Computational Structural Geology and Rock Physics

Rechnergestützte Strukturgeologie und Gesteinsphysik

Habilitation treatise
Habilitationsschrift

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Everything we do in earth sciences is modeling.

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Summary

This Habilitation treatise comprises a selection of my scientific work that I published since finishing my PhD in 2009. My general scientific aim is the mechanical understanding of geological, geodynamical, and geophysical phenomena, for which I primarily employ self-developed numerical simulation tools, but also integrate my theoretical work with field and laboratory data. My process-oriented research that I developed since my PhD may be divided into two main research fields, which also define the outline of this Habilitation treatise:

1. *Computational structural geology*
2. *Computational rock physics*

The Habilitation treatise starts with an overview and some general thoughts about modeling. The three principal purposes a model fulfills are: simplification, generalization, and parameterization of nature. Since it will never be possible to grasp the full complexity of natural processes, simplification is essential in all earth sciences; hence the statement: "*Everything we do in earth sciences is modeling!*"

After providing a brief historical account of both my main research fields, I put my own contribution into the current research landscape. I also provide some personal research perspectives for the future and teaching philisophies that I follow. Finally, I summarize my publications, which are attached to the Habilitation treatise as appendices. Thereby, I do not order my publications chronologically, but after a train-of-thoughts principle, which helps identify connections between my publications and important preceding publications.

My contribution to computational structural geology mainly comprises studies on buckle folding. In a first part, I present some more basic work quantifying strain distribution in and around buckle folds (i.e., neutral line, foliation refraction patterns) and fold growth in 3D. Consecutively, two applications to the Zagros High Folded Zone are presented: a comparison between mechanical and kinematical fold reconstruction and a study on sur-

face morphology based on a digital elevation model. After that, I introduce two detailed 3D structural models in two quite different tectonic setting, one in the southwestern Paris Basin and one for the Säntis area in Switzerland. Finally, I add three publications, which are not directly linked to the other contributions in computational structural geology, but provide a flavor of the breadth of my work.

My contributions to computational rock physics mainly consider fractured rocks and the influence of fluids on the behavior of seismic waves. The first study investigates if and how seismic body waves can trigger so-called Krauklis waves, which is a special guided wave mode in fractured reservoir rocks, and if seismic recordings may therefore contain information about the fractures. In the second study, a new methodology based on EBSD (electron backscatter diffraction) images is proposed to assess seismic anisotropy in heterogeneous and fractured rocks. Finally, two models with increasing complexity are presented that describe the effect of rock-internal oscillations on the propagation of seismic waves. Such oscillations may be caused by fracture resonance or residual saturated fluids in the pore space.

Zusammenfassung

Die vorliegende Habilitationsschrift umfasst eine Auswahl an wissenschaftlichen Arbeiten, die ich seit dem Abschluss meines Doktorats im Jahr 2009 publiziert habe. Mein generelles wissenschaftliche Ziel ist das mechanische Verständnis von geologischen, geodynamischen und geophysikalischen Phänomenen zu verbessern. Dazu verwende ich in erster Linie eigens dafür entwickelte numerische Simulationssoftware. Ich verbinde jedoch meine theoretische Arbeit auch mit Feld- und Labordaten. Meine prozessorientierte Forschungstätigkeit, die ich seit meinem Doktorat entwickelt habe, lässt sich in zwei Schwerpunkte unterteilen, nach welchen auch die vorliegende Habilitationsschrift gegliedert ist.

1. *Rechnergestützte Strukturgeologie*
2. *Rechnergestützte Gesteinsphysik*

Die Habilitationsschrift beginnt mit einem Überblick und einigen allgemeinen Gedanken zur Modellierung. Ein Model erfüllt drei Hauptzwecke: Vereinfachung, Verallgemeinerung und Parametrisierung der Natur. Da es niemals möglich sein wird, natürliche Prozesse in ihrer ganzen Komplexität zu erfassen, spielt die Vereinfachung eine zentrale Rolle in den Erdwissenschaften. Deshalb erlaube ich mir die Aussage: "*Alles was wir tun in den Erdwissenschaften ist Modellierung!*"

Nach einem kurzen historischen Ausflug in meine beiden Forschungsschwerpunkte, platziere ich meinen eigenen wissenschaftlichen Beitrag in die aktualle Forschungslandschaft. Ich erläutere ebenfalls einige persönliche zukünftige Forschungsperspektiven sowie meine Lehr-Philosophien, die ich verfolge. Zum Schluss fasse ich meine wissenschaftlichen Publikationen zusammen, die der Habilitationsschrift als Appendix angehängt sind. Dabei sortiere ich die Publikationen nicht chronologisch, sondern nach einem aufbauenden Gedankengang. Dies hebt die Verbindungen zwischen den einzelnen Publikationen, sowie zu wichtigen früheren Publikationen besser hervor.

Mein Beitrag zur rechnergestützten Strukturgeologie umfasst in erster Linie Studien über geologische Faltung. Zuerst beschreibe ich drei eher theoretische Arbeiten, in denen ich die Deformationsverteilung in und um Falten (Neutrale Line, Schieferungsrefraktionsmuster), sowie das Faltenwachstum in 3D untersuche. Darauf aufbauend präsentiere ich zwei Anwendungen am Beispiel des Zagros Faltengebirges: einen Vergleich zwischen mechanischer und kinematischer Faltenrekonstruktion und eine Studie zur Oberflächenmorphologie basierend auf einem digitalen Höhenmodell. Danach zeige ich zwei detaillierte 3D Strukturmodelle in zwei grundlegend verschiedenen tektonischen Situationen, eines im südwestlichen Pariser Becken und eines für das Säntisgebiet in der Schweiz. Zum Abschluss füge ich drei Publikationen hinzu, die nicht direkt mit den anderen Beiträgen zur rechnergestützten Strukturgeologie verknüpft sind, jedoch die Breite meiner Arbeit aufzeigen sollen.

Meine Beiträge zur rechnergestützten Gesteinsphysik behandeln grösstenteils zerklüftete Reservoirgesteine und den Einfluss von Fluiden auf das Verhalten von seismischen Wellen. Die erste Studie untersucht ob seismische Körperwellen sogenannte Krauklis-Wellen initiieren und seismische Aufzeichnungen somit Informationen über Klüfte im Untergrund enhalten können. Krauklis-Wellen sind dabei spezielle Grenzflächenwellen in zerklüfteten Reservoirgesteinen. In der zweiten Studie wird eine neuartige Methode vorgeschlagen, basierend auf EBSD (*electron backscatter diffraction*) Bildern, um die seismische Anisotropie von heterogenen und zerklüfteten Gesteinen zu untersuchen. Zuletzt präsentiere ich zwei Modelle mit zunehmender Komplexität, die den Einfluss von Gesteins-internen Oszillationen auf die seismische Wellenausbreitung beschreiben. Solche Oszillationen können durch Kluft-Resonanzeffekte oder durch residualgesättigte Fluide im Porenraum hervorgerufen werden.

MAIN PART OF HABILITATION TREATISE

1 Introduction

For many geoscientists, the year 2015 marks the 200^{th} anniversary of geological modeling. It was in 1815, when Sir James Hall presented two analog experiments to study the development of buckle folds under layer-parallel shortening (Hall, 1815), which aimed at explaining folds in the graywacke strata along the coast of SE Scotland near the city of Eyemouth. The European Geosciences Union (EGU) celebrates this anniversary by organizing a dedicated session at its 2015 General Assembly entitled "*200 years of modelling of geological processes*".

For about 150 years, geological structures were modeled exclusively by using experimental deformation machines. In the late 1950'ies and early 1960'ies, mathematical expressions were introduced to the structural geology community to explain buckle folds based on well-established continuum mechanics equations; and in the late 1960'ies, computer models finally entered the scene of geological modeling.

Today, computer modeling is one of the key pillars in geological and geophysical research. Nevertheless, the 200^{th} anniversary of Hall's rudimentary experiments represent an excellent landmark to present my own research in this Habilitation treatise. My main scientific interest is the mechanical understanding of geological, geodynamical, and geophysical processes. My process-oriented research focuses on two main areas:

1. *Computational structural geology*
   (i.e., deformation of rocks, mostly folding)

2. *Computational rock physics*
   (i.e., seismic properties of rocks, mostly fractured reservoir rocks)

Below, I first provide some general thoughts about modeling in geosciences and then give a brief historical context of my two main research areas.

1.1. Some general thoughts about modeling

Except for observing, everything we do in earth sciences is modeling! Models in natural sciences fulfill one or more of three principal purposes: (1) simplification, (2) generalization, and (3) parameterization of nature (Figure 1.1), whereas the first is the primary goal and hence a compulsory characteristic of a model. A model is always designed for a special purpose and has therefore its limitations in terms of applicability, as well as in terms of time and length scales. A model is valid if it reproduces the natural observations on the scale it is designed for. Following this definition, every earth scientist is a modeler, not only those who call themselves a modeler. In structural geology, typical models are (Figure 1.1):

- A geological map or cross-section, and even a sketch in the geological field book, is a model. They all simplify the geology, enhance important features, and suppress or neglect less important ones. A geological map certainly also reproduces observations, namely the distribution of lithologies, and is therefore a valid model.
- In geology, tons of conceptual models exist. Almost every geological text book or scientific paper contains sketches or block diagrams conceptualizing geological observations or processes, such as plate tectonics, paleogeographic situations, or volcanic systems. Such sketches simplify and generalize natural observations and reproduce natural observations; hence they qualify as valid models.
- Earth sciences typically deal with huge amounts of data of all kinds. Data mining techniques or statistical approaches allow identifying trends in such data or correlations between different data sets. The resulting statistical descriptions are valid models because they simplify and parameterize natural observations (the data) and can reproduce observations within the statistical error.
- To describe geological deformations, it is often sufficient to only consider the deformation path (kinematics) without taking into account the deformation mechanics (dynamics). Such purely kinematical models often use quite sophisticated mathematical formulations (parameterization) to describe the deformation. A typical application is the palinspastic reconstruction of geological cross-sections.

- Complementary to kinematical models, physical or mechanical models also consider deformation mechanics (dynamics) and include rheological parameters of rocks. Such physical/mechanical models comprise both laboratory experiments and mathematical models (e.g., continuum mechanics equations); dynamical computer simulations are based on the latter.

- Analog modeling in laboratory sandboxes or fish tanks is one particular type of physical/mechanical modelling. Such models use analog materials with known properties to reproduce tectonic deformation structures in a time and length scale suitable for laboratory experiments.

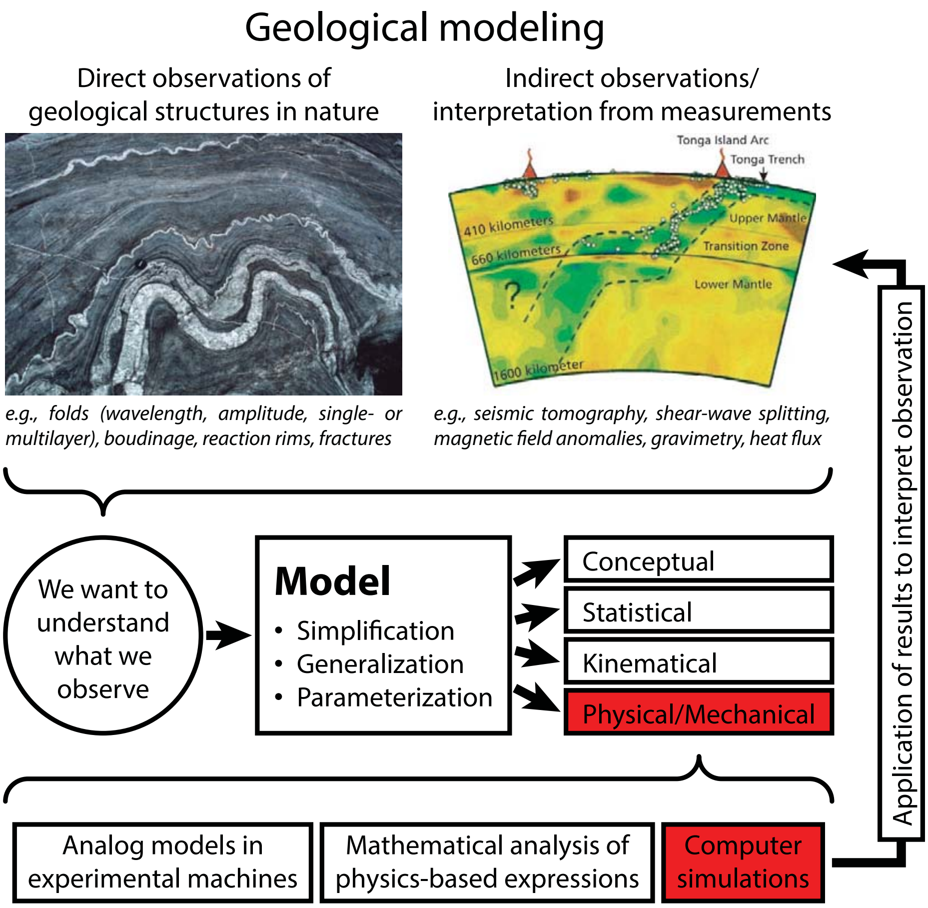

Figure 1.1: Train-of-thoughts diagram supporting the statement: "*Except for observing, everything we do in earth sciences is modeling*". Left picture courtesy of David Chew (University of Dublin); right image modified after van der Hilst (1995).

Because everything we do in earth sciences is modeling, this list can of course be extended at will. Figure 1.2 focuses on the special case of mathematical modeling. First, a physical/mechanical framework has to be identified that is suitable to describe the problem at hand. This depends on the particular application and on the spatio-temporal scale of investigation. The physical/mechanical framework then provides the governing equations (usually in various forms), which are complemented by the constitutive equations. For my particular type of modeling, I use the continuum mechanics framework, which provides the governing conservation equations (e.g., conservation of linear momentum), and I use constitutive rheological equations, such as elastic stress-strain or viscous stress-strain rate relationships.

The governing and constitutive equations together form a closed system of equations that describes the physical material behavior; boundary and initial conditions finally define the particular model setup to be studied. Dimensional analysis provides a possible pre-stage to the full solution of this system of equations. In short, the equations are reformulated, simplified, and analyzed to identify dominating parameters or parameter groups and discard insignificant portions of the system of equations. Ideally, dimensional analysis yields one or few dimensionless parameter(s) (i.e., without units) that allow separating the problem into end-member cases.

A closed-form analytical solution of a particular problem can often be found for relatively simple geometrical setups. Examples relevant for this Habilitation treatise are the analytical solutions for the dominant wavelength of single-layer viscous buckle folds (Biot, 1961; Adamuszek *et al.*, 2013b) or for the scattered seismic wave field around a cylindrical heterogeneity (Liu *et al.*, 2000). Also, all the formulas for the different seismic wave velocities are analytical solutions of the elastic wave equation (Stokes, 1849; Rayleigh, 1885; Love, 1911).

For more complex/realistic geometrical setups, usually no closed-form analytical solution can be derived. In these cases, the system of equations can be solved numerically using a spatio-temporal discretization method, such as the finite-difference or the finite-element method. The application of such methods to problems in structural geology and rock physics is the main topic of this Habilitation treatise.

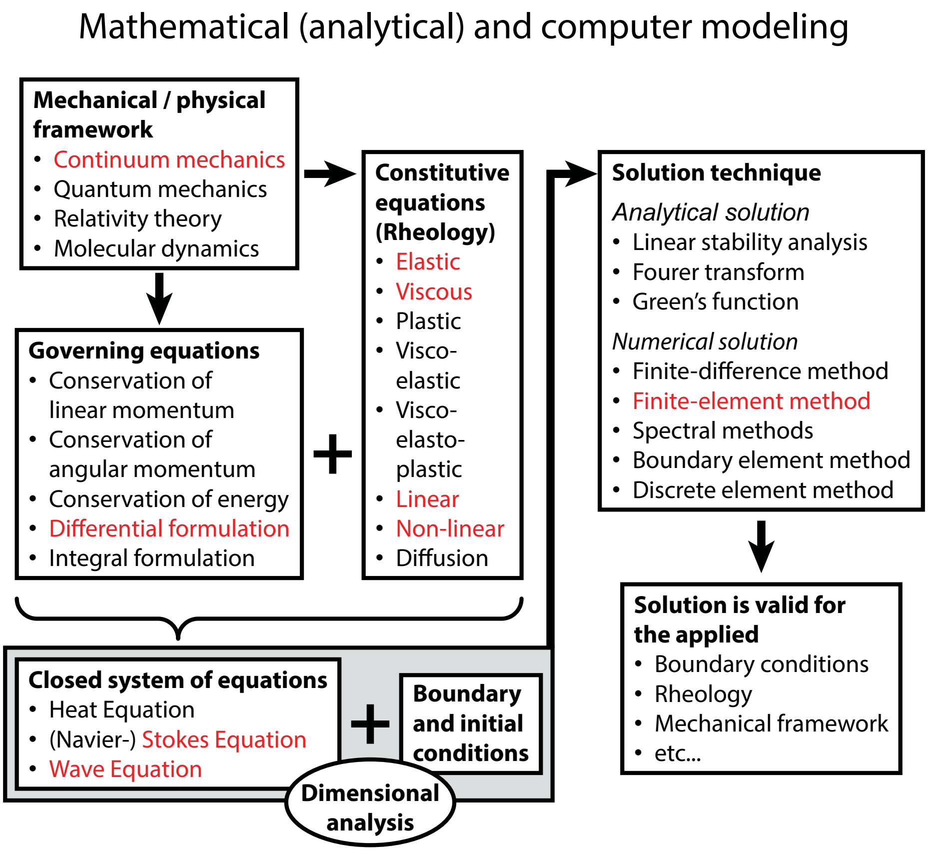

Figure 1.2: Train-of-thoughts diagram visualizing the mathematical analytical and computer modeling workflow.

As mentioned above, every modeling workflow comprises assumptions and simplifications no matter which method is used. Consequently, models are never universally valid. In the case of dynamical computer simulations, results are only valid for the applied boundary and initial conditions, only for the used rheology, and only within the assumed mechanical framework. Outside this range of assumptions and simplifications, other (maybe unexpected) results may occur.

Personally, I believe that modeling studies should start with the simplest possible model to reproduce and understand the first-order observations first. Only after this first step is completed, increasing complexity should be added to the model as is necessary to study more and more details. Depending on the problem to be studied, the "simplest possible" model may already be quite advanced. However, if a modeling study already starts off with a very complex model containing a large number of (possibly inter-dependent) parameters, it will be very difficult to identify the key parameters or processes. Such models may produce realistic-looking results but the fundamental processes responsible for these results are obscured by the complexity of the model. It is also fundamentally important to benchmark a model using an analytical solution for a simple test case before applying it to more complex cases. Only after a successful benchmark, the modeling results are trustworthy. If the starting model is already too complex, there will be no analytical solutions to conduct such a benchmark.

Similar thoughts about the complexity of models have been made many times before, which is exemplified by the following famous citations:

> *It is futile to do with more things that which can be done with fewer.*
>
> (known as Ockham's razor)
> William of Ockham (1287–1347)
>
> *Everything should be made as simple as possible, but not simpler.*
>
> Albert Einstein (1879–1955)
>
> *Essentially, all models are wrong, but some are useful.*
>
> George E. P. Box (1919–2013)

1.2. History of computational structural geology

Sir James Hall was the first to use analog models in geological sciences in 1815 (Figure 1.3). Despite their simplicity, Hall already understood the fundamental boundary condition necessary to reproduce buckle folds in a physical experiment, i.e. layer-parallel shortening, which shall be used in countless analog and numerical folding experiments up to the present day. The early days of geological modeling are very well summarized and illustrated in Ranalli (2001) and Graveleau *et al.* (2012), the latter focusing specifically on models of orogenic wedges.

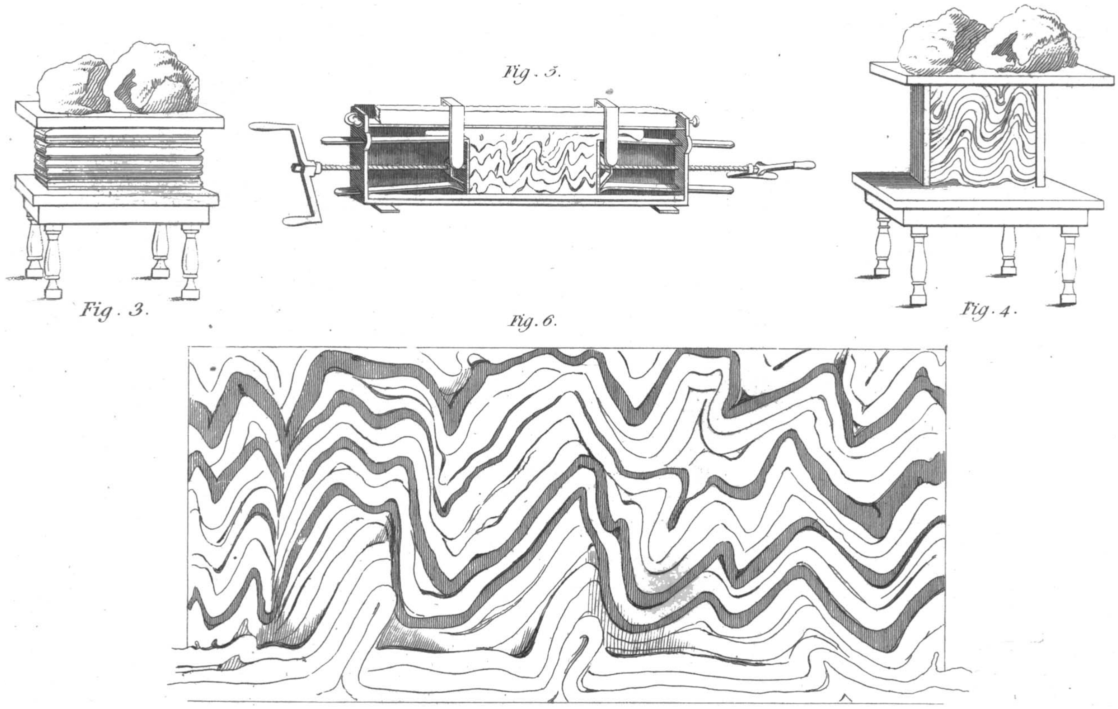

Figure 1.3: Figures 3–6 in Hall (1815) showing the setup (Fig. 3) and resulting geometry (Fig. 4) of the first rudimentary experiment and the setup (Fig. 5) and resulting geometry (Fig. 6) of the second experiment using a more sophisticated experimental machine. Hall used horizontal cloth (first experiment) or clay layers (second experiment), which he then compressed horizontally (i.e., layer-parallel) to obtain buckle folds.

The early physical models merely aimed at reproducing the geometry of geological structures without respecting the correct scales involved in the formation of these structures, for example magnitudes of stresses, viscosities, or strain rates. The seminal work of Hubbert (1937) introduced the concept of scale models to the geological community, a concept already well known at the time in civil engineering, as well as in hydro- and aerodynamics. Dimensionless numbers have been introduced that discriminate between different deformation regimes (Barenblatt, 1987, 1996). The analog material and model design are then chosen such that the dimensionless numbers of the model are the same as of the original (i.e., in nature). In this way, the model effectively behaves similar to its original, even though the model is smaller, the deformation is faster, and the material is weaker. In fluid mechanics (e.g., buckle folding), the dimensionless number most often used is the Reynolds number (Stokes, 1851), which is the ratio between inertial forces and viscous forces of a given flow problem. A properly scaled model (both analog and numerical) can not only reproduce natural geometries and structures, but also allows inferring physical quantities (e.g., stresses, strain rates, viscosities) of the dynamical formative processes. In the case of numerical models, a well-chosen scaling may even help stabilize the numerical algorithm because physical quantities of extremely different orders of magnitudes can be avoided, which, without scaling, would lead to ill-conditioned system matrices.

Even though buckle folding has been mathematically described already in the 18^{th} century, Smoluchowski (1909) was the first to apply such mathematical analysis to folded geological strata, though only for elastic buckling. It was the seminal work of Maurice Biot (Biot, 1957, 1961) and Hans Ramberg (Ramberg, 1959, 1963) that finally consolidated viscous buckle folding as a geological concept. Despite some severe approximations (e.g., large viscosity ratio, infinitesimal amplitudes), Biot and Ramberg mathematically explained a fundamental observation of folding: the wavelength selection process. Even though all wavelengths grow exponentially, there is one wavelength growing with the highest rate, outpacing all other growing wavelengths. Therefore, this wavelength will dominate the fold geometry at a finite-amplitude stage; hence it is called the dominant wavelength. A number of extensions and generalizations have been added to the initial work of Biot and Ramberg, some of which are listed in Table 1.1, resulting in more complete mathematical descriptions of buckle folding. Such analytical expressions are also extremely valuable for validating numerical codes; a numerical model must be able to reproduce the analytical solution if the same assumptions, initial, and boundary conditions are used. A numerical model can therefore be benchmarked for relatively simple geometries, for which the analytical solutions are usually valid, before applying it to more complex problems. A recent review of possible information that can be gained from fold shapes can be found in Hudleston and Treagus (2010).

Publication(s)	Finite amplitude	Small viscosity ratio	Power-law viscous rheology	3D
Biot (1957, 1961); Ramberg (1959, 1963)				
Smith (1975a); Fletcher (1977)		✓		
Fletcher (1974); Smith (1977)		✓	✓	
Schmalholz and Podladchikov (2000)	✓			
Adamuszek *et al.* (2013b)	✓	✓		
Fletcher (1991)		✓		✓
Fletcher (1995)		✓	✓	✓
Kaus and Schmalholz (2006)	✓			✓

Table 1.1: Selection of mathematical buckle folding analyses incorporating different levels of complexity.

Chapple (1968) was the first to publish computer simulations of buckle folding of a viscous layer embedded in a matrix of lower viscosity. Using a variational method, he derived finite-difference equations that are solvable on a computer to simulate fold shapes up to large amplitudes and calculate strain rates and finite strains. The applied computational methods were already described years earlier in his PhD Thesis (Chapple, 1964). The first fully two-dimensional finite-element simulation of viscous buckle folding was performed by Dieterich and Carter (1969), who calculated the stress evolution (magnitude and orientation) in amplifying single-layer folds. Since this pioneering time of computational structural geology, an increasing number of more and more sophisticated numerical models have been published. However, it was not until 2006 that the first fully 3D finite-element simulation of viscous buckle folding has been presented by Kaus and Schmalholz (2006).

1.3. History of computational rock physics

The theory of seismic wave propagation is based on the theory of elasticity, which has been established in the 17$^{\text{th}}$ century by physicist Robert Hooke. At that time, it was common to claim literary property by using an anagram for a particular scientific finding before revealing its meaning. In the postscript of his book from 1676, Hooke wrote a short outlook of his future publication plans; as a third point he wrote:

> *3. The true Theory of Elasticity or Springiness, and a particular Explication thereof in several Subjects in which it is to be found: And the way of computing the velocity of Bodies moved by them. ceiiinosssttuu.*
>
> Hooke (1676)

Two years later, Hooke revealed the anagram by writing:

> *About two years since I printed this Theory in an Anagram at the end of my Book of the Description of Helioscopes, viz. ceiiinosssttuu, id est, Ut tensio sic vis; That is, if one power stretch or bend it one space, two will bend it two, and three will bend it three, and so forward.*
>
> Hooke (1678)

The Latin phrase "*Ut tensio sic vis*" translates to "*As the extension, so the force*"; Hooke described here the linear proportionality between deformation and force, or in a continuum mechanics sense, between strain and stress.

In the early 19$^{\text{th}}$ century, two opposing concepts were used to describe an isotropic elastic body: the concept of material points interacting through center forces and the concept of a continuous medium. Navier (1821) derived the equations of motion using the first concept, which yielded only one elastic material constant. On the other hand, the equations of motion derived by Cauchy (1823) using the continuum approach correctly resulted in two elastic constants.

Based on the principles of elasticity, Poisson (1830) predicted the existence of two propagating waves in an unbounded elastic medium, i.e. the two seismic body waves now referred to as the P- and S-wave, and Stokes (1849) determined the theoretical velocities of these two seismic body waves and expressed them in terms of the two elastic constants (and density). An extensive review of the early days of research on elasticity and the prediction of seismic body waves can be found in Todhunter (1886).

After the two seismic body waves had been mathematically described, other wave modes (in particular surface, interface, and guided waves) followed one after the other. Starting with the Rayleigh wave, Table 1.2 lists those wave modes that are actually named after their first investigator or discoverer.

It is interesting to note that most seismic wave modes were mathematically described long before any observations or experimental evidence were available. This is quite the opposite to the geological investigations described in Chapter 1.2, where mathematical theory was usually developed long after the observations were made. Despite some earlier attempts, quantitative observations of seismic waves began in 1880 with the invention of the seismograph by seismologists John Milne, James Ewing, and Thomas Gray. Nine years later, a teleseismic earthquake (April 18 1889 in Tokyo) was recorded for the first time (von Rebeur-Paschwitz, 1889). An excellent account of the early days of seismology as a scientific discipline can be found in Dewey and Byerly (1969). Observational seismology is beyond the scope of this Habilitation treatise and I will not go in any further details here.

Publication(s)	Seismic wave type
Rayleigh (1885)	Surface wave on an elastic (solid) halfspace
Love (1911)	Guided SH-wave along a low-velocity elastic layer over an elastic halfspace
Lamb (1917)	Guided wave along a thin elastic plate
Stoneley (1924)	Interface wave between two elastic halfspaces
Scholte (1942a,b)	Interface wave between an elastic and an acoustic (fluid) halfspace
Biot (1956a,b)	Slow longitudinal wave in a fluid-saturated poro-elastic medium
Krauklis (1962)	Guided wave along a thin acoustic (fluid) layer sandwiched between two elastic halfspaces (i.e., fluid-filled fracture)

Table 1.2: Seismic waves that are named after their original discoverer or investigator.

The first synthetic seismograms were calculated by Lamb (1904) and showed the arrivals of P-, S-, and Rayleigh waves at the surface of a homogeneous isotropic elastic half-space; Love waves were still unknown at that time, hence the calculated seismograms did not match the observed ones. Lamb's calculations were purely analytical, resulting in closed-form mathematical expressions describing the seismograms. Many studies of the first half of the 20$^{\text{th}}$ century followed the same approach and/or used mathematical approximations and asymptotic formulations to describe more complex problems (Ewing *et al.*, 1957). Abramovici and Alterman (1965) were among the first to use a computer to numerically solve such mathematical expressions. However, this approach still requires that mathematical expressions can actually be derived for the particular geometrical setup through which the propagation of seismic waves is calculated. Such restriction to regular geometries is very severe; hence many general and more complex/realistic problems cannot be described.

To circumvent this issue, various computational methods have been developed for simulating seismic wave propagation; here I only consider those that discretize the wave equation in the space-time-domain (the finite-difference method is certainly the most popular of these methods). It is difficult to identify the first study that uses such a numerical technique; yet Nuckolls (1959) (one-dimensional) and Maenchen and Sack (1963) (two-dimensional) each described a finite-difference computer code to simulate the seismic response of nuclear explosions, and Bertholf (1967) simulated seismic waves in a cylindrical bar using a two-dimensional axisymmetric finite-difference formulation. Finally, the group around Israel-based mathematician Zipora Alterman (Alterman and Kornfeld, 1968; Alterman and Karal, 1968; Alterman and Rotenberg, 1969) established the finite-difference technique as a suitable method for modeling seismic wave propagation. Since these early days, almost uncountable improvements have been added to this very popular method; few milestones are listed in Table 1.3. In addition, Moczo *et al.* (2007) provides a comprehensive overview of the currently popular finite-difference methods.

Publication(s)	Major achievement
Boore (1972); Kelly *et al.* (1976)	Finite-difference algorithm using a single grid; suitable for heterogeneous media
Madariaga (1976); Virieux (1984, 1986)	Second-order staggered grid finite-difference algorithm based on the velocity-stress-formulation; higher accuracy for heterogeneous media
Levander (1988)	Fourth-order staggered grid finite-difference algorithm
Robertsson *et al.* (1994)	Fourth-order staggered grid finite-difference algorithm for visco-elastic media
Saenger *et al.* (2000); Saenger and Bohlen (2004)	Rotated staggered grid finite-difference algorithm; suitable for strongly heterogeneous, visco-elastic, and anisotropic media with very abrupt jumps of elastic parameters

Table 1.3: Selection of milestones in finite-difference wave propagation modeling.

So far, only finite-difference methods have been discussed. However, for my own work I mostly use the finite-element method, which is another numerical discretization technique, yet much less popular for seismic wave propagation modeling. The reason for me to use the finite-element method is threefold: (1) its ability to perfectly match any geometry using an unstructured numerical mesh, (2) its capability to handle extremely large jumps of mechanical properties across material boundaries, and (3) the straightforward implementation of anisotropic elastic properties. These advantages allow me to numerically resolve fluid-filled fractures or to incorporate the crystallographic orientation of different mineral phases into seismic wave propagation models.

Similar to the finite-difference method above, it is difficult to identify the first finite-element wave propagation models. Some pioneering work was certainly done by Berkeley-based geotechnical engineers John Lysmer, Lawrence Drake, and Günter Waas (Lysmer, 1970; Lysmer and Drake, 1971, 1972; Drake, 1972a,b); they used a frequency-domain finite-element method primarily to investigate seismic surface waves. However, the finite-element method appears to have had a slow start in seismic modeling and early publications may only be found sparsely (Smith, 1975b; Marfurt, 1984). At the same time, the finite-element method quickly gained popularity in various engineering communities and several comprehensive textbooks were published in the early 1970'ies (Zienkiewicz, 1971;

Desai and Abel, 1972; Norrie and de Vries, 1973), which are quite general and therefore also (partly) cover the modeling of seismic waves.

Today, there is a large number of numerical methods that derive from the classical finite-difference and finite-element methods, such as the spectral-element method (Komatitsch and Vilotte, 1998; Komatitsch and Tromp, 1999) or the discontinuous Galerkin method (Käser and Dumbser, 2006; Dumbser and Käser, 2006; Käser *et al.*, 2007; de la Puente *et al.*, 2007; Dumbser *et al.*, 2007). The Society of Exploration Geophysicists (SEG) published two books with reprinted articles providing an excellent overview of both more classical (Kelly and Marfurt, 1990) and more modern articles (Robertsson *et al.*, 2012) about numerical methods for seismic wave propagation modeling. Recent comprehensive methodological overviews can also be found in Fichtner (2011) and Virieux *et al.* (2012).

Computational rock physics hereby developed as a sub-discipline that focuses on seismic properties of rocks on the micro- to meso-scale. The aim is to better understand how the seismic wave field is influenced by different rock properties, such as lithology, porosity, permeability, pore fluid content, or fracture density and orientation. To investigate these effects numerically, it is particularly important to implement poro-elastic material properties, fractures, or viscous fluids into the seismic wave propagation simulations. Such implementation may be done in two ways: (1) numerically resolving the respective features (e.g., pore space or fractures) and (2) using an upscaled effective medium description (e.g., poro-elasticity). Both approaches have their advantages and disadvantages. The first approach allows investigating in detail the processes taking place on the pore- or fracture-scale; however it is numerically too expensive to run larger-scale models and still resolving the small-scale features. On the other hand, the second approach cannot directly describe the processes on the pore- or fracture-scale, but describes their effects on a larger scale; hence it is possible to run larger-scale models.

2 My own work placed into the current research landscape

2.1. Computational structural geology

Today, computational methods are one of the key pillars in structural geology research and in earth sciences in general. In structural geology, computer models are used on every possible scale to simulate the development of geological structures, to better understand their geometries and the processes involved in their formation, and to access spatial and temporal scales that are difficult to access in nature or in the laboratory. Depending on the problem at hand, different numerical simulation methods may be applied. Below, I try to illustrate the breadth of computational structural geology by providing some selected (and not representative) recent examples, mostly for ductile processes from the small to the large scale.

- On the grain-scale, laboratory heating experiments have been supported by numerical simulations of the development of microstructures (Piazolo *et al.*, 2004) and of the thermo-elastic stress buildup due to different thermal expansion coefficients of the involved mineral phases (Schrank *et al.*, 2012).

- On the scale of inclusions or particles (e.g., porphyroclasts), the rotational behaviour of individual clasts (Mancktelow, 2013) and the formation of SC- and SC'-structures related to a distribution of multiple clasts (Jessell *et al.*, 2009; Dabrowski *et al.*, 2012) have been investigated using numerical finite-element simulations.

- On the outcrop-scale, a whole range of structures have been modeled, for example so-called chocolate-tablet structures (i.e., bi-directional boudinage) on fold limbs (Reber *et al.*, 2010), the influence of quasi-rigid porphyroblasts on a layer's folding behaviour in pure-shear (Adamuszek *et al.*, 2013a), the opening of outer-arc extension fractures during progressive fold amplification (Jager *et al.*, 2008), folding and unfolding of single layers in simple shear (as opposed to pure shear assumed in most folding studies) (Llorens *et al.*, 2013), and the development of pinch-and-swell (i.e., ductile boudinage) structures and related shear bands (Schmalholz and Maeder, 2012).

- On the thin-skinned mountain-range scale, the natural fold wavelength of the Zagros Simply Folded Belt has been explained (Yamato *et al.*, 2011) and the competition between thrusting and folding in both the Helvetic nappe system and the Jura fold-and-thrust belt has been investigated (Jaquet *et al.*, 2014) by numerical multi-layer folding simulations. Additionally, it has been shown that large elongated folds may efficiently form by lateral linkage of initially isolated fold segments (Grasemann and Schmalholz, 2012) and that lateral mechanical variations of the décollement layer strongly influence the 3D geometry of accretionary wedges (Ruh *et al.*, 2014).

- On the thick-skinned mountain-range scale, the basement-cover interaction and the role of pre-existing basement half-graben structures in the formation of tectonic nappe systems has been investigated (von Tscharner and Schmalholz, 2015).

- On the lithospheric scale, the competition between thrusting and folding has been studied to explain the Himalayan syntaxes (Burg and Schmalholz, 2008) and the effect of the strength and mechanical layering of the lithosphere on the India-Asia collision has been modeled and constrained with geophysical data (Lechmann *et al.*, 2014).

Of course, this list may be extended to the scale of subduction zones, mantle convection, and whole-Earth dynamics. However, I would draw a (quite arbitrary and smooth) line between computational structural geology and computational geodynamics at the mountain-range scale, which is about the upper limit of direct field observations. Therefore, going beyond the mountain-range scale, research slowly changes from a geological character to a geophysical character. Also, the above list becomes almost infinite when incorporating interdisciplinary studies between structural geology and, for example, volcano-tectonics, earthquake seismology, surface dynamics, metamorphic petrology, rock mechanics and rock physics, engineering applications, or material sciences.

My own contribution to structural geology mostly gravitates around the outcrop-scale. I try to explain and understand structures that can directly be observed in the field and investigate the related deformation processes that may result in these structures. As such, I keep a very close link to field geology and try to help geologists in their structural interpretations; in fact, I consider myself a structural geologist and not a modeler.

This approach is only followed by a small scientific community; the community in computational structural geology is substantially smaller than in computational geodynamics. However, computational geodynamicists are often trained physicists or mathematicians, and not geologists. This can lead to miscommunication between modelers and geologists or, in the worst case, to modeling studies completely independent from observations. With my approach, I am trying to bride this gap between modelers and geologists.

For ductile deformation processes, a similar approach is followed by few other research groups, which can be outlined by the following selected publications:

- Adamuszek M., Dabrowski M. and Schmid D.W., 2013: **Interplay between metamorphic strengthening and structural softening in inclusion-bearing layered rocks**, Terra Nova 25, 381–386
- Dabrowski M. and Grasemann B., 2014: **Domino boudinage under layer-parallel simple shear**, Journal of Structural Geology 68, 58–65
- Fernandez N. and Kaus B.J.P., 2014: **Fold interaction and wavelength selection in 3D models of multilayer detachment folding**, Tectonophysics 632, 199–217
- Hobbs B., Regenauer-Lieb K. and Ord A., 2008: **Folding with thermal-mechanical feedback**, Journal of Structural Geology 30, 1572–1592
- Jager P., Schmalholz S.M., Schmid D.W. and Kuhl E., 2008: **Brittle fracture during folding of rocks: A finite element study**, Philosophical Magazine 88, 3245–3263
- Lechmann S.M., Schmalholz S.M., Burg J.P. and Marques F.O., 2010: **Dynamic unfolding of multilayers: 2D numerical approach and application to turbidites in SW Portugal**, Tectonophysics 494, 64–74
- Llorens M.G., Bons P.D., Griera A. and Gomez-Rivas E., 2013: **When do folds unfold during progressive shear?**, Geology 41, 563–566

- Peters M., Veveakis M., Poulet T., Karrech A., Herwegh M. and Regenauer-Lieb K., 2015: **Boudinage as a material instability of elasto-visco-plastic rocks**, Journal of Structural Geology 78, 86–102
- Reber J.E., Schmalholz S.M. and Burg J.P., 2010: **Stress orientation and fracturing during three-dimensional buckling: Numerical simulation and application to chocolate-tablet structures in folded turbidites, SW Portugal**, Tectonophysics 493, 187–195
- Schmalholz S.M. and Schmid D.W., 2012: **Folding in power-law viscous multilayers**, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 370, 1798–1826
- Viola G. and Mancktelow N.S., 2005: **From XY tracking to buckling: Axial plane cleavage fanning and folding during progressive deformation**, Journal of Structural Geology 27, 409–417
- Yamato P., Kaus B.J.P., Mouthereau F. and Castelltort S., 2011: **Dynamic constraints on the crustal-scale rheology of the Zagros fold belt, Iran**, Geology 39, 815–818

2.2. Computational rock physics

Similar to structural geological research, numerical modeling has developed into a fundamental pillar of all research related to seismic wave propagation. High-performance simulations are applied on every possible scale, from the grain-scale of 3D rock core images (Saenger *et al.*, 2007, 2011; Madonna *et al.*, 2012), to the scale of laboratory fish-tank experiments (Vasmel *et al.*, 2013), to 3D active seismic surveys (van Manen *et al.*, 2005; Robertsson *et al.*, 2006; Regone, 2007), and to spherical whole-Earth models for global seismic modeling, tomography, and inversion (Nissen-Meyer *et al.*, 2007, 2008; Tromp *et al.*, 2010; Fichtner *et al.*, 2013).

Even though the numerical methods for wave propagation simulation may be similar, I allow myself again to draw a (quite arbitrary and smooth) line between two sub-disciplines: computational rock physics and computational seismology with a boundary at the scale of dm-sized rock samples. Seismology, the sub-discipline dealing with the larger scale, also embraces a larger scientific community dealing mostly with earthquake-related problems, but also with the Earth's free oscillations, seismic background noise, volcano-related seismic events, and industry and environmental applications of seismic wave propagation.

Rock physics, on the other hand, mostly investigates how the rock's pore space, pore fluids, fractures, anisotropy, and various other rock properties influence the propagation of seismic waves. Such investigations usually take place on small rock samples, often in combination with micro-CT imaging and/or laboratory studies. However, the ultimate aim is to link such small-scale rock physics knowledge with large-scale seismological observations to infer rock properties from seismic attributes.

My own contribution to rock physics mostly considers fractured rocks containing a fluid in the fractures. I investigate how such fractures modify the propagation behavior for seismic waves, which may help seismic interpreters or seismologists to read fracture-related information from seismic data. Besides being scattered and diffracted at fractures, seismic energy can be trapped by fractures leading to fracture-related resonance effects. Such rock-internal resonance effects are one of my major research topics.

My studies are closely related to investigations of seismic tremor, which is often thought of as a resonance effect in fractured reservoir rocks (Ferrazzini and Aki, 1987; Chouet, 1988, 1996; Lipovsky and Dunham, 2015). Such seismic tremor can occur in various settings, such as volcanic systems (Kumagai and Chouet, 1999), geothermal fields (Ferrazzini *et al.*, 1990), hydro-fracking operations (Tary *et al.*, 2014), or even in glaciers (Anandakrishnan and Alley, 1997; Métaxian *et al.*, 2003; Stuart *et al.*, 2005; Winberry *et al.*, 2009; West *et al.*, 2010) and typically consists of a continuous seismic background signal marked by a characteristic frequency corresponding to the supposed resonance frequency. My rock physics studies help better understand the interaction between propagating seismic wave, fractures, and oscillations.

3 Personal research perspectives

My main scientific aim is the mechanical understanding of geological and geophysical phenomena, for which I developed various numerical modeling codes. However, my aim is also to integrate my theoretical/numerical work with field and laboratory data. In my opinion, only this combination enables a better understanding of both the observations and the physical processes causing them.

The first of my two main research fields can be summarized as *computational structural geology*, for which I combine detailed structural field studies with numerical modeling of geological structures to better understand the mechanical behavior of rocks during deformation.

For the second of my main research branches, *computational rock physics*, the aim is to measure seismic properties in partially fluid-saturated porous and/or fractured rocks (e.g., seismic attenuation) both in real rocks and numerically in digital rock samples to gain insight into the micro-scale physics and how to upscale these processes to an effective medium.

Below I outline some possible personal research perspectives for these two main research fields, and in particular the combination and integration of the two.

3.1. Computational structural geology

I spent quite some time of my career developing numerical tools to simulate the deformation of rocks. With this background, I intend to focus more of my future research energy in geological field studies. My aim is to use my mechanical knowledge to better understand the field observations. My ability to combine detailed structural field investigations with numerical simulations puts me in a comfortable situation, from which I can go beyond kinematic and conceptual descriptions.

I want to keep my process-oriented research focus; hence I have no preferred geographical study area. However, my main interest is in collisional orogens. Therefore, the French, Swiss, Italian, and Austrian Alps are ideally situated in central Europe to conduct field studies and will be my primary natural laboratory. Of course, I will participate in studies of other orogens depending on arising opportunities.

One particular research challenge is the mechanically consistent reconstruction of orogens. A number of techniques and software are available to unfold or reconstruct deformed cross-sections; however, all of these techniques use kinematic descriptions and are therefore not mechanically self-consistent. I want to use my experience from numerical forward modeling and apply it to time-reverse modeling (i.e., unfolding). Pilot studies can be done in simple settings with low-amplitude open folds a few thrusts, but the aim is to apply such methodology to entire mountain chains, which is a longer-term research goal.

Computational structural geology also allows conducting short-term research projects, such as Bachelor and Master Theses. Short structural field mapping studies can readily be combined with numerical modeling of an observed structure. This combination leads to an integrated mechanical understanding of a chosen field area, which can be much more satisfying for a student than a pure mapping or a pure modeling exercise.

3.2. Computational rock physics

Even though there is a large theoretical background describing the mechanical properties of porous rocks, the knowledge in fractured rocks is still limited. Fractures, the interaction between fractures and the pore space, and the influence of pore fluids are my primary interest in rock physics. I am on the way to develop tools and the necessary knowledge to extract fracture-related information (e.g., orientation, connectivity, etc.) from seismic recordings; however, this is a long-term research perspective, which I will continue to follow.

One very important aspect of this work is the upscaling of micro- and meso-scale studies to larger scales using effective medium theories. Without such upscaling, the gained insight into the studied processes is useless on a reservoir-scale, which is the scale of seismic or geological studies.

I will integrate my theoretical work with studies conducted at the seismic and rock deformation laboratory at the ETH Zurich, to which I am closely associated. This collaboration allows hand-in-hand studies pushing both theoretical and numerical advancements as well as laboratory confirmation of theoretical predictions. Also, I continue participating in the ROCKETH, which is an international competence center for rock physics research gravitating around the ETH Zurich (hence ROCKETH). Initially fully based at the ETH Zurich, the ROCKETH evolved into an international research network with members and collaborators distributed around the world.

Similar to my structural geological work, also my rock physics research is process-oriented and I am not specifically focusing on a particular application. However, obvious applications include hydrocarbon and geothermal reservoirs studies, as well as underground nuclear waste disposal and CO_2-sequestration.

3.3. Integration

My structural geology and rock physics research has so far been almost independent from each other. In the future, I want to integrate the two fields much more.

The role of pore fluids and fluid flow during the tectonic deformation of rocks is a major topic in such integrated studies. These processes take place on entirely different time scales, which is a major challenge for numerical simulations, but also for theoretical predictions. At the same time, pore fluids influence the propagation of seismic waves, which takes place on yet another time scale. Bridging these time scales is the aim of integrated structural geology-rock physics research.

My primary aim is to first bridge the time scales between tectonic deformation and fluid-related processes, such as fluid flow. Fluids modify the mechanical properties of rocks and therefore have a direct impact on the tectonic deformation. Understanding this feedback requires thorough theoretical work and the development of new numerical modeling tools, but also detailed field work to understand the observable effects of fluids in tectonically active areas and advanced rock characterization in the laboratory to understand the mechanical properties of rocks and how they change when fluids are present.

For rock characterization, I also plan to use both micro-CT data and synchrotron-based X-ray tomography (SRXTM). The high-resolution SRXTM is necessary to gain insight into the micro-scale processes. The combination with micro-CT and medical-CT scans allows developing upscaling algorithms for rock characterization on different scales.

4 Teaching philosophies

Here I state some of my teaching and supervision philosophies. I consider teaching and student supervision a key part of my university life. Discussions with students always have priority above my own daily work.

Generally, my office door is always open and I always take the time for student discussions, whether they participate in one of my lectures or they are my Bachelor-, Master-, or PhD-students.

4.1. Lectures and courses

In the class-room, I am experienced in teaching fundamentals and advanced courses of structural geology and tectonics, particularly focusing on quantitative aspects (e.g., strain analysis, tensor formulations), geological mapping techniques including stereographic projection, and numerical modeling of rock deformation (mainly using the finite-element method). Because I not only use but also develop my own numerical codes, I am ready to teach hands-on programming courses. My teaching also has a strong field component. I am experienced in fundamental and advanced mapping courses, advanced structural geological mapping courses, as well as various 1–10 days excursions.

My teaching portfolio allows me to guide the students through the entire workflow:

- Field observation and mapping
- Code development and testing
- Modeling of the observed structure
- Understanding and generalization of results

My lectures always combine different teaching methodologies, such as frontal teaching at the black board, power-point-based presentations, class-room exercises, computer-exercises, or student presentations. This combination may take place within one lecture (e.g., 1h theory, 1h exercises), or across the semester (e.g., 4 weeks introduction to computer software, 4 weeks theory plus class-room exercises, 4 weeks computer exercises), and always depends on the particular class that I teach.

I strongly believe that Powerpoint-based presentations are often too fast for the students. Therefore, if I teach theoretical concepts, I usually do it on the black board to allow the students to follow and write down themselves all the derivations. By doing it this way, I rather teach less but make sure the students can profit the most. Whenever possible, I appreciate the feedback of students and I am flexible to adapt a course according to the level and needs of the students.

4.2. Innovative teaching methods

I am very open-minded towards new and modern teaching methodologies, such as e-learning tools, problem-based learning, or flipped-classroom teaching, to better activate students during courses and to reach a higher level of student motivation. In fact, I self-developed several innovative teaching programs within our department, in particular to improve classical course assessments.

Particularly on the Master's-level, I strongly believe that students should not only gain knowledge related to their particular field, but also gain soft-skills (e.g., social, presentation, or communication skills). To illustrate this, I explain below the assessment method for my course "Numerical Modeling of Rock Deformation", which is partly a theoretical course on rheology, continuum mechanics, and strain analysis, and partly a practical course on programming the finite-element method for simulating rock deformation.

As a written or oral exam for such an applied course seemed unpractical, I provide the students with applied challenges, which they solve numerically in groups of two using their knowledge from the course. The challenges may range from elastic problems (e.g., stress or pressure distribution around tunnels or boreholes, seismic wave propagation) to viscous flow problems (e.g., buckle folding, diapirism, strain localization in a shear zone, rockglacier flow). Each group of two can choose the challenge according to their interest and finishes by writing a 4-page report and handing in all the numerical codes. Their final mark is the average of three individual marks:

1. a mark from me
2. a mark from a fellow student (peer-evaluation)
3. a mark from themselves (self-evaluation)

With this system, the students not only learn to apply their technical knowledge to a particular problem, but also gain a number of soft-skills important for their future career; for example writing for a semi-expert audience, providing feedback to a colleague in a way that it is acceptable, receiving and accepting feedback from a colleague, evaluate work for which she/he is not 100% expert, self-evaluate her/his own work.

Generally, I believe that we (University teachers) should put more responsibility into the hands of the students. In my experience (example above), the students can deal very well with responsibility if they are guided well by the assistants or teachers. Most importantly, having responsibility significantly increases the student's motivation. In the future, I will certainly continue implementing such innovative teaching and assessment methods and I am ready to push the boundaries in teaching further.

4.3. Student supervision

Generally, I consider a student and myself as a team conducting a project. I try to avoid teacher-student-situations, but rather see both of us on the same level. I strongly believe that even on a Bachelor-level students have their own scientific ideas and opinions. My task as a supervisor is to help the students not to be shy and express their thoughts. They have to learn to see themselves as a researcher rather than a student.

I also believe that high-level research is only one half that is necessary for a successful project; presenting, writing, and selling her/his own research is the other half. Therefore, I strongly support my students in gaining scientific writing and presentation skills and I encourage them to take presentation and writing lectures or attend conferences if possible.

5 Overview of appendices

In this Habilitation treatise I present a selection of my scientific work conducted and published after finishing my PhD in 2009. My research is gravitating around two main research fields, which also provide the subdivision of this chapter and of the appendices:

1. *Computational structural geology*
2. *Computational rock physics*

These two research fields provide the backbone of my research activities. However, since finishing my PhD in 2009, I have broadened my scientific interest and developed quite a diverse set of expertise, such as in geomorphology, structural model building, or signal processing. Since the beginning of my post-doctoral academic career, I have also been strongly involved in university teaching and student supervision. Therefore, a substantial part of the selected publications originates (at least partly) from student theses under my supervision.

Below, I provide an overview of all appended publications and how they are related to each other. For this overview, I do not sort the publications chronologically, but rather according to their logical (train-of-thoughts) relationships. Figure 5.1 emphasizes these relationships graphically and highlights the main influencing publications.

Because my research covers a range of subjects, drawing relationships between publications is not always possible. However, even if the target application can be quite different, there may still be a methodological relationship between different publications. One of the most persistent methodological relationships is through the development and use of my numerical finite-element codes, which is therefore also indicated in Figure 5.1.

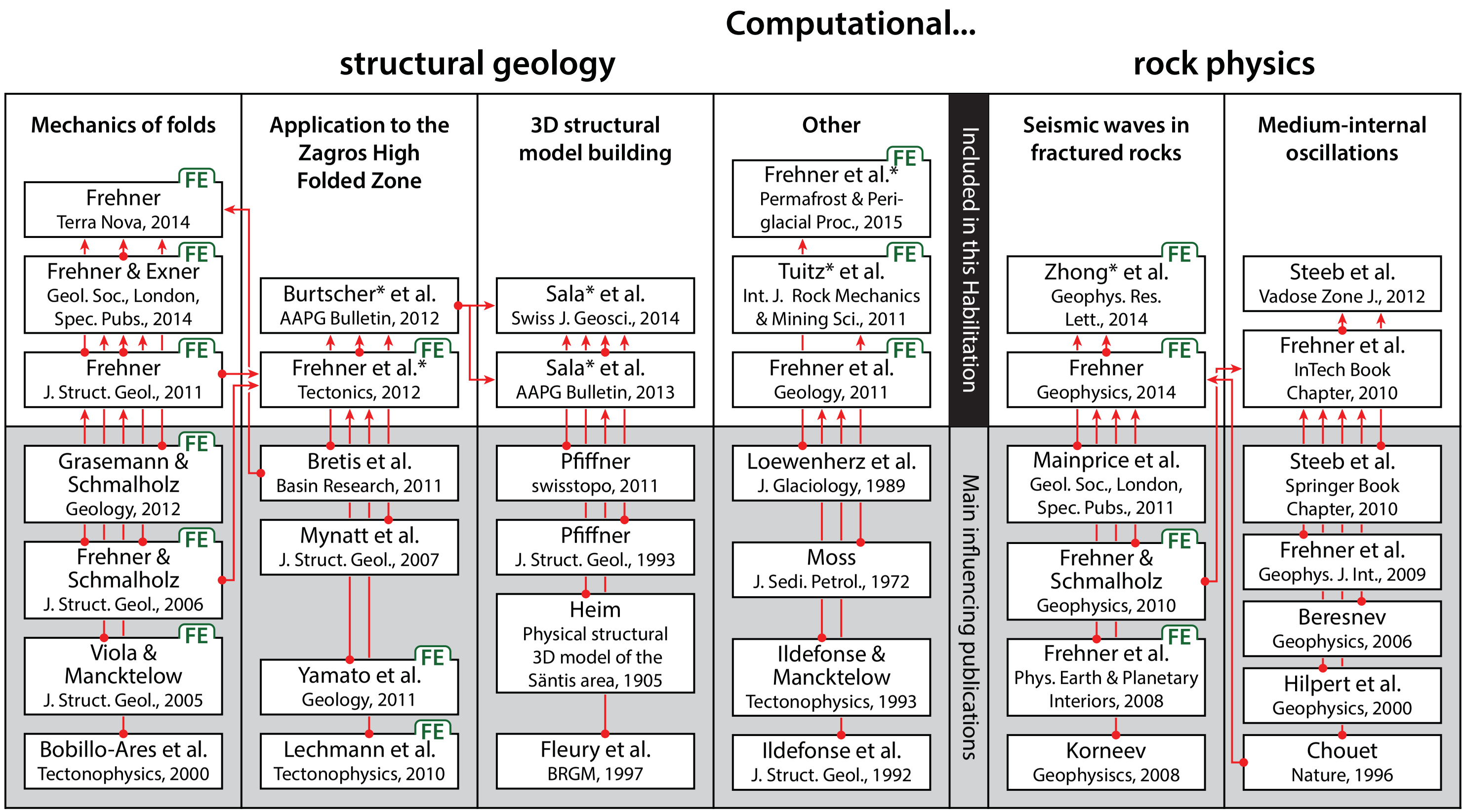

Figure 5.1: Relationships between publications in this Habilitation treatise and the main influencing publications. Red arrows indicate the "train-of-thoughts"-relationships between publications. Green FE-symbols indicate studies applying my various self-developed finite-element codes; this highlights a methodological relationship between studies, whose target application may be quite different. Stars indicate studies conducted with students under my supervision.

5.1. Computational structural geology

The first of my two main research branches can be summarized as *computational structural geology*, for which I combine detailed structural field studies with numerical modeling of geological structures to better understand the mechanical behavior of rocks.

5.1.1. Mechanics of folds

In Frehner (2011) and Frehner and Exner (2014) I investigated phenomena occurring in outcrop-scale folds, and in Frehner (2014a) I studied the growth of folds in 3D. For all three publications I used a very similar numerical finite-element algorithm to investigate the strain distribution in folds.

In **Frehner (2011)** I studied the neutral line in buckle folds, which divides areas of outer-arc extension from areas of inner-arc shortening. By analyzing numerically simulated buckle folds I demonstrate that the neutral line is not a stationary feature during progressive folding, but migrates dynamically through the fold. For some geometrical and rheological situations, the neutral line does not develop at all. Hence, my study questions several assumptions of tangential longitudinal strain folding, which is a common kinematic concept to explain fold geometries.

In **Frehner and Exner (2014)** we investigated the strain and foliation orientation and refraction patterns (foliation fans) in and around both numerically simulated and natural buckle folds. Using a range of different strain measures, we show that the divergent foliation fan in the matrix at the outer arc of a fold does not necessarily reflect the finite strain orientation, as it is often assumed. Alternatively, our results suggest that the convergent foliation fan inside a folded layer is better suited for strain estimates. We also studied foliation fans in and around natural folds in metasedimentary rocks in NW Spain and find a good match between the natural examples and the numerical results.

In **Frehner (2014a)** I quantify the growth of buckle folds in 3D. The three growth directions are defined as *fold amplification* (vertical growth), *fold elongation* (growth parallel to fold axis), and *sequential fold growth* (growth parallel to shortening direction by the appearance of new syn- and antiforms adjacent to the initial isolated fold). I simulated the growth of a 3D fold structure from a point-like perturbation using a finite-element code for 3D viscous deformation. The two lateral fold growths (elongation and sequential growth) exhibit similar growth rates, leading to fold aspect ratios in map view close to 1, while the fold structure amplifies at a slightly higher rate in the vertical direction.

5.1.2. Application to the Zagros High Folded Zone

Building upon the mechanical understanding of small-scale folds described above has allowed me to go a step ahead and apply my numerical tools to larger-scale folds, namely the Zagros High Folded Zone (ZHFZ) of the Kurdistan region in NE Iraq. The ZHFZ is characterized by open to gentle folds with amplitudes of less than 2.5 km and wavelengths of 5–10 km; it is fold-dominated lacking major thrust faults, which makes it ideally suited to apply pure buckle-folding models.

In **Frehner *et al.* (2012)** we compared kinematical and a mechanical fold reconstruction methods to estimate the bulk shortening in the ZHFZ. We discretized a geological cross-section using the finite-element method and extended it numerically during dynamic unfolding simulations. This corresponds to a reverse-time simulation, reversing the folding process. Our study is only the second study after Lechmann *et al.* (2010) that ever applied this methodology to natural fold structures. The dynamic unfolding simulations reveal that interfacial slip and decoupling of the deformation between the mechanically strong units is a key factor controlling the folding processes in the ZHFZ. Parts of Frehner *et al.* (2012) resulted from the PhD Thesis of D. Reif under my supervision.

In **Burtscher *et al.* (2012)** we further studied the geometry of the ZHFZ. We applied differential geometry to a digital elevation model (DEM) to calculate and map various curvature values. Such calculations allow classifying the folded and eroded surface into different geologically relevant shapes. By adjusting two key parameters of the curvature calculation we can separate long-wavelength structures (i.e., folds) from short-wavelength features (i.e., river incisions) and we demonstrate that both tectonic-oriented

and geomorphological-oriented studies are viable using the same DEM.
The largest part of Burtscher *et al.* (2012) resulted from the Bachelor Thesis of A. Burtscher under my supervision.

5.1.3. 3D structural model building

The above mechanical studies explain and quantify certain features of buckle folds for general cases; however, they do not aim at reproducing natural folds one to one. For a comprehensive understanding of natural geological structures, first and foremost detailed geometrical insights are indispensable. Therefore, it is essential to be able to create and analyze detailed 3D structural models.

In **Sala *et al.* (2013)** we present a 3D structural and petrophysical model of the shallow subsurface (top few 100 m) in the Chémery area (southwestern Paris Basin, France). We constructed the structural model based exclusively on lithological well markers (i.e., 1D borehole data); hence we first had to develop a unique model building protocol for this type of data, which is substantially different from standard methods using seismic 2D sections or 3D cubes. The resulting structural model is populated with petrophysical data both from the boreholes (P-wave velocity) and from laboratory testing (P- and S-wave velocity, porosity, density) to produce a comprehensive petrophysical model of the shallow subsurface.
The largest part of Sala *et al.* (2013) resulted from the PhD Thesis of P. Sala under my supervision.

In **Sala *et al.* (2014)** we present a detailed 3D structural model of the Säntis area (Helvetic Zone, NE Switzerland). To create the model, we used published 2D geological cross-sections from various authors and two new self-drawn cross-sections. We also incorporated measured 3D geometries of caves and the known lithologies they follow. The good geometrical match between our 3D structural model and the cave data validates the model at depth. The publicly available model highlights the complex 3D relationship between thrust faults, strike-slip faults, folds, and the distribution of different lithologies.
The largest part of Sala *et al.* (2014) resulted from the PhD Thesis of P. Sala under my supervision.

5.1.4. Other

In this sub-section I summarize three publications that are not directly related to each other or to the publications summarized above.

In **Frehner *et al.* (2011)** we investigated the effects of imperfect boundary conditions in laboratory analog models of simple-shear deformation. Such models are often used for studying, for example, rotation of rigid inclusions or oblique folding. Using a finite-element model that reproduces the deformation in such laboratory equipment we show that imperfect boundary conditions can lead to very large deviations from the desired simple-shear flow. Because it is difficult to obtain perfect boundary conditions in the laboratory, we suggest that a thorough analysis of the flow field is necessary before using a simple-shear apparatus and in particular before quantifying the modeled deformation patterns.

In **Tuitz *et al.* (2012)** we studied the effects of pebble shape and loading configuration on the effective compressive strength of fluvial pebbles. Laboratory point-load tests do not necessarily represent the natural loading configuration during sediment burial. We applied a finite-element code to calculate the orientation and magnitude of elastic stresses within pebbles during mechanical testing. Our results show that laboratory point-load tests correspond to the weakest possible loading configuration and that natural pebbles in gravel are effectively stronger. Therefore, we suggest that a given distribution of broken pebbles in gravel may underestimate their burial depth.
The largest part of Tuitz *et al.* (2012) resulted from the PhD Thesis of C. Tuiz under my supervision.

In **Frehner *et al.* (2015)** we identify gravity-driven buckle folding as the main formative process for the so-called furrow-and-ridge morphology on rockglaciers. Such permafrost bodies often develop a peculiar "wavy" surface morphology when creeping down-slope under their own weight. We chose the Murtèl rockglacier (upper Engadin valley, SE Switzerland) as a case study because of its well-studied kinematic behavior and internal structure. We simulated the dynamic flow of the Murtèl rockglacier using a self-developed finite-element model based on the available digital elevation model. Our simulations demonstrate that the compressive flow regime towards the toe of the rockglacier results

in buckle folding of the top layer and reproduces several key features of the furrow-and-ridge morphology.
Parts of Frehner *et al.* (2015) resulted from the Master Thesis of A.H.M. Ling under my supervision.

5.2. Computational rock physics

For my second main research field, *computational rock physics*, I closely collaborate with the Seismic Attenuation and Rock Deformation Laboratory at the ETH Zurich. The aim is to measure seismic properties in partially fluid-saturated porous or fractured rocks both in real rocks and numerically in digital rock samples. My contribution is mainly on the theoretical and numerical side of rock physics research.

5.2.1. Seismic waves in fractured rocks

Fractures in reservoir rocks are of great scientific and economic interest as they can significantly enhance reservoir performance. The presence of fractures also alters the propagation behavior of seismic waves. For example, fractures can significantly increase the seismic anisotropy of rocks or they give rise to a special fracture-bound wave mode, so-called Krauklis waves. When repeatedly propagating back and forth along a fracture they may fall into resonance, which leads to important frequency-dependent propagation effects. Such resonance effects may also explain seismic tremor generation in volcanic settings or in fractured fluid reservoirs.

In **Frehner (2014b)** I performed high-resolution numerical wave-propagation simulations to investigate if seismic body waves can initiate Krauklis waves when propagating through a fractured rock. Indeed, both P- and S-waves are capable of initiating Krauklis waves with significant amplitude. For both wave modes the initiation strongly depends on the fracture orientation, but S-waves generally initiate larger-amplitude Krauklis waves than P-waves. My results suggest that analyzing S-waves that have propagated through fluid-bearing fractured rocks may reveal fracture-related information.

In **Zhong *et al.* (2014)** we propose a novel method to assess seismic anisotropy in rocks. The method relies on EBSD-scans (Electron Backscatter Diffraction) of thin sections, which provide the distribution of mineral phases and their crystallographic orientation. We incorporate such 2D EBSD-maps into a self-developed finite-element model to simulate the propagation of seismic waves through the fully anisotropic and heterogeneous rock. By simulating wave propagation in different directions we can quantify the effective bulk anisotropy. With this method we can isolate different causes for anisotropy (crystallographic preferred orientation CPO, shape preferred orientation SPO, presence of fractures) and study them and their relative importance separately. In our case study (Finero Peridotite, Ivrea-Verbano Zone, N Italy) we find that CPO is the dominating cause for anisotropy.
The largest part of Zhong *et al.* (2014) resulted from the Master Thesis of X. Zhong under my supervision.

5.2.2. Medium-internal oscillations

As described above, Krauklis waves may lead to resonance effects within a fractured rock. There may be other phenomena leading to medium-internal oscillations and resonance effects such as oscillating fluid blobs or clusters in the pore space or resonant scattering of seismic waves at geometrical heterogeneities characterized by an eigenfrequency. The following two publications present theoretical models with increasing complexity of the interaction between such medium-internal oscillations and propagating seismic waves. The main result of both publications is the phase velocity dispersion and frequency-dependent attenuation curves for these models.

In **Frehner *et al.* (2010)** we present the simplest possible model consisting of oscillations within an acoustic medium (i.e., only P-waves, no S-waves, e.g., water containing oscillating gas bubbles). The model predicts a very strong phase velocity dispersion anomaly and an attenuation peak for P-waves around the resonance frequency of the oscillations. A comparison with more sophisticated models and with laboratory data of acoustic waves propagating through water containing gas bubble demonstrates that our simple model can accurately reproduce the dispersion and attenuation curves.

In **Steeb *et al.* (2012)** we extended our model to describe oscillations within porous media (i.e., fast and slow P-waves and S-waves, e.g., sandstone). We assume two immiscible pore fluids: a continuous (almost full saturation) non-wetting fluid and a discontinuous (residual saturation) wetting fluid. The latter forms isolated fluid bridges or clusters that can oscillate. Our model reduces to Biot's poro-elastic model (Biot, 1962) in the limit of the residual saturation approaching 0%. Our model predicts strong dispersion anomalies and attenuation peaks for the fast P-waves and S-waves, but not for the slow P-waves.

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[15] More sleepless nights at the Synchrotron.
[16] My current office mate.

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