$ such that*

$$\begin{aligned} \langle \mathcal{J} f, v \rangle_{\mathcal{H}} &= \langle f, v \rangle_{\mathcal{H}^* \times \mathcal{H}} \qquad \text{for all } v \in \mathcal{H}, \\ \|\mathcal{J} f\|_{\mathcal{H}} &= \|f\|_{\mathcal{H}^*}, \end{aligned}$$

*meaning that we can always identify elements in $\mathcal{H}^*$ with elements in $\mathcal{H}$.*

**Definition 5.2** (Elliptic Operator)**.** *A linear operator $A$ mapping from a Hilbert space $\mathcal{H}$ into its dual $\mathcal{H}^*$ is called* $\mathcal{H}$-elliptic*, if there exists a positive constant $c_1^A$ such that*

$$\Re\langle Av, v\rangle_{\mathcal{H}^*\times\mathcal{H}} \geq c_1^A \|v\|_{\mathcal{H}}^2$$

*holds for all $v \in \mathcal{H}$.*

**Definition 5.3** (Adjoint, Self-adjointness)**.** *Let $A\colon X \to Y$ be a bounded linear operator between Hilbert spaces. Then the operator $A^*\colon Y^* \to X^*$ defined by*

$$\langle x, A^*y\rangle_{X\times X^*} = \langle Ax, y\rangle_{Y\times Y^*}, \qquad \text{for all } x \in X,\ y \in Y^*$$

*is called the* adjoint *of $A$. If $X = Y$ and $A = A^*$ then $A$ is called* self-adjoint*.*

**Theorem 5.2** (Lemma of Lax-Milgram)**.** *Let $\mathcal{H}$ be a Hilbert space, and $A\colon \mathcal{H} \to \mathcal{H}^*$ be a linear, bounded $\mathcal{H}$-elliptic operator. Then the equation*

$$Au = f$$

*has a unique solution for any $f \in \mathcal{H}^*$ and it holds that*

$$\|u\|_{\mathcal{H}} \leq \frac{1}{c_1^A}\|f\|_{\mathcal{H}^*}$$

*Proof.* See for example [75]. □

**Lemma 5.3.** *Let $A\colon \mathcal{H} \to \mathcal{H}^*$ be a bounded, self-adjoint $\mathcal{H}$-elliptic operator. Then the inverse of $A$, $A^{-1}$ is elliptic.*

*Proof.* See for example [75]. □

**Definition 5.4** (Compact Operator)**.** *Let $X$ and $Y$ be two Banach spaces. A linear operator $K : X \to Y$ is called* compact *if the image of a bounded set $\mathcal{B} \subset X$ is relatively compact. A set is called* relatively compact*, if its closure is compact.*

**Remark 5.3.** *Since we are working in at least Banach spaces we can characterize relatively compact sets equivalently by all those sets which possess a converging subsequence.*

### Banach Space Valued $L^p$ Functions

Proceeding we will introduce the conecept of Banach space valued $L^p$-functions. It is assumed that the reader is familiar with the concept of $L^p(\Omega)$-spaces in general. For details one may refer to [69] The following definition is based on [85, Definition 24.1]:

**Theorem 5.4.** *Let $\mathcal{X}$ be a Banach space and $(0,T) \subset \mathbb{R}^+$ an open measurable interval with $T > 0$. Let further $1 \leq p < \infty$. Define*

$$\|v\|_{L^p((0,T);\mathcal{X})} := \left( \int_0^T \|v(\cdot,t)\|_{\mathcal{X}}^p \ \mathrm{dt} \right)^{\frac{1}{p}}.$$

*Then the space*

$$L^p((0,T);\mathcal{X}) := \left\{ v : (0,T) \to \mathcal{X} \mid \|v\|_{L^p((0,T);\mathcal{X})} < \infty \right\}$$

*defines a Banach space with the norm $\|\cdot\|_{L^p((0,T);\mathcal{X})}$. Furthermore, in the case of $p = \infty$ we can introduce the norm*

$$\|v\|_{L^\infty((0,T);\mathcal{X})} := \operatorname*{ess\,sup}_{t \in (0,T)} \|v\|_{\mathcal{X}}.$$

*Then the above statement remains valid even for $p = \infty$.*

*Proof.* See for example [21, Chapter IV, Theorem 1.11 and Theorem 1.12]. □

For simplicity we abbreviate $L^p((0,T);\mathcal{X})$ by $L^p(0,T;\mathcal{X})$. For the further analysis we also need to know something about the dual spaces of these special $L^p$-spaces. This is covered by:

**Theorem 5.5.** *Let the assumptions of Definition 5.4 hold and assume further that the Banach space $\mathcal{X}$ is reflexive and separable, and that $1 < p < \infty$. Then it holds*

$$(L^p(0,T;\mathcal{X}))^* = L^q(0,T;\mathcal{X}^*)$$

*with $\frac{1}{p} + \frac{1}{q} = 1$.*

*Proof.* See [21, Chapter IV, Theorem 1.14]. □

A very classic concept in connection with these $L^p$-spaces is the *Gelfand triple* or *evolution triple*.

**Definition 5.5.** *Let $\mathcal{X}$ be a separable and reflexive Banach space and $\mathcal{H}$ a separable Hilbert space. Further, let $\mathcal{X}$ be densly embedded in $\mathcal{H}$. Then we call the triple*

$$\mathcal{X} \subset \mathcal{H} \cong \mathcal{H}^* \subset \mathcal{X}^*$$

*a* Gelfand triple *or* evolution triple.

In the analysis of the bi-domain equations we will also need to consider a more generalized version of the Gelfand triple. There we will consider frameworks of the form

$$\mathcal{X} \subset L^p(\Omega) \subset \mathcal{H} \cong \mathcal{H}^* \subset L^{p^*}(\Omega) \subset \mathcal{X}^*.$$

Additionally we will need to use function spaces in the form

$$L^2(0,T;\mathcal{X}) \cap L^p((0,T)\times\Omega).$$

Therefore we will also need the following:

**Theorem 5.6.** *Let $X$ and $Y$ be Banach spaces which are continuously embedded into a locally convex space $V$. Then the following statements hold:*

- *The space $(X \cap Y, \|.\|_{X\cap Y})$ where $\|v\|_{X\cap Y} := \|v\|_X + \|v\|_Y$ is a Banach space.*
- *The space $(X + Y, \|.\|_{X+Y})$ where*

$$\|v\|_{X+Y} := \inf_{\substack{x\in X, y\in Y \\ x+y=v}} \max(\|x\|_X, \|y\|_Y)$$

  *is a Banach space. The direct sum of two spaces $X$ and $Y$ is defined by*

$$X + Y := \{x + y : x \in X \ y \in Y\}.$$

- *Provided $X \cap Y$ is densely embedded in either $X$ or $Y$ with respect to the norm $\|.\|_{X\cap Y}$. Then, $(X \cap Y)^* = X^* + Y^*$ and $(X + Y)^* = X^* \cap Y^*$.*

*Proof.* See [21, Chapter I, Theorem 5.13]. □

## Sobolev spaces

Having defined the $L^p(0,T;\mathcal{X})$ spaces we are getting closer to the framework which will actually be used for the analysis, the *Sobolev spaces*. To this end we need the concept of a weak derivative.

**Definition 5.6.** *Let $\Omega \subseteq \mathbb{R}^3$ and let $m \in \mathbb{N}$ Then we define the following spaces:*

- *$\mathcal{C}^m(\Omega)$ shall be the space of $m$-times continuously differentiable functions mapping from $\Omega$ to either $\mathbb{R}$ or $\mathbb{C}$.*
- *The space of arbitrary continuously differentiable functions*

$$\mathcal{C}^\infty(\Omega) := \bigcap_{m\in\mathbb{N}} \mathcal{C}^m(\Omega).$$

- *The space of arbitrary continuously differentiable functions with compact support,*

$$\mathcal{C}_0^\infty(\Omega) := \{f \in \mathcal{C}_0^\infty(\Omega) \mid \overline{\{\boldsymbol{x} \in \Omega \ : \ f(\boldsymbol{x}) \neq 0\}} \subset \Omega \text{ is compact}\}.$$

**Definition 5.7.** *Let $\Omega \subset \mathbb{R}^3$. Then we define the space $L^1_{loc}(\Omega)$ of locally integrable functions by*

$$L^1_{loc}(\Omega) := \bigcap_{\substack{K \subset \Omega, \\ K \text{ compact}}} L^1(K).$$

**Definition 5.8** (Weak Derivative)**.** *A function $u \in L^1_{loc}(\Omega)$ has a* weak partial derivative *of order $s$, when there exists a function $h \in L^1_{loc}(\Omega)$ such that*

$$\int_\Omega h\phi \ \mathrm{d}\boldsymbol{x} = (-1)^{|s|} \int_\Omega u D^s \phi \ \mathrm{d}\boldsymbol{x} \qquad \text{for all } \phi \in \mathcal{C}_0^\infty(\Omega),$$

*where $s = (s_1, s_2, \ldots, s_n)$ is a multi-index and $D^s := \frac{\partial^{|s|}}{\partial x_1^{s_1} x_2^{s_2} \cdots x_n^{s_n}}$. The function $h$ is usually identified with $D^s u$, when $s$ is a multi-index.*

**Definition 5.9** (Sobolev Norm, Sobolev Space)**.** *Let $\Omega \subseteq \mathbb{R}^d$ and let $k \in \mathbb{N}_0$. Then for $1 \leq p < \infty$ we define the* Sobolev norm $\|\cdot\|_{W^{k,p}(\Omega)}$ *via*

$$\|u\|_{W^{k,p}(\Omega)} := \left( \sum_{|\alpha| \leq k} \|D^\alpha u\|^p_{L^p(\Omega)} \right)^{\frac{1}{p}},$$

*and for the case of $p = \infty$ we define*

$$\|u\|_{W^{k,\infty}(\Omega)} := \max_{|\alpha| \leq k} \|u\|_{L^\infty(\Omega)}.$$

*The* Sobolev space $W^{k,p}(\Omega)$ *is defined by*

$$W^{k,p}(\Omega) := \overline{\mathcal{C}^\infty(\Omega)}^{\|\cdot\|_{W^{k,p}(\Omega)}}.$$

In [1, Theorem 3.3] it is shown, that the space $W^{k,p}(\Omega)$ is a Banach space. Furthermore, it is known, see [1, Theorem 3.17], that we can also write the space $W^{k,p}(\Omega)$ as

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) \ : \ D^\alpha u \in L^p(\Omega) \text{ for } 0 \leq |\alpha| \leq k\}.$$

**Definition 5.10** (Sobolev Spaces with Fractional Order)**.** *Let $s \in \mathbb{R}^+$ with $s = k + \kappa, k \in \mathbb{N}_0$ and $\kappa \in (0, 1)$. Then we define the* Sobolev-Slobodeckii norm

$$\|u\|_{W^{s,p}(\Omega)} := \left( \|u\|^p_{W^{k,p}(\Omega)} + |u|^p_{W^{k,p}(\Omega)} \right)^{\frac{1}{p}},$$

*with the semi-norm*

$$|u|^p_{W^{k,p}(\Omega)} := \sum_{|\alpha|=k} \int_\Omega \int_\Omega \frac{|D^\alpha u(\boldsymbol{x}) - D^\alpha u(\boldsymbol{y})|^p}{|\boldsymbol{x}-\boldsymbol{y}|^{d+p\kappa}} \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}.$$

*The corresponding* Sobolev space *is then defined as*

$$W^{s,p}(\Omega) := \overline{\mathcal{C}^\infty(\Omega)}^{\|\cdot\|_{W^{s,p}(\Omega)}}.$$

**Definition 5.11** (Dual Space of $W^{s,p}(\Omega)$)**.** *Let $s < 0 \in \mathbb{R}$ and $1 < p < \infty$. Then we define the space $W^{s,p}(\Omega)$ via*

$$\widetilde{W}^{s,p}(\Omega) := (W^{-s,q}(\Omega))^*$$

*with $1/p + 1/q = 1$ and the norm*

$$\|u\|_{\widetilde{W}^{s,p}(\Omega)} := \sup_{\substack{v \in W^{-s,q}(\Omega) \\ v \neq 0}} \frac{\left|\langle u, v\rangle_{\widetilde{W}^{s,p}(\Omega)\times W^{-s,q}(\Omega)}\right|}{\|v\|_{W^{-s,q}(\Omega)}}.$$

It is also possible to introduce Sobolev spaces with the help of the Fourier transform, see [44, 75] for details. The spaces introduced this way are then called $H^s(\Omega)$. These Sobolev spaces turn out to be Hilbert spaces and for Lipschitz domains $\Omega$ and $s > 0$ it holds that

$$H^s(\Omega) = W^{s,2}(\Omega)$$

**Remark 5.4.** *We will also use the following notation for the dual spaces:*

$$\widetilde{H}^s(\Omega) := (H^{-s}(\Omega))^* \qquad \text{for } s < 0.$$

**Remark 5.5.** *For the sake of brevity we will hereafter mostly use the notation $\langle\cdot,\cdot\rangle_\Omega$ or $\langle\cdot,\cdot\rangle_{\partial\Omega}$ for denoting the duality pairings in the respective Sobolev spaces in $\Omega$ or on $\partial\Omega$.*

**Definition 5.12** (Trace Operator)**.** *The* trace *of a vector valued function $\boldsymbol{u}$ is defined by*

$$\gamma_0^{int}\boldsymbol{u} := \lim_{\tilde{\boldsymbol{x}} \ni \Omega \to \boldsymbol{x} \in \partial\Omega} \boldsymbol{u}(\tilde{\boldsymbol{x}}).$$

For the later analysis of the system of non-linear elasticity we will use the fact that the trace operator $\gamma_0^{\mathrm{int}}(\cdot)$ considered as an operator between $W^{s,p}(\Omega)$ and $W^{s-1/p,p}(\partial\Omega)$ is continuous and bounded provided $\Omega$ is a Lipschitz domain and $s \in [\frac{1}{p}, 1]$, see [47, Theorem 3.9] for details.

## 5.2 Analysis of the Stationary Equations

We will now turn our attention to the analysis of the decoupled bi-domain equations (2.35)–(2.42). The following part is mainly taken from [9]. As starting point we will reformulate the equations in the following way:

$$\frac{\partial u_{\mathrm{tm}}}{\partial t} + g(u_{\mathrm{tm}}, \boldsymbol{v}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_e) = s_i \tag{5.1}$$

$$- \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e) = s_i + s_e, \tag{5.2}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{f}(u_{\mathrm{tm}}, \boldsymbol{v}) = 0 \tag{5.3}$$

in $\Omega \times (0, T)$, where we have denoted the area occupied by the heart with $\Omega$. We carefully mention that we have

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \boldsymbol{f}(u_{\mathrm{tm}}(\boldsymbol{x}, t), \boldsymbol{v}) = \boldsymbol{f}(\boldsymbol{x}, t).$$

Therefore $\boldsymbol{v}$ will also depend on the position $\boldsymbol{x}$. Therefore we already replaced the ordinary differential by a partial differential in (5.3). For completeness we give again the boundary and initial conditions:

$$\boldsymbol{n} \cdot (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} + \mathbf{M}_i \operatorname{grad} u_e) = g_{N.i} \qquad \text{on } \partial\Omega \times (0, T], \tag{5.4}$$

$$\boldsymbol{n} \cdot (\mathbf{M}_e \operatorname{grad} u_e) = g_{N,e} \qquad \text{on } \partial\Omega \times (0, T], \tag{5.5}$$

$$u_{\mathrm{tm}}(\boldsymbol{x}, 0) = u_{\mathrm{tm}}^0 \qquad \text{in } \Omega, \tag{5.6}$$

$$u_{\mathrm{e}}(\boldsymbol{x}, 0) = u_{\mathrm{e}}^0 \qquad \text{in } \Omega, \tag{5.7}$$

$$\boldsymbol{v}(\boldsymbol{x}, 0) = \boldsymbol{v}_0 \qquad \text{in } \Omega. \tag{5.8}$$

Eventually, we need to enforce the solvability condition:

$$\int_\Omega (s_i + s_e) \ \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} (g_{N,i} + g_{N,e}) \ \mathrm{ds}_{\boldsymbol{x}} = 0.$$

Due to the pure Neumann boundary conditions on $u_e$ we know that $u_e$ will be only uniquely defined up to an constant.

### 5.2.1 The Bi-domain Operator $A_{\mathrm{BD}}$

Before discussing existence and uniqueness of the full bi-domain equations we will analyze a related subproblem. To this end we will, as discussed in [9], consider the subproblem emerging by ignoring the nonlinearities and the time derivatives in the bi-domain equations. This leads to the new classical subproblem

$$- \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_e) = s_i, \tag{5.9}$$

$$- \operatorname{div}(\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}}) - \operatorname{div}((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e) = s_i + s_e, \tag{5.10}$$

which is completed by the boundary conditions

$$\boldsymbol{n} \cdot (\mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} + \mathbf{M}_i \operatorname{grad} u_e) = g_{N.i}, \tag{5.11}$$

$$\boldsymbol{n} \cdot (\mathbf{M}_e \operatorname{grad} u_e) = g_{N,e}. \tag{5.12}$$

At this point we assume knowledge about the analysis of partial differential equations in their weak form. For more details we shall refer to [75]. We multiply the equations (5.9)–(5.10) with suitable test functions $\phi_1, \phi_2$, integrating over $\Omega$, using integration by parts and applying the boundary conditions. This leads to the variational problem: find $(u_{\mathrm{tm}}, u_e) \in V \times V$ such that

$$a_i(u_{\mathrm{tm}}, \phi_1) + a_i(u_e, \phi_1) = \langle s_i, \phi_1 \rangle_\Omega + \left\langle g_{N,i}, \gamma_0^{\mathrm{int}} \phi_1 \right\rangle_{\partial\Omega}, \tag{5.13}$$

$$a_i(u_{\mathrm{tm}}, \phi_2) + a_{i+e}(u_e, \phi_2) = \langle s_i + s_e, \phi_2 \rangle_\Omega + \left\langle g_{N,i} + g_{N,e}, \gamma_0^{\mathrm{int}} \phi_2 \right\rangle_{\partial\Omega}, \tag{5.14}$$

where

$$a_i(u, v) := \int_\Omega (\mathbf{M}_i \operatorname{grad} u) \cdot \operatorname{grad} v \ \mathrm{d}\boldsymbol{x},$$

$$a_{i+e}(u, v) := \int_\Omega ((\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u) \cdot \operatorname{grad} v \ \mathrm{d}\boldsymbol{x}\,.$$

and $\langle \cdot, \cdot \rangle_{\{\Omega, \partial\Omega\}}$ denotes the duality pairing.

In this variational formulation $V$ denotes a suitable Hilbert space. In our analysis we choose the Sobolev space $H^1(\Omega)$ as Hilbert space $V$. This problem can now be treated as a standard Neumann problem in $H^1(\Omega)$ . It is a well-known fact, that the pure Neumann-Problem is not uniquely solvable, as one can add a constant to a solution of the above equation and this would still be a solution. This corresponds to the latter operator formulation of this problem, where the operators have non-trivial kernels. Furthermore, we need to impose a solvability condition, which follows immediately when putting $\phi_1 = \phi_2 = 1$. Then we see that we need to guarantee that

$$\langle s_i, 1 \rangle_\Omega + \langle g_{N,i}, 1 \rangle_{\partial\Omega} = 0, \tag{5.15}$$

$$\langle s_i + s_e, 1 \rangle_\Omega + \langle g_{N,i} + g_{N,e}, 1 \rangle_{\partial\Omega} = 0. \tag{5.16}$$

To circumvent the non-uniqueness of the Neumann-Problem we will work on a factor space of $H^1(\Omega)$ defined by $H^1_*(\Omega) := \{v \in H^1(\Omega) : \int_\Omega v \ \mathrm{d}\boldsymbol{x} = 0\}$. Doing so, we fix the constant part of the solutions. In this setting it would be necessary to search both $u_{\mathrm{tm}}$ and $u_e$ in the factor space $H^1_*(\Omega)$. However, as we will see later it will not be necessary to restrict $u_{\mathrm{tm}}$ to $H^1(\Omega)$. For our purposes as for the numerical treatment of the bi-domain equations, it is quite useful to incorporate this side constraint explicitly in the variational formulation to avoid worrying about constructing the right finite element ansatz spaces for $H^1_*(\Omega)$. The incorporation of the side constraint can now

be accomplished by introducing Lagrange parameters $\lambda, \mu$. This yields the variational problem: Find $(u_{\mathrm{tm}}, u_e, \mu) \in [H^1(\Omega)]^2 \times \mathbb{R}$ such that

$$a_i(u_{\mathrm{tm}}, \phi_1) + a_i(u_e, \phi_1) = \langle s_i, \phi_1 \rangle_\Omega + \left\langle g_{N,i}, \gamma_0^{\mathrm{int}} \phi_1 \right\rangle_{\partial\Omega}, \tag{5.17}$$

$$a_i(u_{\mathrm{tm}}, \phi_2) + a_{i+e}(u_e, \phi_2) + \mu \int_\Omega \phi_2 \ \mathrm{d}\boldsymbol{x} = \langle s_i + s_e, \phi_2 \rangle_\Omega + \left\langle g_{N,i} + g_{N,e}, \gamma_0^{\mathrm{int}} \phi_2 \right\rangle_{\partial\Omega}, \tag{5.18}$$

$$\int_\Omega u_e \ \mathrm{d}\boldsymbol{x} = 0. \tag{5.19}$$

The special choice $\phi_1 = \phi_2 = 1$ and the solvability conditions (5.15)–(5.16) lead to

$$\mu = 0.$$

Thus we can reformulate (5.19) and obtain an equivalent formulation for determining $(u_{\mathrm{tm}}, u_e, \mu) \in [H^1(\Omega)]^2 \times \mathbb{R}$

$$a_i(u_{\mathrm{tm}}, \phi_1) + a_i(u_e, \phi_1) = \langle s_i, \phi_1 \rangle_\Omega + \left\langle g_{N,i}, \gamma_0^{\mathrm{int}} \phi_1 \right\rangle_{\partial\Omega}, \tag{5.20}$$

$$a_i(u_{\mathrm{tm}}, \phi_2) + a_{i+e}(u_e, \phi_2) + \mu \int_\Omega \phi_2 \ \mathrm{d}\boldsymbol{x} = \langle s_i + s_e, \phi_2 \rangle_\Omega + \left\langle g_{N,i} + g_{N,e}, \gamma_0^{\mathrm{int}} \phi_2 \right\rangle_{\partial\Omega}, \tag{5.21}$$

$$\int_\Omega u_e \ \mathrm{d}\boldsymbol{x} - \mu = 0, \tag{5.22}$$

and thus we end up with

$$\mu = \int_\Omega u_e \ \mathrm{d}\boldsymbol{x}\,.$$

Finally we end up with the stabilized subproblem of finding $(u_{\mathrm{tm}}, u_e) \in [H^1(\Omega)]^2$ such that

$$a_i(u_{\mathrm{tm}}, \phi_1) + a_i(u_e, \phi_1) = \langle s_i, \phi_1 \rangle_\Omega + \left\langle g_{N,i}, \gamma_0^{\mathrm{int}} \phi_1 \right\rangle_{\partial\Omega}, \tag{5.23}$$

$$a_i(u_{\mathrm{tm}}, \phi_2) + a_{i+e}(u_e, \phi_2) + \int_\Omega u_e \ \mathrm{d}\boldsymbol{x} \int_\Omega \phi_2 \ \mathrm{d}\boldsymbol{x} = \langle s_i + s_e, \phi_2 \rangle_\Omega + \left\langle g_{N,i} + g_{N,e}, \gamma_0^{\mathrm{int}} \phi_2 \right\rangle_{\partial\Omega}. \tag{5.24}$$

Following [75] we can now reformulate this variational formulation as an equivalent operator equation.

To this end we define the operators $\tilde{A}_{i+e}, \tilde{A}_i, A_i$ for $(u,v) \in H^1(\Omega) \times H^1(\Omega)$ via

$$\begin{aligned} \left\langle \widetilde{A}_{i+e} u, v \right\rangle_\Omega &:= a_{i+e}(u,v) + \int_\Omega u \ \mathrm{d}\boldsymbol{x} \int_\Omega v \ \mathrm{d}\boldsymbol{x}, \\ \langle A_i u, v \rangle_\Omega &:= a_i(u,v). \end{aligned} \tag{5.25}$$

From this definition we can immediately see the mapping properties of the operators:

$$\begin{aligned} \widetilde{A}_{i+e} &\colon H^1(\Omega) \to \widetilde{H}^{-1}(\Omega), \\ A_i &\colon H^1(\Omega) \to \widetilde{H}^{-1}(\Omega). \end{aligned}$$

Thus we can now state the equivalent operator equation in $\widetilde{H}^{-1}(\Omega)$ reading as

$$\begin{aligned} A_i u_{\mathrm{tm}} + A_i u_e &= F_1, \\ A_i u_{\mathrm{tm}} + \widetilde{A}_{i+e} u_e &= F_2, \end{aligned}$$

where $F_1, F_2$ stand for the right hand sides in the variational formulation (5.23) in the sense that for $\phi, \psi \in H^1(\Omega)$ it holds that

$$\begin{aligned} \langle F_1, \phi \rangle_\Omega &:= \langle s_i, \phi \rangle_\Omega + \left\langle g_{N,i}, \gamma_0^{\mathrm{int}} \phi \right\rangle_{\partial\Omega}, \\ \langle F_2, \psi \rangle_\Omega &:= \langle s_i + s_e, \psi \rangle_\Omega + \left\langle g_{N,i} + g_{N,e}, \gamma_0^{\mathrm{int}} \psi \right\rangle_{\partial\Omega}. \end{aligned}$$

We will try to eliminate the variable $u_e$ and thus end up with a single equation, the so-called *Schur complement system*. However, before we can do this we must prove that the stabilized operator $\widetilde{A}_{i+e}$ is invertible. This is stated by the following:

**Lemma 5.7.** *Assume that the coefficient tensors $\mathbf{M}_{\{i,e\}}$ have $L^\infty(\Omega)$ components and satisfy the condition*

$$m \left|\boldsymbol{\xi}\right|^2 \leq \left(\mathbf{M}_{\{i,e\}}(\boldsymbol{x})\boldsymbol{\xi}, \boldsymbol{\xi}\right) \leq M \left|\boldsymbol{\xi}\right|^2, \quad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^3 \text{ and almost every } \boldsymbol{x} \in \Omega$$

*independent of the chosen basis for $\mathbf{M}_{\{i,e\}}$. Then the operator $\widetilde{A}_{i+e}$ is bounded and $H^1(\Omega)$-elliptic.*

*Proof.* We will first show the boundedness of the bilinear-form. Using the assumptions on $\mathbf{M}_{\{i,e\}}$ and the Cauchy-Schwarz inequality, see [82, Theorem I.1.10], in (5.25) we obtain

$$\begin{aligned} a_{i+e}(u,v) + \int_\Omega u \,\mathrm{d}\boldsymbol{x} \int_\Omega v \,\mathrm{d}\boldsymbol{x} &\leq 2M \|\mathrm{grad}\, u\|_{L^2(\Omega)} \|\mathrm{grad}\, v\|_{L^2(\Omega)} + |\Omega|^2 \|u\|_{L^2(\Omega)} \|v\|_{L^2(\Omega)} \\ &\leq \max\{2M, |\Omega|^2\} \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)}. \end{aligned}$$

In the next step we will show the ellipticity. To this end we set $u = v$ in (5.25). Thus we obtain

$$\left\langle \widetilde{A}_{i+e} v, v \right\rangle_{\Omega} = a_{i+e}(v, v) + \left( \int_{\Omega} v \ \mathrm{d}\boldsymbol{x} \right)^2 .$$

Using the assumptions on $\mathbf{M}_{\{i,e\}}$ once again we obtain

$$\begin{aligned} a_{i+e}(v, v) + \left( \int_{\Omega} v \ \mathrm{d}\boldsymbol{x} \right)^2 &\geq 2m \|\mathrm{grad}\, v\|^2_{L^2(\Omega)} + \left( \int_{\Omega} v \ \mathrm{d}\boldsymbol{x} \right)^2 \\ &\geq \min\{2m, 1\} \left( \|\mathrm{grad}\, v\|^2_{L^2(\Omega)} + \left( \int_{\Omega} v \ \mathrm{d}\boldsymbol{x} \right)^2 \right). \end{aligned}$$

With Sobolev's norm equivalence theorem, see [75, Theorem 2.6], we know that the terms in parentheses form an equivalent norm in $H^1(\Omega)$. Thus we finally obtain

$$a_{i+e}(v, v) + \left( \int_{\Omega} v \ \mathrm{d}\boldsymbol{x} \right)^2 \geq \tilde{c}_{i+e} \|v\|^2_{H^1(\Omega)},$$

where the constant $\tilde{c}_{i+e} > 0$ depends only on the eigenvalues of $\mathbf{M}_{\{i,e\}}$ and the constant from the norm equivalence in Sobolev's norm equivalence theorem. □

With this result we can now apply the Lemma of Lax-Milgram (Lemma 5.2), and conclude that the operator $\widetilde{A}_{i+e}$ possesses a bounded inverse, say $\widetilde{A}^{-1}_{i+e}$ and by using the self-adjointness of this operator we can also conclude with Lemma 5.3 that the inverse is elliptic too.

These results can now be used to obtain a Schur complement system. Eliminating $u_e$ in (5.24) we obtain

$$u_e = \widetilde{A}^{-1}_{i+e} \left( F_2 - A_i u_{\mathrm{tm}} \right).$$

This can now be inserted into equation (5.23). Then we arrive at

$$\begin{aligned} A_i u_{\mathrm{tm}} + A_i \widetilde{A}^{-1}_{i+e} \left( F_2 - A_i u_{\mathrm{tm}} \right) &= F_1, \\ \left( A_i - A_i \widetilde{A}^{-1}_{i+e} A_i \right) u_{\mathrm{tm}} &= F_1 - A_i \widetilde{A}^{-1}_{i+e} F_2. \end{aligned}$$

We define the *bi-domain operator* $A_{\mathrm{BD}} := (A_i - A_i \widetilde{A}^{-1}_{i+e} A_i)$ and the modified right hand side $\widetilde{f} := F_1 - A_i \widetilde{A}^{-1}_{i+e} F_2$. Now we have to investigate the properties of $A_{\mathrm{BD}}$. This is answered by:

**Theorem 5.8.** *Let the assumptions of Lemma 5.7 be fulfilled. Then the bi-domain operator $A_{BD}$ is bounded and it holds:*

$$\langle A_{BD}v, v\rangle_\Omega + \|v\|^2_{L^2(\Omega)} \geq c_{BD}\|v\|^2_{H^1(\Omega)}. \tag{5.26}$$

*Proof.* The boundedness of the operator $A_{\mathrm{BD}}$ is obvious, since it is composed of bounded operators. It remains to show that $A_{\mathrm{BD}}$ fulfills (5.26). Recall the full system

$$\begin{aligned} A_i u_{\mathrm{tm}} + A_i u_e &= F_1, \\ A_i u_{\mathrm{tm}} + \widetilde{A}_{i+e} u_e &= F_2. \end{aligned}$$

This can be rewritten as

$$\begin{pmatrix} A_i & A_i \\ A_i & \widetilde{A}_{i+e} \end{pmatrix} \begin{pmatrix} u_{\mathrm{tm}} \\ u_e \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}.$$

We now introduce the operator $\mathcal{A}$ via

$$\mathcal{A} := \begin{pmatrix} A_i & A_i \\ A_i & \widetilde{A}_{i+e} \end{pmatrix} + \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix}$$

where the operator $M\colon H^1(\Omega) \to \widetilde{H}^{-1}(\Omega)$ is defined as

$$\langle Mu, v\rangle_\Omega := \int_\Omega uv \, dx \qquad \text{for all } u, v \in H^1(\Omega).$$

The newly introduced operator $\mathcal{A}$ maps from $H^1(\Omega) \times H^1(\Omega)$ to $\widetilde{H}^{-1}(\Omega) \times \widetilde{H}^{-1}(\Omega)$. We introduce the related norm

$$\|(u_1, u_2)\|_{H^1(\Omega)\times H^1(\Omega)} := \sqrt{\|u_1\|^2_{H^1(\Omega)} + \|u_2\|^2_{H^1(\Omega)}}$$

on the product space $H^1(\Omega) \times H^1(\Omega)$. Assume that $\mathcal{A}$ is $H^1(\Omega) \times H^1(\Omega)$-elliptic, this means

$$\langle \mathcal{A}\boldsymbol{v}, \boldsymbol{v}\rangle_{H^1(\Omega)\times H^1(\Omega)} \geq c_1^{\mathcal{A}} \|\boldsymbol{v}\|^2_{H^1(\Omega)\times H^1(\Omega)} \qquad \text{for all } \boldsymbol{v} \in H^1(\Omega) \times H^1(\Omega). \tag{5.27}$$

Additionally we know that $\widetilde{A}_{i+e}$ is invertible thus we may choose $v_2 := -\widetilde{A}^{-1}_{i+e} A_i v_1$. Using this in the ellipticity condition (5.27) we obtain

$$\begin{aligned} &\left\langle (\widetilde{A}_i - A_i \widetilde{A}^{-1}_{i+e} A_i) v_1, v_1 \right\rangle + \|v_1\|^2_{L^2(\Omega)} \\ &\qquad \geq c_1^{\mathcal{A}} \left( \|v_1\|^2_{H^1(\Omega)} + \left\| -\widetilde{A}^{-1}_{i+e} A_i v_1 \right\|^2_{H^1(\Omega)} \right) \geq c_1^{\mathcal{A}} \|v_1\|^2_{H^1(\Omega)}. \end{aligned}$$

Hence, for concluding the proof we need to show that $\mathcal{A}$ is elliptic. This is equivalent to show that

$$a_i(u_1, v_1) + \langle u_1, v_1\rangle_\Omega + a_i(u_2, v_1) + a_i(u_1, v_2) + a_{i+e}(u_2, v_2) + \langle u_2, 1\rangle_\Omega \langle v_2, 1\rangle_\Omega$$

is elliptic. The last equation can be rewritten as

$$a_i(u_1+u_2,v_1+v_2)+a_e(u_2,v_2)+\langle u_1,v_1\rangle_\Omega+\langle u_2,1\rangle_\Omega\langle v_2,1\rangle_\Omega.$$

Setting $v_1=u_1$ and $v_2=u_2$ we obtain

$$a_i(u_1+u_2,u_1+u_2)+a_e(u_2,u_2)+\|u_1\|^2_{L^2(\Omega)}+\left|\langle u_2,1\rangle_\Omega\right|^2.$$

At this point we use Lemma 5.7 and the definitions of $a_i$ and $a_e$. This results in

$$\begin{aligned}a_i(u_1+u_2,u_1+u_2)+a_e(u_2,u_2)+\|u_1\|^2_{L^2(\Omega)}+\left|\langle u_2,1\rangle_\Omega\right|^2&\\ \geq m\underbrace{\left(|u_1+u_2|^2_{H^1(\Omega)}+|u_2|^2_{H^1(\Omega)}\right)}_{=:(I)}+\|u_1\|^2_{L^2(\Omega)}+\left|\langle u_2,1\rangle_\Omega\right|^2,&\quad(5.28)\end{aligned}$$

where we introduced the $H^1(\Omega)$-semi-norm:

$$|\cdot|_{H^1(\Omega)}:=\|\mathrm{grad}(\cdot)\|_{L^2(\Omega)}.$$

Next we rewrite $(I)$ as

$$(I)=\frac{1}{2}(I)+\frac{1}{2}(I)\geq\frac{1}{2}(I)+\frac{1}{2}|u_2|^2_{H^1(\Omega)}.$$

Finally we use the fact that

$$\frac{1}{2}\|u_1\|^2\leq(I)$$

and conclude that

$$\begin{aligned}(I)=|u_1+u_2|^2_{H^1(\Omega)}+|u_2|^2_{H^1(\Omega)}&\geq\frac{1}{4}|u_1|^2_{H^1(\Omega)}+\frac{1}{2}|u_2|^2_{H^1(\Omega)}\\ &\geq\frac{1}{4}\left(|u_1|^2_{H^1(\Omega)}+|u_2|^2_{H^1(\Omega)}\right)\end{aligned}$$

Going back to (5.28) we get

$$\begin{aligned}m\left(|u_1+u_2|^2_{H^1(\Omega)}+|u_2|^2_{H^1(\Omega)}\right)+\|u_1\|^2_{L^2(\Omega)}+\left|\langle u_2,1\rangle_\Omega\right|^2&\\ \geq\min\left\{\frac{m}{4},1\right\}\underbrace{\left(|u_1|^2_{H^1(\Omega)}+|u_2|^2_{H^1(\Omega)}+\|u_1\|^2_{L^2(\Omega)}+\left|\langle u_2,1\rangle_\Omega\right|^2\right)}_{=:(II)}.&\end{aligned}$$

With Sobolev's norm equivalence theorem we get that $(II)$ defines an equivalent norm in $H^1(\Omega)\times H^1(\Omega)$. Therefore we finally get that the operator $\mathcal{A}$ is $H^1(\Omega)\times H^1(\Omega)$-elliptic. □

**Remark 5.6.** *In Theorem 5.8 we have shown that the operator $A_{BD}$ is* coercive *when considered as operator from $H^1(\Omega) \to \widetilde{H}^{-1}(\Omega)$. On the other hand it can be shown that the operator $A_{BD}\colon H^1_*(\Omega) \to \widetilde{H}^{-1}(\Omega)$ is elliptic and thus invertible. This follows from the fact, that the $H^1(\Omega)$ semi-norm coincides with the full $H^1(\Omega)$-norm in that case, see [75] for details.*

For the analysis hereinafter we need to know more about this operator $A_{\mathrm{BD}}$. The next result is a classic result from spectral theory of compact operators. For more information about spectral theory one should refer to [4, 25, 27, 65, 82].

**Theorem 5.9.** *Let the assumptions of Lemma 5.7 be fulfilled. Then, their exists an increasing sequence of non-zero eigenvalues $\{\lambda_n\}_{n\in\mathbb{N}}$ tending to infinity and a family of eigenfunctions $\{z_n\}_{n\in\mathbb{N}} \subset H^1(\Omega)$, forming an orthonormal basis of $L^2(\Omega)$ such that the operator $A_{BD}$ can be decomposed as*

$$A_{BD}u = \sum_{n=0}^{\infty} \lambda_n \langle u, z_n\rangle_{L^2(\Omega)} z_n, \qquad \text{for all } u \in H^1(\Omega).$$

*Furthermore the functions $\{\lambda_n^{-1/2} z_n\}_{n\in\mathbb{N}}$ form an orthonormal basis of $H^1(\Omega)$ with respect to the induced bilinear-form*

$$a_{BD}(\cdot,\cdot) := \langle A_{BD}\cdot, \cdot\rangle_{\Omega}.$$

*The same decomposition holds for $a_{BD}(\cdot,\cdot)$, this means for $u$ and $v \in H^1(\Omega)$ is holds:*

$$a_{BD}(u,v) = \sum_{n=0}^{\infty} \lambda_n \langle u, z_n\rangle_{L^2(\Omega)} \langle v, z_n\rangle_{L^2(\Omega)}.$$

*Proof.* See [65, Théorème 6.2-1] and [65, Remarque 6.2-2]. □

## 5.3 Analysis of the Bi-Domain Equations

We have analyzed the linear subproblem of the bi-domain equations in the last chapter. This will now be useful when discussing the analysis of the full bi-domain equations. But first of all we need to specify some assumptions to be able to handle the nonlinearities in the full bi-domain equations as suggested in [9]:

**(H1)** The Sobolev embedding, see [1, Theorem 4.12], $H^1(\Omega) \subset L^p(\Omega)$ holds. This is valid for $p \in [2,6]$ and $\Omega \subset \mathbb{R}^3$.

**(H2)** The functions $g, \boldsymbol{f}$ are affine with respect to $\boldsymbol{v}$:

$$g(u_{\mathrm{tm}}, \boldsymbol{v}) = g_1(u_{\mathrm{tm}}) + (\boldsymbol{g}_2(u_{\mathrm{tm}}), \boldsymbol{v}), \qquad \boldsymbol{f}(u_{\mathrm{tm}}, \boldsymbol{v}) = \boldsymbol{f}_1(u_{\mathrm{tm}}) + f_2\boldsymbol{v},$$

where $g_1 \colon \mathbb{R} \to \mathbb{R}$, $\boldsymbol{g}_2 \colon \mathbb{R} \to \mathbb{R}^n$, $\boldsymbol{f}_1 \colon \mathbb{R} \to \mathbb{R}^n$ are continuous functions and $f_2 \in \mathbb{R}$.

**(H3)** There exist constants $c_i \geq 0, i = 1, \ldots, 6$ such that for any $u \in \mathbb{R}$ there holds

$$|g_1(u)| \leq c_1 + c_2 \, |u|^{p-1} , \tag{5.29}$$

$$|\boldsymbol{g}_2(u)| \leq c_3 + c_4 \, |u|^{p/2-1} , \tag{5.30}$$

$$|\boldsymbol{f}_1(u)| \leq c_5 + c_6 \, |u|^{p/2} . \tag{5.31}$$

**(H4)** There exist constants $a > 0, \lambda > 0$ and $b, c \geq 0$ such that for any $(u, \boldsymbol{v}) \in \mathbb{R}^{n+1}$:

$$\lambda u g(u, \boldsymbol{v}) + (\boldsymbol{v}, \boldsymbol{f}(u, \boldsymbol{v})) \geq a \, |u|^p - b \left( \lambda \, |u|^2 + |\boldsymbol{v}|^2 \right) - c. \tag{5.32}$$

For the further analysis we also need the following:

**Lemma 5.10.** *Under the assumptions (H2) and (H3), the mappings $(u, \boldsymbol{v}) \in L^p(\Omega) \times [L^2(\Omega)]^n \mapsto g(u, \boldsymbol{v}) \in L^{p'}$ and $(u, \boldsymbol{v}) \in L^p(\Omega) \times [L^2(\Omega)]^n \mapsto \boldsymbol{f}(u, \boldsymbol{v}) \in [L^2(\Omega)]^n$ are well-defined. Specifically for any $(u, \boldsymbol{v}) \in L^p(\Omega) \times [L^2(\Omega)]^n$ we have*

$$\|g(u, \boldsymbol{v})\|_{L^{p'}(\Omega)} \leq A_1 \, |\Omega|^{1/p'} + A_2 \|u\|^{p/p'}_{L^p(\Omega)} + A_3 \|\boldsymbol{v}\|^{2/p'}_{[L^2(\Omega)]^n},$$

$$\|\boldsymbol{f}(u, \boldsymbol{v})\|_{[L^2(\Omega)]^n} \leq B_1 \, |\Omega|^{1/2} + B_2 \|u\|^{p/2}_{L^p(\Omega)} + B_3 \|\boldsymbol{v}\|_{[L^2(\Omega]^n},$$

*where $A_i \geq 0, i = 1, 2, 3$ and $B_i \geq 0, i = 1, 2, 3$ are some constants that depend only on the constants $c_i$ in the assumption (H3) and $p$.*

*Proof.* See [9, Lemma 25]. □

**Weak Formulation of the Bi-Domain Equations.** Having analyzed the elliptic subproblem (5.9)–(5.10), we can now start to derive a full variational formulation of the bi-domain equations. We will start with the abstract definition, taken and adapted from [9, Definition 26], of a weak solution and motivate it afterwards.

**Definition 5.13** (Weak Solution of the Bi-domain Equations)**.** *Consider $\tau > 0$, a Gelfand triple $V \subset H \subset V^*$ and two functions $u \colon t \in [0, \tau) \mapsto u(t) \in H, \boldsymbol{v} \colon t \mapsto \boldsymbol{v}(t) \in H^n$. Given $(u_0, \boldsymbol{v}_0) \in H^{n+1}$ we say that $(u, \boldsymbol{v})$ is a weak solution of the bi-domain equations if and only if, for any $T \in (0, \tau)$*

1. *$u \colon [0, T] \to H$ and $\boldsymbol{v} \colon [0, T] \to H$ are continuous and $u(0) = u_0$ and $\boldsymbol{v}(0) = \boldsymbol{v}_0$ in the sense of $H$ and $H^n$ respectively.*

*2.* $(u, \boldsymbol{v}) \in (W, \Pi)$ *where*

$$W := \left\{ u \in L^p(Q_T) \cap L^2(0,T;V) \middle| \frac{\partial u}{\partial t} \in L^{p'}(\Omega) + L^2(0,T;V^*) \right\},$$
$$\Pi := \left\{ \boldsymbol{v} \in L^2(0,T;H^n) \middle| \frac{\partial \boldsymbol{v}}{\partial t} \in L^2(0,T;H^n) \right\}.$$

*3.* $(u, \boldsymbol{v})$ *satisfy in* $(C_0^\infty(0,T))^*$

$$\left\langle \frac{\partial u}{\partial t}, w \right\rangle_\Omega + a_{BD}(u(t), v) + \langle g(u(t), \boldsymbol{v}(t)), w \rangle_\Omega = \left\langle \widetilde{f}(t), w \right\rangle_\Omega, \tag{5.33}$$
$$\left\langle \frac{\partial \boldsymbol{v}}{\partial t}, \boldsymbol{\zeta} \right\rangle_\Omega + \langle \boldsymbol{f}(u(t), \boldsymbol{v}(t)), \boldsymbol{\zeta} \rangle_\Omega = 0 \tag{5.34}$$

*for all* $(w, \boldsymbol{\zeta}) \in (V \cap L^p(\Omega), H^n)$.

**Remark 5.7.** *The spaces* $V$ *and* $H$ *will in our case be chosen as* $H^1(\Omega)$ *and* $L^2(\Omega)$.

**Remark 5.8.** *In fact, we may even define the weak solution of the bi-domain equations for more general functions which only possess distributional derivatives with respect to time, see [25] for details. However, it can be shown that by choosing suitable spaces for* $u$ *that the distributional derivative coincides with a weak derivative as in the definition above, see [9, Remark 27].*

At this point we shall give a brief motivation for the abstract Definition 5.13. Consider the full bi-domain equations (5.1)–(5.3). Then we multiply them with test functions $(\phi, \psi, \boldsymbol{\zeta})$ in suitable spaces and integrate over $\Omega$ use integration by parts and include the boundary conditions. Thus we arrive at

$$\int_\Omega \frac{\partial u_{\mathrm{tm}}}{\partial t} \phi \ \mathrm{d}\boldsymbol{x} + \int_\Omega \mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} \operatorname{grad} \phi \ \mathrm{d}\boldsymbol{x} + \int_\Omega \mathbf{M}_i \operatorname{grad} u_e \operatorname{grad} \phi \ \mathrm{d}\boldsymbol{x} + \int_\Omega g(u_{\mathrm{tm}}, \boldsymbol{v}) \phi \ \mathrm{d}\boldsymbol{x} = \int_\Omega s_i \phi \ \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} g_{N,i} \phi \ \mathrm{ds}_{\boldsymbol{x}}, \tag{5.35}$$

$$\int_\Omega \mathbf{M}_i \operatorname{grad} u_{\mathrm{tm}} \operatorname{grad} \psi \ \mathrm{d}\boldsymbol{x} + \int_\Omega (\mathbf{M}_i + \mathbf{M}_e) \operatorname{grad} u_e \operatorname{grad} \psi \ \mathrm{d}\boldsymbol{x} = \int_\Omega (s_i + s_e) \psi \ \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} (g_{N,i} + g_{N,e}) \psi \ \mathrm{ds}_{\boldsymbol{x}}, \tag{5.36}$$

$$\int_\Omega \left( \frac{\partial \boldsymbol{v}}{\partial t}, \boldsymbol{\zeta} \right) \ \mathrm{d}\boldsymbol{x} + \int_\Omega (\boldsymbol{f}(u_{\mathrm{tm}}, \boldsymbol{v}), \boldsymbol{\zeta}) \ \mathrm{d}\boldsymbol{x} = 0.$$

As for the stationary problem (5.9)–(5.10), we may stabilize the operator equation corresponding to equation (5.36) with

$$\int_\Omega u_e \ \mathrm{d}\boldsymbol{x} \int_\Omega \psi \ \mathrm{d}\boldsymbol{x},$$

and thus arrive at the operator $A_{\mathrm{BD}}$ with the corresponding bilinear form $a_{\mathrm{BD}}(u,v)$ which has been analyzed in Theorem 5.8. This now reads as

$$\int_\Omega \frac{\partial u_{\mathrm{tm}}}{\partial t}\phi \ \mathrm{d}\boldsymbol{x} + \int_\Omega g(u_{\mathrm{tm}},\boldsymbol{v})\phi \ \mathrm{d}\boldsymbol{x} + a_{\mathrm{BD}}(u_{\mathrm{tm}},\phi) = \left\langle \widetilde{f},\phi \right\rangle_\Omega,$$
$$\int_\Omega \left(\frac{\partial \boldsymbol{v}}{\partial t},\boldsymbol{\zeta}\right) \ \mathrm{d}\boldsymbol{x} + \int_\Omega (\boldsymbol{f}(u_{\mathrm{tm}},\boldsymbol{v}),\boldsymbol{\zeta}) \ \mathrm{d}\boldsymbol{x} = 0$$

Due to the Riesz representation theorem (Theorem 5.1) we can interpret the scalar product as a duality pairing arriving at the weak form of the bi-domain equations.

Before proving existence and uniqueness for solutions of this variational formulation we may mention that their are also existence and uniqueness theorems for classical or strong solutions available. One may refer to [9, Section 4], their one may also find a statement about the equivalence of strong and weak solutions under the assumption that the boundary $\partial\Omega$ is smooth enough.

For brevity we introduce the notations

$$\begin{aligned}
X &:= L^p(Q_T) \cap L^2(0,T;H^1(\Omega)),\\
X^* &:= L^{p'}(Q_T) + L^2(0,T;\widetilde{H}^{-1}(\Omega)),\\
Y &:= L^p(\Omega),\\
Y^* &:= L^{p'}(\Omega),\\
V &:= H^1(\Omega),\\
V^* &:= \widetilde{H}^{-1}(\Omega),\\
H &:= L^2(\Omega),\\
H_{Q_T} &:= L^2(Q_T),\\
H^n &:= [H]^n,\\
H_T^n &:= [L^2(\Omega)]^n \times L^2((0,T)),\\
u &:= u_{\mathrm{tm}}.
\end{aligned}$$

### 5.3.1 Existence and Uniqueness of the Weak Bi-Domain Equations

In the following we will prove existence and uniqueness for solutions of the weak bi-domain equations under minimal regularity assumptions. The proof will be given in three parts:

1. We will construct a unique approximate solution using the *Galerkin-Faedo*

technique[1].

2. We will show that the constructed approximate solutions are bounded and possess therefore weakly convergent subsequences.

3. We will show that those subsequences converge almost everywhere to a unique weak solution.

**Construction of the approximate solution.** In Theorem 5.9 we have shown that there exists an orthonormal basis $\{z_n\}_{n\in\mathbb{N}}$ of the space $H$ spanned by the eigenvectors of the operator $A_{\mathrm{BD}}$. For $m \geq 1$ arbitrary but fixed let us denote

$$V_m = \operatorname{span}\{z_1, z_2, \ldots, z_m\} \subset V \subset H.$$

With this finite dimensional subspace we now construct approximate solutions by

$$u_m(t) := \sum_{i=0}^{m} u_{im}(t) z_i,$$
$$\boldsymbol{v}_m(t) := \sum_{i=0}^{m} \boldsymbol{v}_{im}(t) z_i.$$

The new unknowns are now the $(m+1)(n+2)$ time-dependent coefficients[2] $u_{im}$ $i = 0, \ldots, m$ and $v_{im}^j$ where $i = 0, \ldots, m$, $j = 0, \ldots, n$. Now we plug the approximate solutions into the variational formulation of the bi-domain equations. Thus we obtain

$$\begin{aligned}
\left\langle \frac{\partial u_m}{\partial t}, \phi \right\rangle_\Omega + \langle g(u_m, \boldsymbol{v}_m), \phi \rangle_\Omega + a_{\mathrm{BD}}(u_m, \phi) &= \left\langle \widetilde{f}, \phi \right\rangle_\Omega, \\
\left\langle \frac{\partial \boldsymbol{v}_m}{\partial t}, \boldsymbol{\zeta} \right\rangle_\Omega + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), \boldsymbol{\zeta} \rangle_\Omega &= 0
\end{aligned}$$

for all $\phi \in V_m$.

Using the definitions of $u_m, \boldsymbol{v}_m$ leads to

$$\begin{aligned}
\sum_{i=0}^{m} \frac{\mathrm{d}u_{im}}{\mathrm{d}t} \langle z_i, \phi \rangle_H + \langle g(u_m, \boldsymbol{v}_m), \phi \rangle_\Omega + \sum_{i=0}^{m} u_{im} a_{\mathrm{BD}}(z_i, \phi) &= \left\langle \widetilde{f}, \phi \right\rangle_\Omega, \\
\sum_{i=0}^{m} \left\langle \frac{\mathrm{d}\boldsymbol{v}_{im}}{\mathrm{d}t}, z_i \boldsymbol{\zeta} \right\rangle_{H^n} + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), \boldsymbol{\zeta} \rangle_\Omega &= 0.
\end{aligned}$$

[1] Techniques for solving abstract operator-valued differential equations of the form $\dot{u} + A(u) = f$, with an arbitrary operator $A$ are called Galerkin-Faedo techniques.

[2] This amount renders as follows: We have $m+1$ unknown coefficients $u_{im}(t)$. Further, we have $m+1$ vector valued coefficients $\boldsymbol{v}_{im}(t)$, each of those having $n+1$ components. Therefore we have $m + 1 + (n+1)(m+1) = (n+2)(m+1)$ unknowns.

This has to be fulfilled for all $(\phi, \boldsymbol{\zeta}) \in V_m \times [V_m]^n$ especially for $\phi = z_j$ and $\zeta = z_j \boldsymbol{e}_j$. Using this, $a_{\mathrm{BD}}(u_m, z_j) = \lambda_j \langle u_m, z_j \rangle_{L^2(\Omega)}$ and the orthonormality of the $z_n$ we can rewrite the above as a system of ordinary linear differential equations in $t$ reading as

$$\frac{\mathrm{d}u_{jm}(t)}{\mathrm{d}t} + \langle g(u_m, \boldsymbol{v}_m), z_j \rangle_\Omega + \lambda_j u_{jm}(t) = \left\langle \widetilde{f}, z_j \right\rangle_\Omega, \tag{5.37}$$

$$\frac{\mathrm{d}\boldsymbol{v}_{jm}(t)}{\mathrm{d}t} + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), z_j \rangle = \boldsymbol{0} \tag{5.38}$$

for $j = 0, \ldots, m$, or equivalently stated in a vector-valued form as

$$\frac{\mathrm{d}\boldsymbol{u}_m}{\mathrm{d}t} + \boldsymbol{d}_1(\boldsymbol{u}_m) + \mathsf{D}_2 \boldsymbol{u}_m = \boldsymbol{F}, \tag{5.39}$$

$$\frac{\mathrm{d}\boldsymbol{v}_{jm}(t)}{\mathrm{d}t} + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), z_j \rangle_\Omega = \boldsymbol{0} \qquad \text{for } j = 1, \ldots, m, \tag{5.40}$$

where

$$\begin{aligned}
\boldsymbol{u}_m &:= (u_{1m}, u_{2m}, \ldots, u_{mm})^\top, \\
\boldsymbol{d}_1(\boldsymbol{u}_m) &:= (\langle g(\boldsymbol{u}_m, \boldsymbol{v}_m), z_1 \rangle, \langle g(\boldsymbol{u}_m, \boldsymbol{v}_m), z_2 \rangle, \ldots, \langle g(\boldsymbol{u}_m, \boldsymbol{v}_m), z_m \rangle)^\top, \\
\mathsf{D}_2 &:= \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m), \\
(\boldsymbol{F})_i &:= \left\langle \widetilde{f}, z_i \right\rangle_\Omega.
\end{aligned}$$

This also means that we have a Galerkin isomorphism between $\boldsymbol{u}_m$ and $u_m$.

We also need to formulate initial values in $t = 0$ for $u_m$ and $\boldsymbol{v}_m$, let us call them $u_{m0}, \boldsymbol{v}_{m0}$. When we assume that the initial conditions $u_0(\boldsymbol{x})$ and $\boldsymbol{v}_0(\boldsymbol{x})$ are in $H$ and $H^n$ respectively we may choose the initial values $u_{m0}, \boldsymbol{v}_{m0}$ to be the $H$-Projection and the $H^n$-Projection of $u_0(\boldsymbol{x})$ and $\boldsymbol{v}_0(\boldsymbol{x})$ on $V_m$, which means that

$$\left\| u_{m0} - u_{\mathrm{tm}}^0 \right\|_H \to 0, \qquad \|\boldsymbol{v}_{m0} - \boldsymbol{v}_0\|_{H^n} \to 0 \quad \text{as } m \to \infty. \tag{5.41}$$

Equations (5.37)–(5.38) make sense because $u_m(t) \in V \subset Y, \boldsymbol{v}_m(t) \in H^n$ for each $t$ and so that by Lemma 5.10 $g(u_m, \boldsymbol{v}_m) \in Y^*$ and $\boldsymbol{f}(u_m, \boldsymbol{v}_m) \in H^n$ for each $t$ and $z_i \in V \subset Y$. We also know, by hypothesis (H2), that the right hand side of the system of ordinary differential equations is continuous. Therefore we may use the Theorem of Cauchy-Peano, see [13, Chapter 1, Theorem 1.2], and deduce that their exists a solution $(\boldsymbol{u}_m, \boldsymbol{v}_{im}) \in [C^1([0, t_m))]^{(n+2)(m+1)}$ of the initial value problem for all $t \in [0, t_m)$. These coefficients determine the solutions $(u_m, \boldsymbol{v}_m)$, which will be investigated hereafter.

**Boundedness of the Approximate Solutions.** The parameter $t_m$ stands for the maximal rectangle in which the solution may be defined. The following lemma states that the case of a *blow-up*, that means that the solutions become unbounded for $t > t_m$, can be excluded, which means that $t_m = \infty$.

**Lemma 5.11.** *The unique solution* $(u_m, \boldsymbol{v}_m)$ *of* (5.37)–(5.38) *is defined for every* $t \in [0, \infty]$*, i.e.:* $t_m = \infty$ *and it holds for any* $T > 0$ *that*

$$\lambda \|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2 \leq \mathcal{C}_1 \qquad \text{for all } t \in [0, T],$$

*where* $\mathcal{C}_1$ *is a constant and* $\lambda$ *is defined in (H4).*

Before proving Lemma 5.11 we need to formulate the well-known *Gronwall Lemma* in its differential form:

**Theorem 5.12** (Gronwall's Lemma, Differential Form)**.** *If* $u(t) \in \mathcal{C}^1([a, b])$ *fulfills*

$$\dot{u}(t) \leq \alpha(t) + \beta(t)u(t) \qquad \text{for all } t \in [a, b]$$

*for some given functions* $\alpha, \beta$*, then it follows that*

$$u(t) \leq u(a)e^{\int_{s=a}^{t} \beta(s)\,\mathrm{ds}} + \int_{s=a}^{t} \alpha(s)e^{\int_{s}^{t} \beta(\tau)d\tau}\ \mathrm{ds}\,.$$

*Proof.* Define

$$v(t) := e^{-\int_{s=a}^{t} \beta(s)\ \mathrm{ds}}.$$

The function $v$ satisfies the differential equation

$$\dot{v} = -\beta(t)v(t), \qquad v(a) = 1$$

Now we take a closer look at the derivative of $uv$:

$$\frac{\mathrm{d}}{\mathrm{d}t}(uv) = \dot{u}v + u\dot{v} = \dot{u}v - uv\beta \leq \beta uv - \beta uv + v\alpha = \alpha v.$$

Here it does not matter, whether we write $t$ or $s$ as the dependent variable. So we may switch from $t$ to $s$ and integrate both sides from $[a, t]$, where $t \in (a, b)$ and obtain

$$u(t)v(t) - u(a) \leq \int_{s=a}^{t} \alpha(s)v(s)\ \mathrm{ds},$$

$$u(t)v(t) \leq u(a) + \int_{s=a}^{t} \alpha(s)v(s)\ \mathrm{ds}\,.$$

Hence we conclude the proof by multiplying with $\frac{1}{v} = e^{\int_{s=a}^{t} \beta(s)\ \mathrm{ds}}$. □

Now we are able to prove Lemma 5.11.

*Proof of Lemma 5.11.* We take the inner product with $\lambda u_{im}(t)$ and $\boldsymbol{v}_{im}$ in (5.39)–(5.40). Thus we obtain

$$\lambda\left(\frac{\mathrm{d}\boldsymbol{u}_m}{\mathrm{d}t}, \boldsymbol{u}_m\right) + \lambda(\boldsymbol{d}_1(\boldsymbol{u}_m), \boldsymbol{u}_m) + (\mathsf{D}_2\boldsymbol{u}_m, \boldsymbol{u}_m) = \lambda(\boldsymbol{F}, \boldsymbol{u}_m),$$
$$\left(\frac{\mathrm{d}\boldsymbol{v}_{im}(t)}{\mathrm{d}t}, \boldsymbol{v}_{im}(t)\right) + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), z_i\boldsymbol{v}_{im}\rangle = 0.$$

Here we can see that

$$\left(\frac{\mathrm{d}\boldsymbol{u}_m}{\mathrm{d}t}, \boldsymbol{u}_m\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left|\boldsymbol{u}_m(t)\right|^2$$

and

$$\left(\frac{\mathrm{d}\boldsymbol{v}_m(t)}{\mathrm{d}t}, \boldsymbol{v}_m(t)\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left|\boldsymbol{v}_m(t)\right|^2.$$

Using Parseval's identity, see for example [82, Theorem V.4.9], we conclude that

$$|\boldsymbol{u}_m(t)|^2 = \|u_m(t)\|_H^2.$$

The same is also valid for the term $|\boldsymbol{v}_{im}(t)|^2$. Next, the term $(\mathsf{D}_2\boldsymbol{u}_m, \boldsymbol{u}_m)$ can be written as $a_{\mathrm{BD}}(u_m, u_m)$, due to

$$\begin{aligned} a_{\mathrm{BD}}(u_m, u_m) &= a_{\mathrm{BD}}\left(\sum_{i=1}^m u_{im}(t)z_i, \sum_{j=1}^m u_{jm}(t)z_j\right) = \sum_{i,j=1}^m u_{im}(t)u_{jm}(t)a_{\mathrm{BD}}(z_i, z_j) \\ &= \sum_{i,j=1}^m u_{im}(t)u_{jm}(t)\lambda_i \underbrace{\langle z_i, z_j\rangle}_{=\delta_{ij}} = \sum_{i=0}^m \lambda_i u_{im}^2(t) = (\mathsf{D}_2\boldsymbol{u}_m, \boldsymbol{u}_m). \end{aligned}$$

Next we use the Galerkin isomorphism for the non-linear terms and arrive at

$$\begin{aligned} &\frac{\lambda}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_m(t)\|_H^2 + \lambda a_{\mathrm{BD}}(u_m(t), u_m(t)) + \langle g(u_m, \boldsymbol{v}_m), \lambda u_m\rangle_\Omega = \lambda\left\langle \widetilde{f}, u_m\right\rangle_\Omega, \\ &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{v}_m(t)\|_{H^n} + \langle \boldsymbol{f}(u_m, \boldsymbol{v}_m), \boldsymbol{v}_m\rangle_\Omega = 0. \end{aligned}$$

Now we sum up all the equations and obtain

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) + \lambda a_{\mathrm{BD}}(u_m(t), u_m(t)) \\ &+ \langle g(u_m(t), \boldsymbol{v}_m(t)), \lambda u_m(t)\rangle_\Omega + \langle \boldsymbol{f}(u_m(t), \boldsymbol{v}_m(t)), \boldsymbol{v}_m(t)\rangle_\Omega = \lambda\left\langle \widetilde{f}, u_m(t)\right\rangle_\Omega. \end{aligned} \tag{5.42}$$

This auxiliary result will be helpful in a few moments. Consider

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) + c_{\mathrm{BD}}\lambda\|u_m(t)\|_V^2 + a\|u_m(t)\|_Y^p.$$

Now we may use for any $t \in [0, t_m)$ the estimate (5.26), hence

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) + c_{\mathrm{BD}}\lambda\|u_m(t)\|_V + a\|u_m(t)\|_Y^p \\ \leq \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) \\ + \lambda a_{\mathrm{BD}}(u_m(t), u_m(t)) + \lambda\|u_m(t)\|_H^2 + a\|u_m(t)\|_Y^p.\end{aligned}$$

Now we may rewrite hypothesis (H4) as

$$a\,|u|^p \leq \lambda u g(u, \boldsymbol{v}) + (\boldsymbol{f}(u, \boldsymbol{v}), \boldsymbol{v}) + \lambda b\,|u|^2 + b\,|\boldsymbol{v}|^2 + c,$$

from which we conclude that

$$a\|u\|_Y^p \leq \lambda\langle g(u, \boldsymbol{v}), u\rangle_\Omega + \langle \boldsymbol{f}(u, \boldsymbol{v}), \boldsymbol{v}\rangle_\Omega + \lambda b\|u\|_H^2 + b\|\boldsymbol{v}\|_{H^n} + c\,|\Omega|\,.$$

Using this result together with (5.42) we obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) \\ \leq \lambda\left\langle \widetilde{f}, u_m(t)\right\rangle_\Omega - c_{\mathrm{BD}}\lambda\|u_m(t)\|_V^2 + \|u_m(t)\|_H^2 - a\|u_m(t)\|_Y^p \\ + \lambda b\|u_m(t)\|_H^2 + b\|\boldsymbol{v}_m\|_{H^n} + c\,|\Omega|\,, \quad (5.43)\end{aligned}$$

and hence

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) \\ \leq \lambda\left\|\widetilde{f}(t)\right\|_{V^*}\|u_m(t)\|_V + c\,|\Omega| + 2b\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right).\end{aligned}$$

The first terms on the right hand side are bounded by hypothesis. Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right) \leq 2\tilde{c} + 4b\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right).$$

Now we are able to use Gronwall's lemma (Theorem 5.12 which gives us

$$\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2 \leq \widetilde{C}\left(\lambda\|u_{m0}\|_H^2 + \|\boldsymbol{v}_{m0}\|_{H^n}^2\right).$$

By assumption, the initial values $u_{m0}, \boldsymbol{v}_{m0}$ are both in $H$. Thus we have proved the second statement of the lemma. This statement now holds for all $t \in [0, t_m)$. For proving that $t_m = \infty$ we may use a corollary to be found in [6, Chapter 2, Corollary 7] and the corresponding remarks, which tells us that we can extend the solutions $u_m(t)$ and $\boldsymbol{v}_m(t)$ to infinity when the right hand sides of the differential equations can be bounded by its arguments, in that case $u_m, \boldsymbol{v}_m$. This can easily be deduced from the results stated above. □

The Lemma 5.11 tells us, that we can find for each $T \in [0,\infty)$ a constant $\mathcal{C}_1$ such that the statement is valid, and so we can conclude the following:

**Corollary 5.1.** *There holds*

$$\|u_m(t)\|_{L^\infty(0,T;L^2(\Omega))} < \infty,$$
$$\|\boldsymbol{v}_m(t)\|_{L^\infty(0,T;H^n)} < \infty,$$

*for each* $T \in [0,\infty)$ *and therefore also*

$$\|\boldsymbol{v}_m(t)\|_{L^2(Q_T)} < \infty.$$

Now we will use this result to state the first important theorem:

**Theorem 5.13.** *For any* $T \in (0,\infty)$ *it holds:*

$$\|u_m\|_X \leq \mathcal{C}_2 < \infty,$$

*where the norm* $\|\cdot\|_X$ *is defined as in Theorem 5.6.*

*Proof.* We start from rewriting the inequality (5.43) as

$$c_{\mathrm{BD}}\lambda\|u_m(t)\|_V^2 + a\|u_m(t)\|_Y^p \leq \lambda\left\langle \widetilde{f}, u_m\right\rangle_\Omega + 2b\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m\|_{H^n}\right) + c\,|\Omega| - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right).$$

Now we use Lemma 5.11 and obtain

$$c_{\mathrm{BD}}\lambda\|u_m(t)\|_V^2 + a\|u_m(t)\|_Y^p \leq \lambda\left\langle \widetilde{f}, u_m\right\rangle_\Omega + 2b\mathcal{C}_1 + c\,|\Omega| - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\lambda\|u_m(t)\|_H^2 + \|\boldsymbol{v}_m(t)\|_{H^n}^2\right).$$

The duality pairing appearing on the right hand side of the inequality may also be bounded by

$$\left\langle \widetilde{f}(t), u_m(t)\right\rangle_\Omega \leq \left\|\widetilde{f}(t)\right\|_{V^*}\|u_m(t)\|_V \leq \frac{1}{2}\left\|\widetilde{f}(t)\right\|_{V^*}^2 + \frac{1}{2}\|u_m(t)\|_V^2.$$

Next we integrate on both sides from $[0,T)$. Thus we obtain

$$\begin{aligned}\left(c_{\mathrm{BD}}\lambda - \frac{1}{2}\right)\|u_m\|_{L^2(0,T;H^1(\Omega))}^2 + a\|u_m\|_{L^p(Q_T)}^p &\leq \lambda\left\|\widetilde{f}\right\|_{L^2(0,T;\widetilde{H}^{-1}(\Omega))} + 2b\mathcal{C}_1 T + cT\,|\Omega| \\ &\quad - \left(\lambda\|u_m(T)\|_H^2 + \|\boldsymbol{v}_m(T)\|_{H^n}^2 - \lambda\|u_{m0}\|_H^2 - \|\boldsymbol{v}_{m0}\|_{H^n}^2\right) \\ &\leq \underbrace{\lambda\left\|\widetilde{f}\right\|_{L^2(0,T;\widetilde{H}^{-1}(\Omega))} + 2b\mathcal{C}_1 T + cT\,|\Omega| + \lambda\|u_{m0}\|_H^2 + \|\boldsymbol{v}_{m0}\|_{H^n}^2}_{=:C_T}.\end{aligned}$$

Define $\widetilde{C} := \min\{c_{\mathrm{BD}}\lambda - \frac{1}{2}, a\} > 0$ by hypothesis (H4). Then we end up with the result

$$\|u_m\|_X \leq \mathcal{C}_2 < \infty \qquad \text{for any } T \in (0,\infty),$$

with

$$\mathcal{C}_2 := \max\left\{\left(\frac{C_T}{\widetilde{C}}\right)^{1/2}, \left(\frac{C_T}{\widetilde{C}}\right)^{1/p}\right\}.$$

□

We will also need the boundedness of the derivatives $\frac{\partial u_m}{\partial t}, \frac{\partial \boldsymbol{v}_m}{\partial t}$ defined by

$$\dot{u}_m = \frac{\partial u_m}{\partial t} = \sum_{i=0}^{m} \dot{u}_{im}(t) z_i,$$
$$\dot{\boldsymbol{v}}_m = \frac{\partial \boldsymbol{v}_m}{\partial t} = \sum_{i=0}^{m} \dot{\boldsymbol{v}}_{im}(t) z_i,$$

which is given by the following result:

**Theorem 5.14.** *For any $T \in (0,\infty)$ it holds that*

$$\|\dot{u}_m\|_{X^*} \leq \mathcal{C}_3 < \infty,$$
$$\|\dot{\boldsymbol{v}}_m\|_{[L^2(Q_T)]^n} \leq \mathcal{C}_4 < \infty.$$

*Proof.* We start with the bound on $\dot{u}_m$. Following [9] we introduce the operator $P_m : V^* \to V_m \subset V \subset V^*$ by

$$P_m f := \sum_{i=0}^{m} \langle f, z_i\rangle_\Omega z_i, \qquad \text{for } f \in V^*.$$

It can be shown that this operator defines a projection, i.e. $P_m^2 = P_m$. Consider an element $f \in V$. Since, $z_i \in V$ for all $0 \leq i \leq m$ and $V \subset H$ we can interpret $f$ and $z_i$ as functions in $H$. Therefore we may interpret the duality pairing $\langle\cdot,\cdot\rangle_\Omega$ as inner product in $H$. This means

$$P_m f := \sum_{i=0}^{m} \langle f, z_i\rangle_H z_i, \qquad \text{for } f \in V.$$

To circumvent ambiguities we will denote the projection $P_m f$ for $f \in V$ with $P_m^V f$. For $f \in H$ the projection $P_m^V f$ is the orthogonal projection from $H$ to $V_m$, i.e.

$$\left\langle P_m^V u, v\right\rangle_H = \langle u, v\rangle_H \qquad \text{for } u, v \in H.$$

Further we obtain with the Cauchy-Schwarz inequality that

$$\left\|P_m^V u\right\|_H \leq \|u\|_H \qquad \text{for } u \in H.$$

Then by applying [4, Lemma 7.5] we conclude that $P_m^V$ is self-adjoint. Using again, that we can switch between the $H$-inner product and the duality pairing in $V$ we conclude that

$$\left(P_m^V\right)^* = P_m.$$

Next by using [82, Satz III.4.2], we obtain that

$$\left\|P_m^V\right\|_{V\to V} = \|P_m\|_{V^*\to V^*} \tag{5.44}$$

where the operator norm $\|\cdot\|_{V\to V}$ is defined as

$$\|P_m\|_{\mathcal{X}\to\mathcal{X}} := \sup_{\substack{f\in\mathcal{X}\\ \|f\|_{\mathcal{X}}\neq 0}} \frac{\|P_m f\|_{\mathcal{X}}}{\|f\|_{\mathcal{X}}}.$$

We will use this result later. From the Riesz representation theorem (Theorem 5.1) we know that for any $t \in (0,T)$ there holds

$$\langle \dot{u}_m(t), v\rangle_\Omega = (\mathcal{J}\dot{u}_m(t), v)_V.$$

Strictly we would have to define $\tilde{\dot{u}}_m := \mathcal{J}\dot{u}_m(t)$, however, it is quite common in literature to override this and use again $\dot{u}_m(t)$. Therefore we may rewrite the equations (5.33) as

$$\langle \dot{u}_m(t), v\rangle_\Omega = -\left\langle A_{\mathrm{BD}} u_m(t) + g(u_m(t), \boldsymbol{v}_m(t)) - \widetilde{f}, v\right\rangle_\Omega,$$

We can regard $g(u_m(t), \boldsymbol{v}_m(t))$ as element of $L^{p'}(\Omega) \subset V^*$ by Lemma 5.10. Using now the above defined projection operator $P_m$ this is equivalent to

$$\dot{u}_m = -P_m\left(A_{\mathrm{BD}} u_m(t) + g(u_m(t), \boldsymbol{v}_m(t)) - \widetilde{f}\right)$$

in $V^*$. Therefore,

$$\begin{aligned}\|\dot{u}_m\|_{V^*} &\leq \left\|P_m\left(A_{\mathrm{BD}} u_m(t) + g(u_m(t), \boldsymbol{v}_m(t)) + \widetilde{f}\right)\right\|_{V^*}\\ &\leq \|P_m\|_{V^*\to V^*}\left\|A_{\mathrm{BD}} u_m(t) + g(u_m(t), \boldsymbol{v}_m(t)) + \widetilde{f}\right\|_{V^*}.\end{aligned}$$

To conclude the proof we therefore have to bound the operator norm of $P_m$, the other norms can be bounded by previous estimates. With the result from (5.44) we see that

it suffices to bound $P_m^V$. To this end we consider the bilinear form $a_{\mathrm{BD}}(\cdot,\cdot)$ induced by the bi-domain operator $A_{\mathrm{BD}}$ for an $u \in V$:

$$\begin{aligned} a_{\mathrm{BD}}(P_m^V u, P_m^V u) &= \sum_{i=0}^{\infty} \lambda_i \left(P_m^V u, z_i\right)_H \left(P_m^V u, z_i\right)_H = \sum_{i=0}^{m} \lambda_i (u, z_i)_H (u, z_i)_H \\ &\leq \sum_{i=0}^{\infty} \lambda_i \left|(u, z_i)_H\right|^2 = a_{\mathrm{BD}}(u, u). \end{aligned}$$

Therefore we obtain

$$c_{\mathrm{BD}} \left\| P_m^V u \right\|_V^2 \leq a_{\mathrm{BD}}(P_m^V u, P_m^V u) + \left\| P_m^V u \right\|_H^2 \leq a_{\mathrm{BD}}(u, u) + \|u\|_H^2 \leq (M+1)\|u\|_V^2$$

and from that we conclude that

$$\|P_m\|_{V^* \to V^*} = \left\| P_m^V \right\|_{V \to V} \leq \frac{M+1}{c_{\mathrm{BD}}}.$$

Application of Lemma 5.10 and the other boundedness results yields the result

$$\|\dot{u}_m\|_{V^*}^2 \leq c < \infty, \tag{5.45}$$

which especially means that $\dot{u}_m \in V^*$. With the definition of the space

$$X^* = L^{p'}(Q_T) + L^2(0, T; V^*)$$

we first see that the estimate

$$\|\dot{u}_m\|_{L^2(0,T;V^*)} \leq c_2 < \infty$$

follows immediately from (5.45). From the definition for the space

$$X^* = L^{p'}(Q_T) + L^2(0, T; \widetilde{H}^{-1}(\Omega))$$

we see that we can write $\dot{u}_m = 0 + \dot{u}_m$ and obtain an element in $X^*$. Therefore we also conclude that

$$\|\dot{u}_m\|_{X^*} \leq \mathcal{C}_2 < \infty$$

The proof for $\dot{\boldsymbol{v}}_m$ goes in an analogous way, by rewriting the second equation in (5.33) as

$$\dot{\boldsymbol{v}}_m = -\mathsf{P}_m \boldsymbol{f}(u_m, \boldsymbol{v}_m)$$

where $\mathsf{P}_m : H^n \to H^n$ is defined by

$$(\mathsf{P}_m \boldsymbol{f})_i := \sum_{j=0}^{m} \langle f_i, z_j \rangle_H z_j.$$

□

Gathering all the last results we have shown the following four statements:

$$\begin{aligned}
\|u_m\|_X &\leq \mathcal{C}_1 < \infty, \\
\|\dot{u}_m\|_{X^*} &\leq \mathcal{C}_2 < \infty, \\
\|\boldsymbol{v}_m\|_{[L^2(Q_T)]^n} &\leq \mathcal{C}_3 < \infty, \\
\|\dot{\boldsymbol{v}}_m\|_{[L^2(Q_T)]^n} &\leq \mathcal{C}_4 < \infty,
\end{aligned}$$

meaning that the constructed approximate solutions are bounded.

**Convergence Towards a Solution of the Bi-Domain Equations.** From these results we may now apply the theorem of Eberlein-Šmulian, see [27, Chapter V, Theorem 4], and conclude that their exist weakly converging subsequences, still denoted by $u_m, \dot{u}_m, \boldsymbol{v}_m, \dot{\boldsymbol{v}}_m$ such that

$$\begin{aligned}
u_m &\rightharpoonup u \qquad \text{in } X, \\
\dot{u}_m &\rightharpoonup u^* \qquad \text{in } X^*, \\
\boldsymbol{v}_m &\rightharpoonup \boldsymbol{v} \qquad \text{in } L^2(Q_T), \\
\dot{\boldsymbol{v}}_m &\rightharpoonup \boldsymbol{v}^* \qquad \text{in } L^2(Q_T),
\end{aligned}$$

where "$\rightharpoonup$" indicates weak convergence. However, we can conclude even more. We can immediately see that $X^* \subseteq L^{p'}(0,T;\widetilde{H}^{-1}(\Omega))$, since $p' \leq 2$ and $L^{p'}(\Omega) \subset V^*$, and that $X \subseteq L^2(0,T;H^1(\Omega))$. Hence we may formally define the space

$$\widetilde{W} := \left\{ u : u \in L^2(0,T;H^1(\Omega)),\ \dot{u} \in L^{p'}(0,T;\widetilde{H}^{-1}(\Omega)) \right\} \supset W.$$

Obviously it holds that $u_m \in \widetilde{W}$. The space $\widetilde{W}$ fits the compactness theorem of Lions, to be found in [42, Chapter 5, Theorem 5.1], and we conclude that the embedding

$$\widetilde{W} \hookrightarrow L^2(0,T;H) = L^2(Q_T)$$

is compact. Therefore we can use a well-known result, see for example [27, Chapter 5, Theorem 6], that the subsequence $u_m$ converges strongly in $L^2(Q_T)$, denoted by $u_m \to u$ in $L^2(Q_T)$. Next we will show, that the subsequences defined above converge to a solution of the bi-domain equations. Therefore we will check if each term of the weak bi-domain equations is fulfilled by the weak limits of the sequences. It was already shown in (5.41) that the initial values $u_{m0}, \boldsymbol{v}_{m0}$ converge to the initial values $u_0, \boldsymbol{v}_0$. Hence we will start with the weak derivatives. We know for a fixed $\psi \in \mathcal{C}_0^\infty(0,T)$ and $\phi \in L^2(\Omega)$ that

$$\int_0^T \int_\Omega \dot{u}_m \phi \psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} = -\int_0^T \int_\Omega u_m \phi \dot{\psi} \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}\,.$$

The last term converges to

$$\int_0^T \int_\Omega u\phi\dot{\psi} \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}$$

in the sense of $L^2(Q_T)$ due to

$$\left| \int_0^T \int_\Omega (u-u_m)\phi\dot{\psi} \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} \right| \leq T\,|\Omega|\,\|u-u_m\|_{L^2(Q_T)}\|\phi\|_{L^2(\Omega)}\left\|\dot{\psi}\right\|_{L^\infty(0,T)}$$

and the term on the right hand side goes to zero because of the strong convergence of $u_m$. Thus we conclude that

$$\lim_{m\to\infty} \int_0^T \int_\Omega \dot{u}_m\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} = -\int_0^T \int_\Omega u\phi\dot{\psi} \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}\,.$$

The term $\int_0^T \int_\Omega \cdot\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}$ can be interpreted as an element of $X^*$ and therefore we use the uniqueness of weak limits and obtain that

$$\lim_{m\to\infty} \int_0^T \int_\Omega \dot{u}_m\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} = \int_0^T \int_\Omega u^*\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}\,.$$

Putting together these results, we observe that the weak derivative of $u$ coincides with $u^*$. In an analogous way we see that the weak derivative of $\boldsymbol{v}$ coincides with $\boldsymbol{v}^*$. The next term on our list is the bilinear form $a_{\mathrm{BD}}(u_m,\phi)$. We know, that the bilinear form is induced by the bounded linear operator $A_{\mathrm{BD}}$ and is therefore continuous. From a classical theorem of measure theory we know that if a sequence converges in a $L^p$ norm for $1 \leq p \leq \infty$ than it possesses a subsequence which converges point-wise almost everywhere, i.e.: $u_n(x) - u(x) \to 0$ almost everywhere. Thus for any $\psi \in \mathcal{C}_0^\infty(0,T)$ we have

$$\left| \int_0^T a_{\mathrm{BD}}(u,\phi)\psi \ \mathrm{dt} - \int_0^T a_{\mathrm{BD}}(u,\phi)\psi \ \mathrm{dt} \right| \leq \int_0^T |a_{\mathrm{BD}}(u-u_m,\phi)|\,|\psi| \ \mathrm{dt}$$

and hence

$$\lim_{m\to\infty} \int_0^T |a_{\mathrm{BD}}(u-u_m,\phi)|\,|\psi| \ \mathrm{dt} = \int_0^T \left| a_{\mathrm{BD}}(\underbrace{\lim_{m\to\infty}(u-u_m)}_{(I)},\phi) \right| |\psi| \ \mathrm{dt}\,.$$

We may interchange the limit and the integral due to the monotone convergence theorem, see [69] for details. The term $(I)$ is zero almost everywhere, therefore the

bilinear form is zero almost everywhere and therefore the outer integral is zero almost everywhere and hence

$$\int_0^T a_{\mathrm{BD}}(u,\phi)\psi \ \mathrm{dt} = \lim_{m\to\infty} \int_0^T a_{\mathrm{BD}}(u_m,\phi)\psi \ \mathrm{dt}\,.$$

The last terms remaining are the non-linear terms. We will start with the function $g(u,\boldsymbol{v})$. By hypothesis (H2) we can write $g$ as

$$g(u_m,\boldsymbol{v}_m) = g_1(u_m) + (\boldsymbol{g}_2(u_m),\boldsymbol{v}_m) = g_1(u_m) + (\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u),\boldsymbol{v}_m)+(\boldsymbol{g}_2(u),\boldsymbol{v}_m).$$

Again we note that $u_m \to u$ point-wise almost everywhere in $Q_T$ and so also $g_1(u_m)$ converges to $g_1(u)$ almost everywhere in $Q_T$ due to the continuity of $g_1$. Furthermore, $g_1(u_m)$ is uniformly bounded in $L^{p'}$ for a fixed $T$. This follows from Lemma 5.10 by integrating the bound in $L^{p'}(\Omega)$ with respect to the time $t$. Therefore we can apply a lemma, to be found in [42, Chapter 1, Lemma 1.3] and conclude that $g_1(u_m)$ converges weakly to $g(u_m)$ in the sense of $L^{p'}(Q_T)$ which means that for any $\psi$ in $C_0^\infty(0,T)$ we have that

$$\int_0^T \langle g_1(u_m),\phi\rangle_H \psi \ \mathrm{dt} \to \int_0^T \langle g_1(u),\phi\rangle_H \psi \ \mathrm{dt}\,.$$

The same argument holds for $\boldsymbol{f}_1(u_m)$.

We have that

$$\int_0^T\int_\Omega (\boldsymbol{g}_2(u),\boldsymbol{v}_m)\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} = \int_0^T\int_\Omega (\phi\psi\boldsymbol{g}_2(u),\boldsymbol{v}_m) \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}\,.$$

Hence, by hypothesis (H3) we can interpret $\phi\psi\boldsymbol{g}_2(u)$ as an element in $H_{Q_T}$ and therefore we can conclude by the weak convergence of $\boldsymbol{v}_m$ that

$$\lim_{m\to\infty}\int_0^T\int_\Omega (\boldsymbol{g}_2(u),\boldsymbol{v}_m)\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} = \int_0^T\int_\Omega (\boldsymbol{g}_2(u),\boldsymbol{v})\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt}\,.$$

The remaining term is $(\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u),\boldsymbol{v}_m)$. We take a look at the integral

$$\int_0^T\int_\Omega (\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u),\boldsymbol{v}_m)\phi\psi \ \mathrm{d}\boldsymbol{x}\,\mathrm{dt} \le \| |\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u)|\,\phi\psi\|_H \|\boldsymbol{v}_m\|_{H_{Q_T}}.$$

Taking a closer look at the norm of the difference we may rewrite

$$\| |\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u)|\,\phi\psi\|_H^2 = \left\langle |\boldsymbol{g}_2(u_m)-\boldsymbol{g}_2(u)|^2,\phi\psi\right\rangle_H.$$

This inner product may now also be interpreted as a duality pairing between $L^\beta(Q_T)$ and $L^{p/2}(Q_T)$, because $\phi\psi \in L^p(Q_T)$ by hypothesis and so $(\phi\psi)^2 \in L^{p/2}(\Omega)$. The term $\beta$ is chosen such that $\frac{1}{\beta} + \frac{2}{p} = 1$. Then we may use Lemma 5.10 and conclude that $|\boldsymbol{g}_2(u_m) - \boldsymbol{g}_2(u)|^2$ is an element of $L^\beta(Q_T)$. We also know that $\boldsymbol{g}_2(u_m) \to \boldsymbol{g}_2(u)$ point-wise almost everywhere, due to the continuity of $\boldsymbol{g}_2$. Therefore we can use [42, Lemma 1.3] and conclude that

$$\left\langle |\boldsymbol{g}_2(u_m) - \boldsymbol{g}_2(u)|^2, \phi\psi \right\rangle_\Omega \to 0$$

and therefore also the norm goes to zero.

**Summary.** Gathering all the results from above we have now shown that the limits of the weakly converging subsequences $u_m, \dot{u}_m, \boldsymbol{v}_m, \dot{\boldsymbol{v}}_m$ fulfill

$$\int_0^T \left\langle \frac{\partial u}{\partial t}, \phi \right\rangle_H \psi \,\mathrm{dt} + \int_0^T a_{\mathrm{BD}}(u(t), \phi)\psi \,\mathrm{dt} + \int_0^T \langle g(u(t), \boldsymbol{v}(t)), \phi \rangle_H \psi \,\mathrm{dt} = \int_0^T \left\langle \widetilde{f}(t), \phi \right\rangle_H \psi \,\mathrm{dt}$$

$$\int_0^T \left\langle \frac{\partial \boldsymbol{v}}{\partial t}, \boldsymbol{\zeta} \right\rangle_{H^n} \theta \;\,\mathrm{dt} + \int_0^T \langle \boldsymbol{f}(u(t), \boldsymbol{v}(t)), \boldsymbol{\zeta} \rangle_{H^n} \theta \;\,\mathrm{dt} = 0$$

for all $(\phi, \boldsymbol{\zeta}) \in (V \cap L^p(\Omega)) \times [L^2(\Omega)]^n$ and $(\psi, \theta) \in [C_0^\infty((0,T))]^2$. This means, that we have found a solution to the variational formulation of the bi-domain equations.

**Uniqueness of weak solutions.** As a last point we will investigate briefly under which assumptions we can guarantee uniqueness of the weak solutions of the bi-domain equations. This is covered by the following result:

**Theorem 5.15.** *Let the non-linear functions $g, \boldsymbol{f}$ be continuously differentiable. The solutions to the weak bi-domain equations are unique if the symmetric gradient*

$$\frac{1}{2}\left(\mathrm{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z}) + (\mathrm{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z}))^\top\right)$$

*is positive semi-definite, where*

$$\boldsymbol{z} := (u, \boldsymbol{v})^\top,$$
$$\boldsymbol{F}(\boldsymbol{z}) := (g(u, \boldsymbol{v}), \boldsymbol{f}(u, \boldsymbol{v}))^\top.$$

*Proof.* We take two solutions $(u_1, \boldsymbol{v}_1), (u_2, \boldsymbol{v}_2)$ of the bi-domain equations . Then the differences $(u_1 - u_2, \boldsymbol{v}_1 - \boldsymbol{v}_2)$ solve in $C_0^\infty(0,T)$

$$\left\langle \frac{\partial(u_1 - u_2)}{\partial t}, w \right\rangle_\Omega + a_{\mathrm{BD}}(u_1(t) - u_2(t), w) + \langle g(u_1(t), \boldsymbol{v}_1(t)) - g(u_2(t), \boldsymbol{v}_2(t)), w \rangle_\Omega = 0$$

$$\left\langle \frac{\partial(\boldsymbol{v}_1 - \boldsymbol{v}_2)}{\partial t}, \boldsymbol{\zeta} \right\rangle_\Omega + \langle \boldsymbol{f}(u_1(t), \boldsymbol{v}_1(t)) - \boldsymbol{f}(u_2(t), \boldsymbol{v}_2(t), \boldsymbol{\zeta} \rangle_\Omega = 0$$

for all $(\phi, \boldsymbol{\zeta}) \in (V \cap L^p(\Omega) \times H^n)$. Especially for $\phi = u_1 - u_2$ and $\boldsymbol{\zeta} = \boldsymbol{v}_1 - \boldsymbol{v}_2$ and by using this and the Riesz representation theorem (Theorem 5.1) gives

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_1 - u_2\|_H^2 + a_{\mathrm{BD}}(u_1 - u_2, u_1 - u_2) + \langle g(u_1, \boldsymbol{v}_1) - g(u_2, v_2), u_1 - u_2\rangle_H = 0,$$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{v}_1 - \boldsymbol{v}_2\|_{H^n}^2 \quad + \quad \langle \boldsymbol{f}(u_1, \boldsymbol{v}_1) - \boldsymbol{f}(u_2, v_2), u_1 - u_2\rangle_{H^n} \quad = \quad 0.$$

Summing up the two equations yields

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u_1 - u_2\|_H^2 + \|\boldsymbol{v}_1 - \boldsymbol{v}_2\|_{H^n}^2\right) + a_{\mathrm{BD}}(u_1 - u_2, u_1 - u_2) \\ + \langle g(u_1, \boldsymbol{v}_1) - g(u_2, v_2), u_1 - u_2\rangle_H \\ + \langle \boldsymbol{f}(u_1, \boldsymbol{v}_1) - \boldsymbol{f}(u_2, v_2), u_1 - u_2\rangle_{H^n} = 0. \quad (5.46)\end{aligned}$$

Using the function $\boldsymbol{F}(\boldsymbol{z}) := (g(\boldsymbol{z}), \boldsymbol{f}(\boldsymbol{z}))^\top$ where $z := (u, \boldsymbol{v})^\top$ we can now define

$$\Phi(z_1, z_2) := \langle \boldsymbol{F}(z_1) - \boldsymbol{F}(z_2), \boldsymbol{z}_1 - \boldsymbol{z}_2\rangle_{H^{n+1}}.$$

By assumption the function $\boldsymbol{F}$ is continuously differentiable with respect to $\boldsymbol{z}$, so we can make a Taylor expansion, hence

$$\boldsymbol{F}(\boldsymbol{z}_1) - \boldsymbol{F}(\boldsymbol{z}_2) = \operatorname{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z})\big|_{\boldsymbol{z}=\boldsymbol{\xi}} \cdot (\boldsymbol{z}_1 - \boldsymbol{z}_2),$$

with $\xi = \theta \boldsymbol{z}_1 + (1-\theta)\boldsymbol{z}_2$ and $\theta \in (0, 1)$. At this point we cannot say much about the eigenvalues of the gradient, but we know that the eigenvalues of the symmetric gradient

$$\frac{1}{2}\left(\operatorname{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z}) + (\operatorname{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z}))^\top\right)$$

have to be real-valued. Denote the eigenvalues by $\lambda_1(\boldsymbol{z}) \le \lambda_2(\boldsymbol{z}) \le \cdots \le \lambda_{n+1}(\boldsymbol{z})$. By assumption those eigenvalues have to be greater or equal to zero due to the positive semi-definiteness of the symmetric gradient. Using this we can estimate

$$\begin{aligned}\Phi(\boldsymbol{z}_1, \boldsymbol{z}_2) = \left\langle \operatorname{grad}_{\boldsymbol{z}} \boldsymbol{F}(\boldsymbol{z})\big|_{\boldsymbol{z}=\boldsymbol{\xi}}(\boldsymbol{z}_1 - \boldsymbol{z}_2), \boldsymbol{z}_1 - \boldsymbol{z}_2\right\rangle_{H^{n+1}} \\ \ge \lambda_1 \|\boldsymbol{z}_1 - \boldsymbol{z}_2\|_{H^{n+1}}^2 = \lambda_1\left(\|u_1 - u_2\|_H^2 + \|\boldsymbol{v}_1 - \boldsymbol{v}_2\|_{H^{n+1}}^2\right). \quad (5.47)\end{aligned}$$

Going back to equation (5.46) we see that

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u_1 - u_2\|_H^2 + \|\boldsymbol{v}_1 - \boldsymbol{v}_2\|_{H^n}^2\right) = -a_{\mathrm{BD}}(u_1 - u_2, u_1 - u_2) \\ - \langle g(u_1, \boldsymbol{v}_1) - g(u_2, v_2), u_1 - u_2\rangle_H \\ - \langle \boldsymbol{f}(u_1, \boldsymbol{v}_1) - \boldsymbol{f}(u_2, v_2), u_1 - u_2\rangle_{H^n},\end{aligned}$$

which may be rewritten as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right) \;=\; -a_{\mathrm{BD}}(u_1-u_2,u_1-u_2)-\Phi(\boldsymbol{z}_1,\boldsymbol{z}_2)$$

Next we see that

$$-a_{\mathrm{BD}}(u_1-u_2,u_1-u_2)\le -c_{\mathrm{BD}}\|u_1-u_2\|_V^2+\|u_1-u_2\|_H^2\le\|u_1-u_2\|_H^2.$$

Together with the estimate (5.47) we obtain

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right)&\le\|u_1-u_2\|_H^2\\ -\lambda_1\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right)&\le(1-\lambda_1)\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right).\end{aligned}$$

Here we can apply Gronwall's lemma (Lemma 5.12) and conclude that

$$\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right)\le\widetilde{C}\left(\|u_1(0)-u_2(0)\|_H^2+\|\boldsymbol{v}_1(0)-\boldsymbol{v}_2(0)\|_{H^n}^2\right),$$

hence

$$\left(\|u_1-u_2\|_H^2+\|\boldsymbol{v}_1-\boldsymbol{v}_2\|_{H^n}^2\right)=0,$$

which proves the uniqueness. □

## 5.4 Analysis of the Non-Linear Elasticity Models

We will now turn our attention to the decoupled models of non-linear incompressible quasi-static elasticity with the special constitutive model by Holzapfel as discussed in Section 3.4.2. The governing equations in material coordinates are to find $(\boldsymbol{U},\tilde{p})$ in suitable spaces such that

$$\begin{aligned}\operatorname{Div}\mathbf{S}&=0 && \text{in }\Omega, && (5.48)\\ \det\mathbf{F}&=1 && \text{in }\Omega, && (5.49)\\ \gamma_0^{\mathrm{int}}\boldsymbol{U}&=\boldsymbol{g}_D && \text{on }\Gamma_D, && (5.50)\\ \mathbf{S}^\top\boldsymbol{N}&=\boldsymbol{g}_N && \text{on }\Gamma_N, && (5.51)\\ \mathbf{S}&=\frac{\partial W(\mathbf{F})}{\partial\mathbf{F}}-\tilde{p}\mathbf{F}^{-1} && && (5.52)\end{aligned}$$

holds. The special form of $\frac{\partial W(\mathbf{F})}{\partial\mathbf{F}}$ is given by the Holzapfel model and reads as

$$\begin{aligned}\frac{\partial W(\mathbf{F})}{\partial\mathbf{F}}=\;&a\exp(b(I_1-3))\mathbf{F}^\top+\exp(b_f(I_{4f}-1)^2)\boldsymbol{f}_0\otimes\boldsymbol{f}_0\\ &+2a_s(I_{4s}-1)\exp(b_s(I_{4s}-1)^2)\boldsymbol{s}_0\otimes\boldsymbol{s}_0\\ &+a_{fs}I_{8fs}\exp(b_{fs}I_{8fs}^2)(\boldsymbol{f}_0\otimes\boldsymbol{s}_0+\boldsymbol{s}_0\otimes\boldsymbol{f}_0),\end{aligned}$$

which was introduced and discussed in Section 3.4.2. For the mathematical analysis we will stay with the Lagrangian form of the equilibrium equations. In the analysis of non-linear elasticity it is usual to treat an equivalent minimization problem instead of analyzing the partial differential equations. But before doing this we need to introduce some basic tools from variational calculus.

### 5.4.1 Tools from Variational Calculus

For proving the existence of solutions to the problem of non-linear elasticity we need some well-known tools from variational calculus.

**Definition 5.14.** *Let $X$ be a Banach space. A functional $I\colon X \to \mathbb{R} \cup \{\infty\}$ is called* sequentially weakly lower semi-continuous *if for any sequence $\{u_n\}_{n\in\mathbb{N}} \subset X$ which converges weakly to a limit $u \in X$ it holds that*

$$I(u) \leq \liminf_{n\to\infty} I(u_n).$$

**Definition 5.15.** *Let $X$ be a Banach space. A functional $I\colon X \to \mathbb{R} \cup \{\infty\}$ is called* coercive *if for any sequence $\{u_n\}_{n\in\mathbb{N}} \subset X$ with $\|u_n\|_X \to \infty$ it holds that $I(u_n) \to \infty$.*

With these two important definitions we can state a rather abstract existence theorem from variational calculus:

**Theorem 5.16** (Tonelli's Theorem)**.** *Let $X$ be a reflexive Banach space and let there be given a coercive and sequentially weakly lower semi-continuous functional $I\colon X \to \mathbb{R} \cup \{\infty\}$. Then the minimization problem of finding $u \in X$ such that*

$$I(u) = \inf_{v\in X} I(v)$$

*admits at least one solution.*

*Proof.* We choose an infimizing sequence $\{u_n\}_{n\in\mathbb{N}}$ which means that

$$\lim_{n\to\infty} u_n = \inf_{v\in X} I(v).$$

Due to the coercivity of $I$ the sequence $u_n$ has to be bounded, otherwise we could choose a subsequence $u_{n'}$ with $\|u_{n'}\|_X \to \infty$ and with the coercivity of $I$ we would conclude that $\lim_{n'\to\infty} I(u_{n'}) = \infty$ which is a contradiction. Therefore the sequence $u_n$ is a bounded sequence in $X$. With the reflexivity of $X$ and the theorem of Eberlein-Šmulian we conclude that we can extract a subsequence $u_{n_k}$ in $M$ with $u_{n_k} \rightharpoonup u$. Now we know that $I$ is sequentially weakly lower semi-continuous and hence

$$I(u) \leq \liminf_{k\to\infty} I(u_{n_k}) = \lim_{k\to\infty} I(u_{n_k}) = \inf_{v\in X} I(v) \leq I(u),$$

therefore $I(u) = \inf_{v\in X} I(v)$. □

This rather straight-forward result is the key ingredient for proofing existence of solutions to the problem of non-linear elasticity, by reformulating the non-linear partial differential equations as an equivalent minimization problem. It remains to show that the occurring functional fulfills the assumptions of Tonelli's theorem and we are pretty much done. For the concrete application to non-linear elasticity we need to introduce some new concepts of convexity.

**Definition 5.16.** *Let* $\boldsymbol{u}\colon \mathbb{R}^3 \to \mathbb{R}$ *be a function. We say that* $u$ *is* convex *if for all* $\theta \in [0,1]$ *and for all* $\lambda, \mu \in \mathbb{R}^3$ *it holds that*

$$\boldsymbol{u}(\theta\boldsymbol{\lambda} + (1-\theta)\boldsymbol{\mu}) \leq \theta\boldsymbol{u}(\boldsymbol{\lambda}) + (1-\theta)\boldsymbol{u}(\boldsymbol{\mu}).$$

**Definition 5.17** (Polyconvexity)**.** *A function* $F\colon \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{\infty\}$ *is called* polyconvex *if there exists a convex function* $P\colon \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R}$ *which for any* $\mathsf{A} \in \mathbb{R}^{3\times 3}$ *has the form*

$$P(\mathsf{A}) = P(\mathsf{A}, \operatorname{Adj}\mathsf{A}, \det \mathsf{A}),$$

*and it holds that*

$$F(\mathsf{A}) = P(\mathsf{A}).$$

*Here the* adjugate *of* $\mathsf{A}$ *is defined as* $\operatorname{Adj}\mathsf{A} := \det(\mathsf{A})\mathsf{A}^{-1}$*, provided* $\mathsf{A}$ *is invertible.*

**Remark 5.9.** *The definition of polyconvexity as given above is not unique, i.e. there are many possibilities of choosing the function* $P$*, see [15, p. 157–158] for details.*

The two convexity properties are connected through the following theorem:

**Theorem 5.17.** *If* $F\colon \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{\infty\}$*. Suppose* $F$ *is convex. Then* $F$ *is also polyconvex.*

*Proof.* See [15, Theorem 5.3]. □

Next we are going to introduce some notations for differentiating matrix or tensor-valued functions similar to the definitions already made in Chapter 3.

**Definition 5.18.** *Let* $\mathsf{A}, \mathsf{B} \in \mathbb{R}^{3\times 3}$*. A scalar product on* $R^{3\times 3}$ *is defined by*

$$(\mathsf{A}, \mathsf{B})_F := \mathsf{A} : \mathsf{B} = \operatorname{tr}(\mathsf{B}^\top \mathsf{A})$$

*which induces the* Frobenius norm

$$\|\mathsf{A}\|_F := \sqrt{(\mathsf{A}, \mathsf{A})_F}.$$

**Definition 5.19.** *Let* $\Omega \subset \mathbb{R}^3$ *be a bounded domain. Let* $f\colon \Omega_r \times \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ *be a function. We then define:*

- $\partial_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A}) := \operatorname{grad} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A}) = (\frac{\partial f}{\partial x_i})_{1 \leq i \leq 3} \in \mathbb{R}^3$.
- $\partial_{\boldsymbol{u}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A}) := (\frac{\partial f}{\partial u_i})_{1 \leq i \leq 3} \in \mathbb{R}^3$.
- $\partial_{\mathsf{A}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A}) := (\frac{\partial f}{\partial A_{ij}})_{\substack{1 \leq i \leq 3 \\ 1 \leq j \leq 3}} \in \mathbb{R}^{3\times 3}$.
- $D_{\boldsymbol{u}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A})[\boldsymbol{v}] := (\partial_{\boldsymbol{u}} f, \boldsymbol{v})$.
- $D_{\mathsf{A}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A})[\mathsf{B}] := \langle \partial_{\mathsf{A}} f, \mathsf{B} \rangle$.
- $D^2_{\mathsf{A}} f(\boldsymbol{x}, \boldsymbol{u}, \mathsf{A})[\mathsf{B}, \mathsf{C}] := \sum_{i,j,k,l=1}^{3} \frac{\partial^2 f}{\partial A_{ij} \partial A_{kl}} B_{ij} C_{kl}$.

**Remark 5.10.** *The two definitions above can also be applied to second–order tensors* $\mathbf{F}$.

The next lemma is going to turn out very useful for our purposes.

**Lemma 5.18.** *Let* $K$ *be a convex subset of* $\mathbb{R}^{3\times 3}$ *and let* $F\colon K \to \mathbb{R}$ *be two times continuously differentiable. Then the following statements are equivalent:*

1. $F$ *is convex.*
2. $D^2_{\mathsf{A}} F(\mathsf{A})[\mathsf{H}, \mathsf{H}] \geq 0$ *for all* $\mathsf{A} \in K$ *and for all* $\mathsf{H} \in \operatorname{Lin}(K)$*, where* $\operatorname{Lin}(K)$ *is the linear hull of* $K$.

*Proof.* See [67]. □

Summarizing all the lemmatas and theorems above we can state the very useful connection between polyconvexity and sequential weak lower semi-continuity.

**Theorem 5.19.** *Let* $\Omega \subset \mathbb{R}^3$ *be a bounded Lipschitz-domain. Let there be given a polyconvex continuous coercive function* $f\colon \mathbb{R}^{3\times 3} \to [0, \infty]$*. Then the functional*

$$\begin{aligned} I\colon W^{1,p}(\Omega) &\to [0, \infty] \\ u &\mapsto \int_{\Omega} f(\mathbf{F}) \ \mathrm{d}\boldsymbol{X} \end{aligned}$$

*is sequentially weakly lower semi-continuous provided* $p > 3$.

*Proof.* See [15, Theorem 3.20 and Theorem 8.16]. □

### 5.4.2 The Equivalent Minimization Problem

As discussed above we will focus on a minimization problem which will turn out to be equivalent to finding solutions for the governing equations of non-linear elasticity. Therefore we will briefly discuss some physical aspects of non-linear elasticity. The most deep result in classical mechanics is the *Hamiltonian principle* or *principle of least action*. It states that the dynamics of a physical system is determined by a variational problem for a functional based on a single function, the *Lagrangian*, which contains all physical information concerning the system and the forces acting on it. We will not go into the details of classical mechanics as this is beyond the scope of this thesis. For details one may start with [5].

What we will actually use is the fact that we can equivalently minimize a functional instead of solving a system of non-linear partial differential equations. However, for convenience we will show how one can derive the system of incompressible non-linear elasticity from a Lagrangian.

**Theorem 5.20.** *Let $\Omega \subset \mathbb{R}^3$ be an bounded Lipschitz domain and let $\partial\Omega = \bar{\Gamma}_D \cup \bar{\Gamma}_N$. Further assume a given strain energy function $W(\mathbf{F})$ corresponding to a hyper-elastic material law and $p > 3$. Then any solution to the minimization problem to find $\boldsymbol{U} \in M$ such that*

$$\boldsymbol{u} = \inf_{\boldsymbol{y} \in M} I(\boldsymbol{y}), \tag{5.53}$$

$$M := \left\{ \boldsymbol{y} \in [W^{1,p}(\Omega)]^3 \mid \gamma_0^{int} \boldsymbol{y} = \boldsymbol{g}_D \text{ on } \Gamma_D \text{ and } \det \mathbf{F} = 1 \right\}, \tag{5.54}$$

$$I(\boldsymbol{x}) := \int_\Omega W(\mathbf{F}) \ \mathrm{d}\boldsymbol{X} - \int_{\Gamma_N} (\boldsymbol{g}_N, \boldsymbol{x}) \ ds_{\boldsymbol{X}} \tag{5.55}$$

*solves the weak system of partial differential equations of non-linear incompressible elasticity, i.e.$(\boldsymbol{U}, \tilde{p}) \in [W^{1,p}_{g_D}(\Omega)]^3 \times L^{p/d}(\Omega)$ solves*

$$\int_\Omega \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}} : \operatorname{Grad} \boldsymbol{y} \ \mathrm{d}\boldsymbol{X} + \int_\Omega (\tilde{p}\mathbf{F}^{-\top}) : \operatorname{Grad} \boldsymbol{y} \ \mathrm{d}\boldsymbol{X} = \int_{\Gamma_N} \left\langle \boldsymbol{g}_N, \gamma_0^{int}(\boldsymbol{v}) \right\rangle \ \mathrm{ds}_{\boldsymbol{X}}, \tag{5.56}$$

$$\int_\Omega \det \mathbf{F} \mu \ \mathrm{d}\boldsymbol{X} = \int_\Omega \mu \ \mathrm{d}\boldsymbol{X}, \tag{5.57}$$

*for all $\boldsymbol{y} \in [W^{-1,q}(\Omega)]^d$ and $\mu \in L^{\frac{p}{p-d}}(\Omega)$, where we have*

$$[W^{1,p}_{g_D}(\Omega)]^d := \left\{ \boldsymbol{y} \in [W^{1,p}(\Omega)]^d \;\middle|\; \gamma_0^{int} \boldsymbol{y} = \boldsymbol{g}_D \text{ on } \Gamma_D \right\}.$$

*Proof.* We consider the stationary points of the first variation of the functional $I(\boldsymbol{x})$. However we need to incorporate the incompressibility constraint. Therefore we

introduce a Lagrange-functional $F(\boldsymbol{U}, \lambda)$ defined by

$$F(\boldsymbol{U}, \lambda) := I(\boldsymbol{U}) + \lambda(\det \mathbf{F} - 1).$$

Now we calculate the stationary points of the first variation of this Lagrangian, thus we obtain

$$\nabla_{s,t} F(\boldsymbol{U} + s\boldsymbol{y}, \lambda + t\mu)\big|_{s,t=0} = \mathbf{0},$$

for arbitrary $\boldsymbol{y} \in [W^{1,p}_{g_D}(\Omega)]^3$ and $\mu \in L^{p/3}(\Omega)$ where $\nabla_{s,t} = (\partial_s, \partial_t)^\top$. Applying the chain rule this yields

$$\begin{aligned}
&\partial_s F(\boldsymbol{U} + s\boldsymbol{y}, \lambda + t\mu)\big|_{s,t=0} = \\
&\qquad \int_\Omega \frac{\partial W}{\partial \mathbf{F}} : \operatorname{Grad} \boldsymbol{y} \, \mathrm{d}\boldsymbol{X} - \int_{\Gamma_N} \langle \boldsymbol{g}_N, \boldsymbol{y} \rangle \, \mathrm{ds}_{\boldsymbol{X}} + \int_\Omega (\lambda \det(\mathbf{F}) \mathbf{F}^{-\top}) : \operatorname{Grad} \boldsymbol{y} \, \mathrm{d}\boldsymbol{X}, \\
&\partial_t F(\boldsymbol{U} + s\boldsymbol{y}, \lambda + t\mu)\big|_{s,t=0} = \int_\Omega (\det \mathbf{F} - 1)\mu \ \mathrm{d}\boldsymbol{X},
\end{aligned}$$

where we used that $\frac{\partial \det \mathbf{F}}{\partial \mathbf{F}} = \det(\mathbf{F})\mathbf{F}^{-\top}$ see for example [31, Chapter 1]. Now we introduce a new variable $\tilde{p} := \lambda \det \mathbf{F}$ and set both equations to zero, arriving at the desired result. □

**Remark 5.11.** *It is also possible to include the essential Dirichlet boundary conditions with the help of a Lagrangian. For more details the reader may refer to [75].*

**Remark 5.12.** *The procedure used in the proof is applicable to many physical phenomenas. The Hamiltonian principle can be reformulated in a way, that the stationary points of the functional solves the* weak Euler-Lagrange equations*, see [12, 15] for details*

**Remark 5.13.** *One can even show that the minimization problem is* equivalent *to solving the weak Euler-Lagrange equations. See [12, 15] for details.*

We have seen that it suffices to look for solutions of the minimization problem (5.53)–(5.55). The existence of minimizers can be guaranteed with a result from John Ball first published in [7], but it may also be found in [12, 15]. We state the result in a way that fits our purposes better.

**Theorem 5.21.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, $p > 3$, $\boldsymbol{g}_N \in L^1(\Gamma_N)$ and $\boldsymbol{g}_D \in W^{1-1/p,p}(\Gamma_D)$. Further, let $W \colon \mathbb{R}^{3\times 3} \to [0, \infty]$ be polyconvex and coercive. Finally let the set $M$ be defined as*

$$M := \left\{ \boldsymbol{y} \in [W^{1,p}(\Omega_r)]^3 \mid \gamma_0^{int} \boldsymbol{y} = \boldsymbol{g}_D \text{ on } \Gamma_D \right\}$$

*and there exists an element $\boldsymbol{y}_0 \in M$ such that*

$$\int_\Omega W(\operatorname{Grad} \boldsymbol{y}_0) \ \mathrm{d}\boldsymbol{X} < \infty.$$

*Then there exists at least one element* $\boldsymbol{U} \in M$ *which minimizes* $I(\boldsymbol{y})$*:*

$$I(\boldsymbol{U}) \leq I(\boldsymbol{y}) \qquad \text{for all } \boldsymbol{y} \in M,$$
$$I(\boldsymbol{y}) := \int_{\Omega} W(\mathbf{F}) \ \mathrm{d}\boldsymbol{X} - \int_{\Gamma_N} (\boldsymbol{g}_N, \boldsymbol{y}) \ ds_{\boldsymbol{X}}.$$

*Proof.* See [12, Theorem 7.7-1]. □

We can not apply this theorem directly as we have an incompressible material. Therefore we need to have a set $\widetilde{M}$ defined as

$$\widetilde{M} := \left\{ \boldsymbol{y} \in [W^{1,p}(\Omega_r)]^3 \mid \gamma_0^{\text{int}} \boldsymbol{y} = \boldsymbol{g}_D \text{ on } \Gamma_D \text{ and } \det \mathbf{F} = 1 \right\}.$$

To bypass this we will define the following new strain energy function

$$\widetilde{W}(\mathbf{F}) := \begin{cases} W(\mathbf{F}) & \text{if } \det \mathbf{F} = 1, \\ \infty & \text{else.} \end{cases} \tag{5.58}$$

Then minimizing $\widetilde{W}(\mathbf{F})$ over the same set as in Theorem 5.21 is equivalent to minimize $W(\mathbf{F})$ over the set $\widetilde{M}$. Thus we have to show that $\widetilde{W}$ fulfills the assumptions of Theorem 5.21. The first one is covered by the following result:

**Lemma 5.22.** *Let* $W \colon K \subset \mathbb{R}^{3\times 3} \to [0, \infty]$*,* $K$ *convex, be a convex function. Then the function* $\widetilde{W}$ *as defined in* (5.58) *is polyconvex.*

*Proof.* We have to show that there exists a convex function $\mathcal{W}$ such that

$$\mathcal{W}(\mathbf{F}, \mathrm{Adj}\mathbf{F}, \det \mathbf{F}) = \widetilde{W}(\mathbf{F}).$$

Therefore we define

$$\mathcal{W}(\mathbf{F}, \det \mathbf{F}) = \widetilde{W}(\mathbf{F}, \det \mathbf{F}).$$

Then we see immediately that the function $\mathcal{W}$ is convex with respect to the new variables $\mathbf{F}$ and $\det \mathbf{F}$ as

$$\mathcal{W}(\lambda_1 \mathbf{F} + (1-\lambda_1)\mathbf{G}, \lambda_2 \det \mathbf{F} + (1-\lambda_2) \det \mathbf{G}) = \begin{cases} W(\lambda_1 \mathbf{F} + (1-\lambda_1)\mathbf{G}) & \lambda_2 \det \mathbf{F} + (1-\lambda_2) \det \mathbf{G} = 1, \\ \infty & \text{else.} \end{cases}$$

Next we use the convexity of $W$ and we can conclude the statement. □

Due to Lemma 5.22, it remains to show that the given strain energy function is convex. Therefore we will investigate the structure of the Holzapfel model.

**Theorem 5.23.** *The function* $W(\mathbf{F}) = W(\mathbf{C})\colon K \subset \mathbb{R}^{3\times 3} \to [0,\infty]$, $K$ *convex, as defined by the Holzapfel model* (3.34) *is convex.*

Before proving this lemma we need the following technical result:

**Lemma 5.24.** *It holds:*

$$\begin{aligned}\frac{\partial}{\partial \mathbf{C}} \operatorname{tr} \mathbf{C} &= \mathbf{I},\\ \frac{\partial}{\partial \mathbf{C}}(\boldsymbol{v}, \mathbf{C}\boldsymbol{v}) &= \boldsymbol{v} \otimes \boldsymbol{v},\\ \frac{\partial}{\partial \mathbf{C}}(\boldsymbol{v}, \mathbf{C}\boldsymbol{w}) &= \frac{1}{2}\left(\boldsymbol{v} \otimes \boldsymbol{w} + \boldsymbol{w} \otimes \boldsymbol{v}\right).\end{aligned}$$

*Proof.* We start with the first one:

$$\left(\frac{\partial}{\partial \mathbf{C}} \operatorname{tr} \mathbf{C}\right)_{ij} = \frac{\partial}{\partial C_{ji}} \operatorname{tr} \mathbf{C} = \frac{\partial}{\partial C_{ji}} \sum_{i=1}^{d} C_{ii} = \delta_{ij}.$$

For the second statement we obtain:

$$\left(\frac{\partial}{\partial \mathbf{C}}(\boldsymbol{v}, \mathbf{C}\boldsymbol{v})\right)_{ij} = \frac{\partial}{\partial C_{ji}} \sum_{t,s=1}^{3} C_{ts} v_s v_t = \delta_{js}\delta_{it} v_s v_t = v_i v_j = (\boldsymbol{v} \otimes \boldsymbol{v})_{ij}.$$

Finally, for the last statement we can write

$$\begin{aligned}\left(\frac{\partial}{\partial \mathbf{C}}(\boldsymbol{v}, \mathbf{C}\boldsymbol{w})\right)_{ij} &= \frac{\partial}{\partial C_{ji}} \sum_{s,t=1}^{3} C_{st} v_s w_t = \frac{\partial}{\partial C_{ji}} \sum_{s,t=1}^{3} C_{st} \frac{1}{2}\left(v_s w_t + v_t w_s\right)\\ &= \delta_{js}\delta_{it} \frac{1}{2}\left(v_s w_t + v_t w_s\right) = \left(\frac{1}{2}\left(\boldsymbol{v} \otimes \boldsymbol{w} + \boldsymbol{w} \otimes \boldsymbol{v}\right)\right)_{ij}.\end{aligned}$$

□

With these auxiliary results we are now able to prove Theorem 5.23.

*Proof of Theorem 5.23.* We first state again the definition of $W(\mathbf{C})$ from (3.34):

$$\begin{aligned}W(\mathbf{C}) := \frac{a}{2b} \exp\left(b(I_1(\mathbf{C}) - 3)\right) + \sum_{i=f,s} \frac{a_i}{2b_i}\left(\exp\left(b_i(I_{4i}(\mathbf{C}) - 1)^2\right) - 1\right)\\ + \frac{a_{fs}}{2b_{fs}}\left(\exp\left(b_{fs} I_{8fs}(\mathbf{C})^2\right) - 1\right).\end{aligned}$$

For showing convexity we need to check the equivalent characterization of convexity as given in Lemma 5.18. Therefore we need to check whether

$$D^2_{\mathbf{C}} W(\mathbf{C})[\mathbf{D},\mathbf{D}] \geq 0$$

holds for arbitrary second-order tensors $\mathbf{C} \in K$ and $\mathbf{D} \in \mathrm{Lin}K$. To this end we rewrite the strain energy function in four terms:

$$\begin{aligned}
\mathrm{I}(\mathbf{C}) &:= \frac{a}{2b} \exp\left(b(I_1(\mathbf{C})-3)\right), \\
\mathrm{II}(\mathbf{C}) &:= \frac{a_f}{2b_f} \left(\exp\left(b_f(I_{4f}(\mathbf{C})-1)^2\right)-1\right), \\
\mathrm{III}(\mathbf{C}) &:= \frac{a_s}{2b_s} \left(\exp\left(b_s(I_{4s}(\mathbf{C})-1)^2\right)-1\right), \\
\mathrm{IV}(\mathbf{C}) &:= \frac{a_{fs}}{2b_{fs}} \left(\exp\left(b_{fs} I_{8fs}(\mathbf{C})^2\right)-1\right).
\end{aligned}$$

Therefore, using Lemma 5.24 we obtain

$$\begin{aligned}
D^2_{\mathbf{C}} I(\mathbf{C})[\mathbf{D},\mathbf{D}] &= ab \exp\left(b(I_1(\mathbf{C})-3)\right) \sum_{i,j,k,l=1}^{3} \delta_{ij}\delta_{kl} D_{ij} D_{kl} \\
&= ab \exp\left(b(I_1(\mathbf{C})-3)\right) (\mathrm{tr}\,\mathbf{D})^2,
\end{aligned}$$

and hence we need that $ab \geq 0$. Proceeding in the same way we can build

$$\begin{aligned}
&D^2_{\mathbf{C}} II(\mathbf{C})[\mathbf{D},\mathbf{D}] = \\
&\quad a_f \exp\left(b_f(I_{4f}(\mathbf{C})-1)^2\right) \left(2b_f(I_{4f}-1)^2+1\right) \sum_{i,j,k,l=1}^{3} (\boldsymbol{f}_0)_i (\boldsymbol{f}_0)_j (\boldsymbol{f}_0)_k (\boldsymbol{f}_0)_l D_{ij} D_{kl} \\
&\qquad = a_f \exp\left(b_f(I_{4f}(\mathbf{C})-1)^2\right) \left(2b_f(I_{4f}-1)^2+1\right) |(\mathbf{D}\boldsymbol{f}_0, \boldsymbol{f}_0)|^2 .
\end{aligned}$$

This results in claiming that

$$a_f \geq 0 \quad \text{and} \quad b_f \geq -\frac{1}{2(I_{4f}(\mathbf{C})-1)^2}.$$

The same results hold for the summand $III(\mathbf{C})$. To finish up we finally look at the summand $IV$. For the derivative we obtain in a similar way as for the summand $II(\mathbf{C})$

$$D^2_{\mathbf{C}} IV(\mathbf{C})[\mathbf{D},\mathbf{D}] = a_{fs} \exp\left(b_f I_{8fs}^2\right) \left(2b_{fs} I_{8fs}^2 + 1\right) |(\mathbf{D}\boldsymbol{f}_0, \boldsymbol{s}_0)|^2 ,$$

yielding

$$a_{fs} \geq 0 \quad \text{and} \quad b_{fs} \geq -\frac{1}{2I_{8fs}(\mathbf{C})^2}.$$

By choosing all the constants appropriately we see that the sum of all the second-order derivatives is always greater or equal than zero and thus we can apply Lemma 5.18 and conclude that $W(\mathbf{C})$ is convex. □

Having shown Theorem 5.23 we can now finally prove the existence theorem for the problem of incompressible non-linear elasticity, which is just an application of Theorem 5.21.

**Theorem 5.25.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain and $p > 3$. Furthermore, let the assumptions of Theorem 5.21 be fulfilled. Then the weak system of partial differential equations of non-linear incompressible elasticity* (5.56)–(5.57) *has at least one solution* $(\boldsymbol{U}, \tilde{p}) \in [W^{1,p}(\Omega)]^3 \times L^{p/3}(\Omega)$.

*Proof.* The proof follows by applying Theorem 5.21 to the polyconvex strain energy function $\widetilde{W}$. □

# Summary & Outlook

This thesis can be categorized in two classes namely:

- The modelling of the coupled electro–mechanical activation of the human heart:
  - general physiological details about the human heart.
  - the modelling of the electrical activation of the human heart.
  - the modelling of the mechanical activation of the human heart.
  - some aspects about the coupling of the two different models.
- The mathematical analysis of the decoupled models:
  - existence and uniqueness of solutions to the governing equations in the electrical model.
  - existence of solutions to the governing equations of the mechanical model.

In Chapter 1 we discussed the main physiological properties of the human heart. This involved basic facts about the structure and its shape but also a rather vivid description of the cardiac cycle. This chapter was mainly a motivation for the following chapters.

In Chapter 2 we went into the details of the electrical activation of the human heart. Firstly, we presented the historic dipole model, going back to Einthoven, for the human heart. Therefore we introduced the Maxwell equations and made some simplifications and arrived at a standard Poisson equation for finding the dipole distribution of the human heart. This model, however, did not suffice for developing more sophisticated and physiological more relevant models. As mentioned in the introduction, the future of cardiomechanics is to be found in multi-scale and multi-physics problems. Therefore we started from scratch and introduced the well-known bi-domain model of Tung, which is motivated by a homogenization procedure of myocardial tissue. This model is more accurate to describe the electrical activation of the human heart, with the drawback of resulting in a coupled system of essentially non-linear partial and ordinary differential equations.

In Chapter 3 we discussed the mechanical activation of the human heart. There we started with introducing the common notations from tensor algebra and non-linear continuum mechanics. The governing equations in non-linear continuum mechanics, which are fairly standard, though essential non-linear in type, and well-known, were also introduced. We focused on incompressible material behavior, which lead to major simplifications in the models. The interesting aspects in this chapter were about choosing a material model for describing the passive mechanical behavior of myocardial tissue. To this end we considered the incompressible Holzapfel model [32] and discussed it in a quite detailed way.

In Chapter 4 we then started to consider the coupling of the two distinct models discussed in the preceding chapters. The coupling of the two models was done by a volume coupling. We first started to couple the bi-domain equations with the mechanic feedback of the myocardial tissue. This was achieved by transforming the equations from Eulerian to Lagrangian coordinates. Furthermore we had to include the mechanic feedback in the system of ordinary differential equations which arose in the derivation of the bi-domain equations. On the other hand we coupled the system of non-linear elasticity by introducing a new material model which depends on the electrical changes. We presented two possibilities to do this, the active strain and active stress formulation and focused on the active stress formulation.

In Chapter 5 we presented the analysis for both decoupled models. For the electrical model we first considered a time-independent elliptic sub-system. This was done in an abstract operator setting. In this setting we were able to eliminate one of the occurring variables, via a Schur complement. This leads to the definition of the bi-domain operator $A_{\mathrm{BD}}$. We then studied the properties of this operator and derived a spectral decomposition of it. The eigenvectors of the bi-domain operator $A_{\mathrm{BD}}$ turned out to be very useful in the construction of a unique weak solution to the full bi-domain equations. This was achieved with a Faedo-Galerkin technique, inspired by [9].

For the analysis of the system of non–linear elasticity we draw on tools from variational calculus. The main statement was that solving the partial differential equations is equivalent to finding minimizers of a particular functional. We first introduced the most important tools and theorems from variational calculus. The most essential property in this context was the concept of sequential weak lower semi-continuity. With this we could show that we can find minimizers to a given integral functional provided this functional has this special property. In the special case of non-linear elasticity this result was achieved by John Ball [7]. We also introduced the concept of polyconvex functions which is the right classification of physical strain energy functions in classical continuum mechanics. In the rest of the chapter we showed that polyconvex strain energy functions lead to sequentially weak lower semi-continuous functionals and showed that the specific strain energy function introduced by Holzapfel [32] has the property of polyconvexity. With this we were able to show that the system

of incompressible non-linear elasticity, modeling the passive mechanical behavior of the human heart, admits at least one solution.

For the future there is a broad range of perspectives to be attacked. It would be interesting to incorporate electrochemical models which take account of sub-cellular activities. This builds a bridge to biophysics. In the mechanic modeling one could think about the incorporation of residual stresses in biological tissue. Furthermore, in the coupling of the two distinct models we did not focus on the active strain formulation. This may also be an interesting aspect.

From a mathematical point of view, we still lack of a sound numerical analysis for the coupled equations. From the perspective of numerics it is very interesting how to actually solve such multi-scale multi-physics problems in an efficient way using the finite element method. For the pure electric activation of the human heart there can already be found software, like CARP [62], which are able to solve large problems. More specifically, it would be interesting to use domain decomposition methods, like the *Finite Element Tearing and Interconnecting Method (FETI)*, and combine existing codes for solving the pure mechanic and the pure electric problem in view of a real clinical application.

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