The University of Würzburg
Department of Mathematics

Mathematical Modeling of Complex Fluids

Master's Thesis

submitted by

Johannes Forster
Matr.-Nr. 1596004

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Advisor/reviewer: Prof. Dr. Anja Schlömerkemper
Department of Mathematics
University of Würzburg

Second reviewer: Prof. Dr. Chun Liu
Department of Mathematics
Penn State University, USA

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Zusammenfassung

Die vorliegende Masterarbeit beschäftigt sich mit der mathematischen Modellierung komplexer Flüssigkeiten.
Nach einer Einführung in das Thema der komplexen Flüssigkeiten werden grundlegende mechanische Prinzipien im zweiten Kapitel vorgestellt. Im Anschluss steht eine Einführung in die Modellierung mit Hilfe von Energien und eines variationellen Ansatzes.
Dieser wird im vierten Kapitel auf konkrete Beispiele komplexer Flüssigkeiten angewendet. Dabei werden zunächst viskoelastische Materialien (z.B. Muskelmasse) angeführt und ein Modell für solche beschrieben, bei dem Eigenschaften von Festkörpern und Flüssigkeiten miteinander kombiniert werden.
Anschließend untersuchen wir den Ursprung solcher Eigenschaften und die Auswirkungen von bestimmten Molekülstrukturen auf das Verhalten der umgebenden Flüssigkeit. Dabei betrachten wir zunächst ein Mehrskalen-Modell für Polymerflüssigkeiten und damit eine Kopplung mikroskopischer und makroskopischer Größen. In einem dritten Beispiel beschäftigen wir uns dann mit einem Model für nematische Flüssigkristalle, die in technischen Bereichen, wie beispielsweise der Displaytechnik, Anwendung finden.
Geschlossen wird mit einem Ausblick auf weitere Anwendungsgebiete und mathematische Probleme.

Wir folgen einer Vorlesung von Professor Dr. Chun Liu von der Penn State University, USA, die er im Sommer 2012 im Rahmen einer Giovanni-Prodi Gastprofessur an der Universität Würzburg über komplexe Flüssigkeiten gehalten hat. Bei der Ausarbeitung werden ebenfalls Teile seiner Veröffentlichungen aufgegriffen und die Vorlesung durch eigene Rechnungen und Argumentationsschritte deutlich erweitert.

1 Introduction

This thesis gives an overview over mathematical modeling of complex fluids with the discussion of underlying mechanical principles, the introduction of the energetic variational framework, and examples and applications.

The purpose is to present a formal energetic variational treatment of energies corresponding to the models of physical phenomena and to derive PDEs for the complex fluid systems.

The advantages of this approach over force-based modeling are, e.g., that for complex systems energy terms can be established in a relatively easy way, that force components within a system are not counted twice, and that this approach can naturally combine effects on different scales.

We follow a lecture of Professor Dr. Chun Liu from Penn State University, USA, on complex fluids which he gave at the University of Würzburg during his Giovanni Prodi professorship in summer 2012. We elaborate on this lecture and consider also parts of his work and publications, and substantially extend the lecture by own calculations and arguments (for papers including an overview over the energetic variational treatment see [HKL10], [Liu11] and references therein).

It is, of course, vital to understand what the term "complex fluids" is about, and what are, in contrast, "simple fluids". When we talk about fluids we think of a certain state of matter. Usually, from our daily experience, everyone knows three states of matter. These are, in particular, the solid, the liquid, and the gas phase. In order to illustrate the three phases in a certain way, we come up with a simple line which stands for an increase of temperature in the direction of the arrow: Figure 1.1 shows what we have learned from our day to day life: If one takes, for example, a pot of water and heats it up, the water becomes steam, i.e., liquid becomes gas.

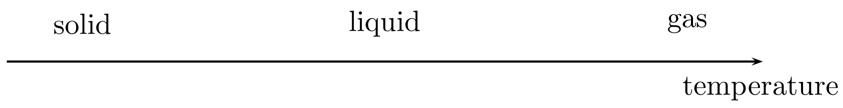

Figure 1.1: States of matter changing with temperature

If, on the other hand, one takes the pot of water and puts it into the freezer, the water becomes ice, i.e., liquid becomes solid while the temperature is decreasing. So far we talked about three distinct phases. However, temperature varies continuously. So the question arises if there can be certain intermediate states of matter between liquid and solid or between liquid and gas.

First, we need to consider what a (simple) state of matter is actually about. For this, we have a closer look at the materials, that means we look at the particles inside the material. If one takes a rigid piece of iron, a piece of ice or a grain of salt and studies the structure with the help of a microscope, it can be observed that the atoms are quite close together and form certain lattice structures.
In the gas phase, however, the atoms have greater distances between each other and are free to move around. The atoms that form a liquid phase are somehow in between: They are closer together but do not form rigid lattices, so they can move quite freely around, i.e., the degree of freedom in motion is higher than within rigid solid lattices but lower than within gas phases.

Next we specify in more detail what is meant by "degree of freedom to move" within the phases. Here we talk about *order* and *interactions*.

In terms of order we can distinguish between different sorts: *Orientational* and *positional order*.

In the lattice structures of solid materials – we stick to the example of water, ice and steam for the moment – there is a high degree of positional order: The atoms are not free to move within the lattice which is due to strong interactions among the atoms. The atoms only vibrate on their fixed position within the structure.
If we let the temperature increase, the vibrations of the atoms also increase and the interactions are "weakened", thus ice becomes water. In this phase, there is also no positional order compared to the rigid lattice.
Letting the temperature increase even more, liquid water reaches the gas phase, where interactions and order are even lower.

A material which exhibits orientational order is called liquid crystalline material. A basic yet interesting material of this kind are nematic liquid crystals: It is like a bunch of rod shaped molecules which are free to move but tend to align in one common direction. Liquid crystals are widely seen in technical applications, such as displays or self-shading windows. The nematics, e.g., give name to the display technology "TN" which stands for "twisted nematic". In fact, liquid crystals are an example for complex fluids: They can flow like a fluid but exhibit certain order or microstructures. We discuss liquid crystals later in Section 4.3.

Complex fluids can exhibit fluid properties (flow) as well as properties usually found in solid materials (order/structure). They form intermediate phases between solids and fluids. Further examples are gels or volcanic lava: They flow but if one looks closer, certain solid structures can be found. These materials are called viscoelastic materials. Certain examples are discussed in Section 4.1.

The theory of complex fluids has also applications in biological and biochemical settings. Ionic solutions that run through our body are complex fluids, so the models can be used to understand chemical processes within our body or special organs.

The main part of this work is organized in three chapters with an additional appendix. The purpose of Chapter 2 is an introduction into basic mechanics. The notation we use for the forthcoming analysis as well as the setting we consider are defined there. This chapter also deals with several mechanical properties of matter.

Chapter 3 introduces the Energetic Variational Framework for the analysis of mechanical systems, kinematics and transport theory, and principles for Hamiltonian and dissipative systems. We also give basic examples of simple solid and fluid systems and discuss what characterizes solid and fluid materials.

Models for complex fluids are then discussed in Chapter 4 with the use of formal energetic variational treatments. The first topic is a model for incompressible viscoelasticity to combine solid and fluid properties. We continue with a model for micro-macro-interactions in polymeric fluids and consider the coupling of microscopic and macroscopic variables. Afterwards we discuss (nematic) liquid crystalline material. Both the polymeric fluids and the nematics are considered in order to study the effect of embedded structures onto fluid flow properties.
This chapter in particular contains elaborate calculations to derive the systems of partial differential equations from the energy laws of the different models. These calculations were left out for brevity in publications and the lecture.

Moreover, several fundamental technical details, which are necessary to understand the calculations, are exhibited in the appendix.

2 Basic Mechanics

In this chapter we present the general setting we consider when studying complex fluids (c.f. [HKL10]). Moreover, we define several objects that help us to model, understand, and study these materials.

2.1 Coordinate Systems and Deformation

First, we define the deformation and talk about the different coordinate systems.

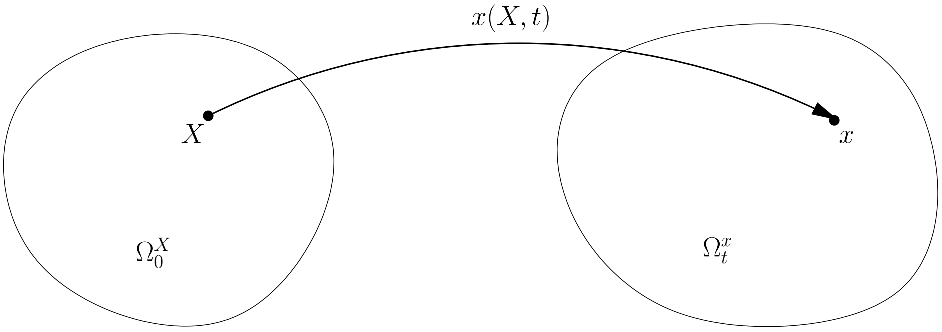

Figure 2.1: Deformation mapping between reference configuration Ω_0^X and deformed configuration Ω_t^x

Definition 1. *Let* $\Omega_0^X,\ \Omega_t^x \subset \mathbb{R}^n$, $n \in \mathbb{N}$, *be domains with smooth boundaries,* $t \in \mathbb{R}_0^+$ *be time and let* $u = (u^1, \ldots, u^n)$ *be a smooth vector field in* $\mathbb{R}^n$ *depending smoothly on time* t*. The deformation or flow map* $x(X,t) : \Omega_0^X \to \Omega_t^x$ *is defined as a solution map of*

$$\begin{cases} \frac{d}{dt}x(X,t) = u(x(X,t),t), \quad t > 0, \\ x(X,0) = X, \end{cases} \tag{2.1}$$

where $X = (X^1, \ldots, X^n) \in \Omega_0^X$ *and* $x = (x^1, \ldots, x^n) \in \Omega_t^x$*.*
The coordinate system X *is called the Lagrangian coordinate system and refers to* Ω_0^X *which we call the reference configuration; the coordinate system* x *is called the Eulerian coordinate system and refers to* Ω_t^x *which we call the deformed configuration.*

In other words, we start from a domain Ω_0^X, the reference configuration which changes over time. At any given time t the deformed configuration is Ω_t^x. The superscripts x and X just indicate the different coordinate systems. Later we consider integrals over the reference or deformed configuration. Then we also use x and X as integration variables.

The special term *flow map* is due to the dependency on two variables: If t is fixed, $X \mapsto x(X,t)$ maps the reference configuration Ω_0^X onto the deformed configuration Ω_t^x. We assume that this map is bijective since we map each particle in the reference configuration to its new position in the deformed configuration, this should be one-to-one and onto.
On the other hand, if X is fixed, i.e., we look at one special point or particle in the reference configuration, the map $t \mapsto x(X,t)$ denotes the changing position or the flow or trajectory of this particle over time.
These two ways of interpreting the deformation $x(X,t)$ lead to the term *flow map*.

The vector field u is the velocity, i.e., the derivative of the flow map with respect to time. The flow map is actually defined using the velocity vector field.

The Lagrangian coordinate system is usually used to describe the elastic behavior of solid materials where one looks at each particle X. However, the Eulerian coordinate system is used to model fluid materials where one looks at special positions x instead of single particles. Equation (2.1) links the two coordinate systems: Both sides describe the velocity of a particle labeled with X at position x and time t.

In the following we always assume that the flow map is smooth in both time and spatial variables, so all the calculations are well-defined. In particular, partial derivatives can be interchanged.

2.2 Deformation Gradient

In this section we take a look at the derivative of the flow map with respect to X and the properties of this important entity.

Definition 2. *Let $\widetilde{F}$ be the Jacobian matrix of the map $X \mapsto x(X,t)$ defined by*

$$\begin{aligned} \widetilde{F}(X,t) &:= \frac{\partial x(X,t)}{\partial X} := \nabla_X x(X,t) \\ &= \left(\frac{\partial x^i}{\partial X^j}\right)_{1\le i,j\le n} = \begin{pmatrix} \frac{\partial x^1}{\partial X^1} & \cdots & \frac{\partial x^1}{\partial X^n} \\ \vdots & & \vdots \\ \frac{\partial x^n}{\partial X^1} & \cdots & \frac{\partial x^n}{\partial X^n} \end{pmatrix}. \end{aligned} \tag{2.2}$$

$\widetilde{F}$ is called the deformation gradient.

Remark 3. *We denote the partial derivative of the flow map with respect to time by $x_t(X,t) := \frac{\partial}{\partial t} x(X,t)$.*

The deformation gradient, by definition, carries the information about how the configuration is deformed with respect to the reference configuration. That means, $\widetilde{F}$ carries all the information about structures and patterns.

We assume that $\det \widetilde{F} > 0$, so that the deformation gradient is an invertible matrix.

The following proposition gives an important result for the deformation gradient. We use it as a natural kinematic equation if the deformation gradient is involved in the model of a physical system. At first, we do a *push forward* for $\widetilde{F}$, i.e., we express the deformation gradient by the *Eulerian coordinate system.* Therefore, set

$$\widetilde{F}(X,t) = F(x(X,t),t).$$

Proposition 4. *F satisfies the equation*

$$\frac{\partial F}{\partial t} + (u \cdot \nabla_x)F = \nabla_x u \cdot F. \tag{2.3}$$

Proof. By the chain rule, we obtain from the push forward

$$\frac{d}{dt}F(x(X,t),t) = \frac{\partial}{\partial t}F(x(X,t),t) + (u(x(X,t),t) \cdot \nabla_x)\, F(x(X,t),t).$$

Furthermore, by using Definition 2 and the chain rule, we get

$$\begin{aligned}
\frac{d}{dt}\widetilde{F}(X,t) &= \frac{d}{dt}\left(\frac{\partial x^i(X,t)}{\partial X^j}\right)_{1\leq i,j\leq n} = \left(\frac{\partial x^i_t(X,t)}{\partial X^j}\right)_{1\leq i,j\leq n} \\
&= \left(\frac{\partial u^i(x(X,t),t)}{\partial X^j}\right)_{1\leq i,j\leq n} = \left(\sum_{k=1}^{n} \frac{\partial u^i(x(X,t),t)}{\partial x^k}\frac{\partial x^k(X,t)}{\partial X^j}\right)_{1\leq i,j\leq n} \\
&= \nabla_x u(x(X,t),t) \cdot \widetilde{F}(X,t).
\end{aligned}$$

Since F is defined by $\widetilde{F}(X,t) = F(x(X,t),t)$, both equations are equal. Thus

$$\frac{\partial}{\partial t}F(x(X,t),t) + (u(x(X,t),t) \cdot \nabla_x)\, F(x(X,t),t) = \nabla_x u(x(X,t),t) \cdot \widetilde{F}(X,t),$$

and with the push forward applied once again, we obtain

$$\frac{\partial}{\partial t}F(x(X,t),t) + (u(x(X,t),t) \cdot \nabla_x)\, F(x(X,t),t) = \nabla_x u(x(X,t),t) \cdot F(x(X,t),t),$$

which can be written in the Eulerian coordinate system as

$$\frac{\partial}{\partial t}F(x,t) + (u(x,t) \cdot \nabla_x)\, F(x,t) = \nabla_x u(x,t) \cdot F(x,t).$$

This concludes the proof. □

For the forthcoming analysis we also need the notion of a matrix divergence. Therefore, we give the definition here.

Definition 5. *Let $M : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ be a differentiable matrix field. The divergence of M, denoted by $\nabla \cdot M$, is defined by*

$$(\nabla \cdot M)_i = \sum_{j=1}^{n} \frac{\partial}{\partial x^j} M_{ij} = \nabla_j M_{ij}$$

for $i = 1, \ldots, n$. In the second equation the Einstein summation convention is applied with the simplified notation $\nabla_j := \frac{\partial}{\partial x^j}$.

By definition, the divergence of a matrix field is a vector field.

2.3 Incompressibility

In this section we turn to a very important property of materials. From a physical point of view, incompressible flows are flows where the material density is constant in an infinitesimal volume element which moves along with the velocity of the fluid. We now give a mathematical definition.

Definition 6. *Let $x(X,t)$ be the deformation of a material. The material is said to be incompressible if* $\det \widetilde{F} \equiv 1$.

The formulation above is in the *Lagrangian coordinate system*, but by using the push forward $\widetilde{F}(X,t) = F(x(X,t),t)$ the same equation holds for F in the *Eulerian coordinate system.*
However, there is another characterization of incompressibility in the *Eulerian coordinate system*, given by the following proposition.

Proposition 7. *Let $x(X,t)$ be the deformation of a material, $\widetilde{F}(X,t)$ the deformation gradient and $u(x(X,t),t)$ the velocity. It holds*

$$\det \widetilde{F} \equiv 1 \quad \forall X \in \Omega_0^X, t \geq 0 \quad \Longrightarrow \quad \nabla_x \cdot u = 0 \quad \forall X \in \Omega_0^X, t \geq 0.$$

The converse is true if the initial data $\det \widetilde{F}(X,0) = 1$ *is given.*

To be able to prove the proposition, we need two lemmas first.

Lemma 8. *The inverse of the deformation gradient is $\widetilde{F}^{-1} = \frac{\partial X}{\partial x}$.*

Proof. Since the flow map is assumed to be smooth, the bijective map $X \mapsto x(X,t)$ is a diffeomorphism from the reference configuration onto the deformed configuration. By the Inverse Function Theorem (c.f. [Kna05, Theorem 3.17]), the inverse mapping $x \mapsto X$ is also smooth and the Jacobian is exactly the inverse of the deformation gradient, so $\frac{\partial X}{\partial x} = \widetilde{F}^{-1}$. □

Lemma 9. *Let $A : \mathbb{R}_0^+ \to GL(n, \mathbb{R}) \subset \mathbb{R}^{n\times n}$ be a time dependent differentiable field of invertible matrices and let* $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$ *be the determinant. Then the derivative of $t \mapsto \det A(t)$ with respect to time t is given by*

$$\frac{d}{dt}\det A(t) = (\det A)\operatorname{tr}\left(A^{-1}\frac{d}{dt}A\right),$$

where $\operatorname{tr}(\cdot)$ *denotes the trace of a matrix.*

Proof. The derivative of the determinant $\det A$ with respect to the argument A (for a calculation see Appendix A.3) is

$$\frac{\partial(\det A)}{\partial A} = A^{-T}\det A.$$

Now, since $\det A(t) = \det \circ A(t)$, where $A : \mathbb{R}_0^+ \to \mathbb{R}^{n\times n}$ and $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$, we use the chain rule from Appendix A.2 and the product defined in Appendix A.1. We obtain

$$\begin{aligned}\frac{d}{dt}\det A(t) &= \frac{\partial(\det A)}{\partial A} : \left(\frac{d}{dt}A\right) = (\det A)A^{-T} : \left(\frac{d}{dt}A\right)\\ &= (\det A)\operatorname{tr}\left(A^{-1}\frac{d}{dt}A\right).\end{aligned}$$

This concludes the proof. ☐

Now we give a proof of Proposition 7:

Proof. (Prop. 7) With the lemmas above and (2.1) we get for any $X \in \Omega_0^X, t \geq 0$

$$\begin{aligned}\det\widetilde{F} = 1 \overset{*}{\Longrightarrow} \frac{d}{dt}\det\widetilde{F} = 0 &\iff \left(\det\widetilde{F}\right)\operatorname{tr}\left(\widetilde{F}^{-1}\frac{d}{dt}\widetilde{F}\right) = 0\\ \iff \operatorname{tr}\left(\sum_{k=1}^{n}\frac{\partial X^k}{\partial x^i}\frac{\partial x_t^j(X,t)}{\partial X^k}\right) = 0 &\iff \operatorname{tr}\left(\frac{\partial u^j(x(X,t),t)}{\partial x^i}\right) = 0\\ \iff \operatorname{tr}\left(\frac{\partial u^j(x,t)}{\partial x^i}\right) = 0 &\iff \sum_{i=1}^{n}\frac{\partial u^i(x,t)}{\partial x^i} = 0 \iff \nabla_x \cdot u = 0.\end{aligned}$$

The converse of $*$ is true if $\det\widetilde{F}(X,0) = 1$, otherwise it just gives that $\det\widetilde{F}$ is a constant. ☐

2.4 Conservation of Mass

In this section we phrase some mathematical formulations and consequences from the law of conservation of mass. This is a basic principle of classical mechanics. It states that mass is a fixed quantity that can only be deformed, but not created or destroyed (c.f. [TME12, Section 4.1], [Gur81, Chapter IV]). Here we consider configurations where the mass is distributed continuously. To this end, let $\rho(x,t) \geq 0$ be the mass density in the *Eulerian coordinate system* depending on time. Moreover, we assume that $\rho(x,t)$ is continuously differentiable and bounded on $\mathbb{R}^n \times \mathbb{R}_0^+$. Then the mass contained in a subdomain E_t^x of $\Omega_t^x \subset \mathbb{R}^n$ is given by

$$m(t) = \int_{E_t^x} \rho(x,t)\ dx. \tag{2.4}$$

The subdomain $E_t^x \subset \Omega_t^x$ is the deformed configuration of a certain subdomain $E_0^X \subset \Omega_0^X$ of the reference configuration.

The mass $m(t)$ depends on time. However, if mass is conserved within the domain, then $m(t)$ is constant over time. Thus, $\frac{d}{dt}m(t) = 0$ holds. Since not only the integrand but also the domain is time-dependent, the derivative of $m(t)$ with respect to time is quite delicate. In order to make the calculation simpler, we pull everything back to write the integral over the reference configuration in the *Lagrangian coordinate system*. We obtain

$$m(t) = \int_{E_t^x} \rho(x,t)\ dx = \int_{E_0^X} \rho(x(X,t),t)\ \det \widetilde{F}\ dX.$$

Here the domain of integration does not depend on time and we can take the derivative of $m(t)$ with respect to time. By the assumptions on the mass density, we can interchange differentiation and integration ([Els11, Proposition/Satz 5.7]). Using the product rule and the chain rule, we get

$$\begin{aligned} 0 = \frac{d}{dt}m(t) &= \frac{d}{dt}\int_{E_0^X} \rho(x(X,t),t)\ \det \widetilde{F}\ dX \\ &= \int_{E_0^X} \Big(\rho_t(x(X,t),t) + (u(x(X,t),t) \cdot \nabla_x)\, \rho(x(X,t),t) \Big) \det \widetilde{F} \\ &\qquad + \left(\det \widetilde{F}\ \operatorname{tr}\left(\widetilde{F}^{-1} \frac{d}{dt} \widetilde{F} \right) \rho(x(X,t),t) \right)\ dX \\ &= \int_{E_0^X} \left(\rho_t + (u \cdot \nabla_x)\, \rho + \rho \nabla_x \cdot u \right) \det \widetilde{F}\ dX. \end{aligned}$$

Now, we write everything in the *Eulerian coordinate system* again and obtain that for every E_t^x

$$\int_{E_t^x} \left(\rho_t + (u \cdot \nabla_x)\, \rho + \rho \nabla_x \cdot u \right)\ dx = 0,$$

and thus

$$\rho_t + (u \cdot \nabla_x)\, \rho + \rho \nabla_x \cdot u = 0.$$

or equivalently

$$\rho_t + \nabla_x \cdot (u\rho) = 0. \tag{2.5}$$

Remark 10. *The last step holds since the integral is identically zero for every subdomain* $E_t^x \subset \Omega_t^x$ *and therefore equation* (2.5) *must be satisfied pointwise, c.f. Lebesgue-Besicovitch differentiation theorem [EG92, Section 1.7.1].*

The following results connect incompressibility with conservation of mass and the properties of the mass density.

Proposition 11. *1. If* $\rho \neq 0$ *is constant in time and space, then* $\nabla_x \cdot u = 0$*, i.e., the incompressibility condition holds.*
2. If the incompressibility condition holds, then $\rho(x(X,t),t) = \rho_0(X)$*, i.e., the density is constant with respect to time. In particular, equation* (2.5) *becomes* $\rho_t + u \cdot \nabla_x \rho = 0$*.*

Proof. The proposition can be easily derived from equation (2.5).
1. If $\rho = const.$, then $\rho_t = 0$ and $\nabla_x \rho = 0$. By plugging this into equation (2.5) we obtain $\rho \nabla_x \cdot u = 0$ or equivalently $\nabla_x \cdot u = 0$.
2. If $\nabla_x \cdot u = 0$ then $\rho_t + u \cdot \nabla_x \rho = 0$. This is equivalent to $\frac{d}{dt}\rho(x(X,t),t) = 0$ which implies that the density is the same as the initial data at time $t = 0$. Thus, $\rho(x(X,t),t) = \rho_0(X)$. ☐

Now we derive a similar relation between the mass densities as in Proposition 11 but for the general case when there is no incompressibility condition.

Proposition 12. *A system satisfies the conservation of mass if and only if*

$$\rho(x(X,t),t) = \frac{\rho_0(X)}{\det \widetilde{F}} \tag{2.6}$$

for all $X \in \Omega_0^X$ *and* $t \geq 0$*.*

Proof. To prove this we consider the mass density $\rho_0(X)$ of the reference configuration and the mass contained within a subdomain $E_0^X \subset \Omega_0^X$ given by

$$m_0 = m(0) = \int_{E_0^X} \rho_0(X)\ dX.$$

Since the mass is conserved, the mass of any deformed configuration $E_t^x \subset \Omega_t^x \subset \mathbb{R}^n$ must be equal to m_0. Thus, we connect this with formula (2.4) which yields

$$\int_{E_0^X} \rho_0(X)\ dX = \int_{E_t^x} \rho(x,t)\ dx.$$

As before, we change variables on the right-hand side and get

$$\int_{E_0^X} \rho_0(X)\ dX = \int_{E_0^X} \rho(x(X,t),t)\ \det \widetilde{F}\ dX$$

which is equivalent to

$$\int_{E_0^X} \left(\rho_0(X) - \rho(x(X,t),t) \;\det \widetilde{F} \right) \; dX = 0.$$

Since this is true for all subbodies E_0^X of Ω_0^X, it must be satisfied pointwise, thus

$$\rho(x(X,t),t) = \frac{\rho_0(X)}{\det \widetilde{F}}.$$

□

Equations (2.5) and (2.6) are needed as kinematic assumptions in the following energetic variational analysis. We then use (2.6) for integral transformations and (2.5) to complete systems of differential equations for material models.

3 Energetic Variational Approach

When we look at physical or biological phenomena and try to build up a mathematical model for them, i.e., a mathematical description, we can do this in different ways.
At first, we could try to analyze the forces of the system and directly write down differential equations describing the given phenomenon.
Secondly, we could look at the energies that are present within the given system. The differential equations then need to be derived from these energies.

Let us consider a Hookean spring as an easy physical system (c.f., e.g., [LL81], [Bra79, Section 2.6]) and let us look at the forces occurring within this system. This example is also important for further discussions later in this thesis (see page 19 for the energetic approach to the spring; see Section 4.2 for application within the micro-macro model). Figure 3.1 shows a spring, of which one end is attached to the ceiling and the other end to a mass m. By empirical observation through experiments, one can check that the force $\mathbf{F}$ that the spring exerts on the mass is in constant proportion to the displacement x of (the lower end of) the spring from its equilibrium position, i.e., when no mass is attached to the

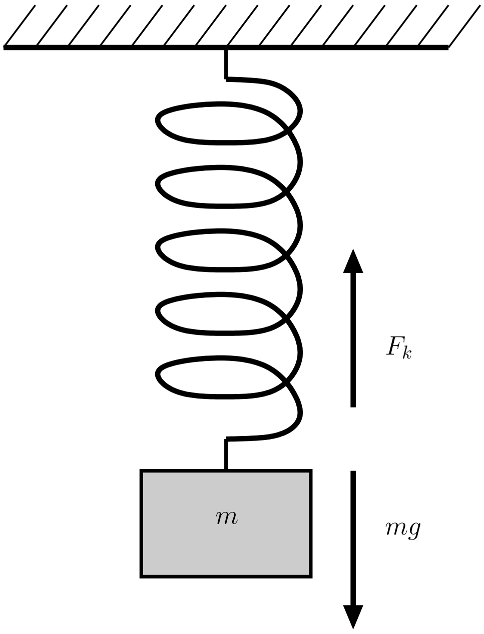

Figure 3.1: Mass attached to a Hookean spring

spring. This means that

$$\mathbf{F} = -kx$$

for some material parameter $k > 0$. The negative sign is due to the fact that the exerted force is in opposite direction to the displacement[1].

When the system moves up and down, the force $\mathbf{F}$ is described by Newton's law $\mathbf{F} = ma$, where the acceleration is $a = x_{tt}$. Plugging force and acceleration into the equation above yields

$$mx_{tt} + kx = 0.$$

Now, one can solve this ordinary differential equation (with suitable initial conditions) to obtain the trajectories for the movement of the spring.

Moreover, we can add a term representing damping (due to friction; assumed to be linear in the velocity) within the system, so we end up with the differential equation

$$mx_{tt} + \gamma x_t + kx = 0,$$

where $\gamma > 0$ is the damping coefficient and x_t is the velocity of the lower end of the spring.

Now we consider the energetic approach. This leads to the same equation for the Hookean spring. To this end, we introduce the framework and the underlying principles first and come back to the spring at the end of Section 3.1.

3.1 General Approach

In 1873 and 1931, Lord Rayleigh (John William Strutt) and Lars Onsager, respectively, published works ([Str73], [Ons31a, Ons31b]) where they developed the general energetic variational framework (c.f. [Liu11], [HKL10]). This approach is based on the following concepts that are outlined below: energy dissipation law, least action principle, maximum dissipation principle, and Newton's force balance law.

3.1.1 Energy Dissipation Law

The starting point for the energetic variational framework is the energy dissipation law (c.f. [HKL10]),

$$\frac{d}{dt}E^{total} + \Delta = 0 \quad \Longleftrightarrow \quad \frac{d}{dt}E^{total} = -\Delta, \tag{3.1}$$

---

[1] If one pulls the spring and makes it longer, so the direction of the displacement is outward, the spring "wants" to shrink, so the force is introverted.

where the total energy E^{total} includes both kinetic and free internal energy, and Δ is the dissipation functional (here this is equal to the entropy production, see (3.3), which is modeled as a quadratic function of certain rates such as the velocity x_t).
The energy dissipation law (3.1) states that (in isothermal situations) the total energy is conserved over time (this is when $\Delta = 0$), unless the energy is dissipated into Δ.

Equation (3.1) can be derived from the first and second law of thermodynamics. The first law states that the rate of change of the kinetic energy $\mathcal{K}$ plus the internal energy $\mathcal{U}$ is due to the rates of change of work $\mathcal{W}$ and heat $\mathcal{Q}$, so

$$\frac{d(\mathcal{K}+\mathcal{U})}{dt} = \frac{d\mathcal{W}}{dt} + \frac{d\mathcal{Q}}{dt}. \tag{3.2}$$

In other words, the first law of thermodynamics states that energy can only be changed by applied work and heat, so this is the conservation of energy. The second law is given in the isothermal case, i.e., when temperature is not time-dependent, by

$$T\frac{d\mathcal{S}}{dt} = \frac{d\mathcal{Q}}{dt} + \Delta, \tag{3.3}$$

where T is the temperature, $\mathcal{S}$ is the entropy and $\Delta \geq 0$ is the entropy production equal to the dissipation in (3.1) which is always nonnegative.
Now, we subtract (3.3) from (3.2) and find that (in the isothermal case)

$$\frac{d}{dt}(\mathcal{K}+\mathcal{U}-T\mathcal{S}) = \frac{d\mathcal{W}}{dt} - \Delta, \tag{3.4}$$

where $\mathcal{F} := \mathcal{U} - T\mathcal{S}$ is the Helmholtz free energy and $\mathcal{K}+\mathcal{F}$ is equal to the total energy E^{total}. Thus, if no external forces are applied, i.e., if $\frac{d\mathcal{W}}{dt} = 0$, the above expression yields the energy dissipation law (3.1).

Next we describe the energies of a system and make use of the energy dissipation law. Therefore, it is necessary to set up corresponding energy and dissipation functionals for the system. Then we derive differential equations of motion for the system. How this is done is described in the following sections.

3.1.2 Least Action Principle

We distinguish two different types of systems, on the one hand, *Hamiltonian systems*, also referred to as *conservative systems*, and, on the other hand, *dissipative systems.*
As the name implies, energy is dissipated within the latter systems, while energy is conserved within *Hamiltonian systems.* Thus, the energy dissipation functional for such a system is identically zero.

Let us consider a (conservative) physical system where we want to derive the trajectories of particles X occurring within this system, i.e., the paths on which the particles are moving from position $x(X,0)$ at time $t=0$ to position $x(X,t^*)$ at time $t=t^*$. In particular, these trajectories of particles X are those which minimize the action functional defined below. Since we look only at one particle X, we write $x(t)$ instead of $x(X,t)$ here.

Definition 13. *Let $L=\mathcal{K}-\mathcal{F}$ be the Lagrangian function of a conservative system, where $\mathcal{K}$ is the kinetic and $\mathcal{F}$ is the free energy, depending on $x(t)$ and the velocity $x_t(t)$. Then the action functional for this system is defined by*

$$A(x(t)) := \int_0^{t^*} L(x(t), x_t(t))\ dt. \tag{3.5}$$

The least action principle states that one can obtain the equation of motion for a Hamiltonian system by taking the variation of the action functional with respect to the flow maps $x(t)=x(X,t)$. To this end, we consider a variation $x(t)+\varepsilon y(t)$ of the minimizing trajectory $x(t)$ for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, $\varepsilon_0>0$, and $y(t)$ an arbitrary smooth and compactly supported test function.
Since $x(t)$ is a minimizer of $A(x(t))$, the function $\varepsilon \mapsto A(x(t)+\varepsilon y(t))$ must have a minimum point in $\varepsilon=0$. Hence, we calculate (assuming L of class C^2)

$$\begin{aligned}
0 &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x+\varepsilon y)\\
&= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^{t^*} L(x+\varepsilon y, x_t+\varepsilon y_t)\ dt\\
&= \int_0^{t^*} \left(\frac{\partial L}{\partial x}(x,x_t)\right)\cdot y + \left(\frac{\partial L}{\partial (x_t)}(x,x_t)\right)\cdot y_t\ dt\\
&= \int_0^{t^*} \left(\frac{\partial L}{\partial x}(x,x_t) - \frac{d}{dt}\left(\frac{\partial L}{\partial (x_t)}(x,x_t)\right)\right)\cdot y\ dt.
\end{aligned}$$

The last step is an integration by parts with respect to t. Since this is true for any y, by the fundamental lemma of the calculus of variations (see, e.g., [JLJ08, Lemma 1.1.1]) the following equation holds:

$$\frac{\partial L}{\partial x}(x,x_t) - \frac{d}{dt}\left(\frac{\partial L}{\partial\,(x_t)}(x,x_t)\right) = 0. \tag{3.6}$$

This is the so-called *Euler-Lagrange equation* or equation of motion and a necessary condition for the minimizing trajectories.

Moreover, the equation of motion of the conservative system gives the conservative force. So, the principle of least action can be interpreted as the manifestation of the general rule ([Liu11], [HKL10])

$$\delta E^{total} = \text{force}_{conservative}\cdot \delta x,$$

where δ refers to the variation of the respective quantity (principle of virtual work). In other words, work is equal to force times the distance.

3.1.3 Maximum Dissipation Principle and Force Balance

The maximum dissipation principle, however, leads to the dissipative force for a (dissipative) system. This is done by variation of the dissipation functional (in fact, $\frac{1}{2}\Delta$ is used here, since Δ is said to be quadratic in the rates, so the force is linear in the respective rates) with respect to the rate such as the velocity:

$$\delta\left(\frac{1}{2}\Delta\right) = \text{force}_{dissipative} \cdot \delta x_t.$$

So, by the least action principle and the maximum dissipation principle we obtain all the forces for the system we consider.
The final step is to combine these forces with *Netwon's force balance law.* The law states that all forces, both conservative and dissipative in kind, added up is equal to zero, or alternatively, “actio” is equal to “reactio”:

$$\text{force}_{conservative} = \text{force}_{dissipative}.$$

After we obtained the conservative and dissipative forces, the force balance yields the differential equation of motion for the entire system.

3.1.4 Hookean Spring Revisited

We now come back to the example from the beginning of this chapter, the Hookean spring. Again, x denotes the displacement of the lower end of the spring from its equilibrium position. Firstly, we have a look at the energies of the system. The kinetic energy is given by

$$\mathcal{K} = \frac{1}{2}mx_t^2,$$

and the free energy is given by the elastic energy

$$\mathcal{F} = \frac{1}{2}kx^2.$$

Secondly, we give a dissipation term which is due to the damping / friction and depends on the velocity:

$$\Delta = \gamma x_t^2.$$

Note that if the system would be frictionless, thus a conservative system, this function would be zero.
Equation (3.1) gives the following energy dissipation law for the Hookean spring:

$$\frac{d}{dt}\left(\frac{1}{2}mx_t^2 + \frac{1}{2}kx^2\right) = -\gamma x_t^2.$$

From here we can now derive the force balance law we found at the beginning of this chapter using energy variation. Therefore, we set up the action functional $A(x)$ and take the variation with respect to x. The action is given by

$$A(x) = \int_0^{t^*} \left(\frac{1}{2} m x_t^2 - \frac{1}{2} k x^2 \right) \, dt.$$

We can use the Euler-Lagrange equation (3.6) from above, so with the Lagrangian function $L = \frac{1}{2} m x_t^2 - \frac{1}{2} k x^2$ we get immediately

$$-m x_{tt} - kx = 0. \tag{3.7}$$

This is exactly the conservative force for the Hookean spring.

Next we treat the dissipative part, hence, we calculate the variation of $\frac{1}{2}\Delta$ with respect to the velocity. To this end, let y_t be a smooth test function:

$$0 = \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \frac{1}{2} \Delta \left(x_t + \varepsilon y_t \right) = \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \left(\frac{1}{2} \gamma (x_t + \varepsilon y_t)^2 \right) = \left(\gamma x_t \cdot y_t \right).$$

Since this equation must hold for any y_t, this yields the dissipative force and the equation

$$\gamma x_t = 0. \tag{3.8}$$

Now we have both the dissipative part (3.8) and the Hamiltonian part (3.7) of the system. The equation for the entire system then comes from Newton's force balance law force$_{conservative}$ = force$_{dissipative}$:

$$-m x_{tt} - kx = \gamma x_t$$

or equivalently

$$m x_{tt} + kx + \gamma x_t = 0. \tag{3.9}$$

This is exactly the equation we obtained earlier by looking directly at the forces exerted on the spring. For this example, however, the energetic approach seems to be quite complicated. As already pointed out in the introduction, the fact that for more complex systems energy terms are relatively easy to establish, that force components within systems are not counted twice and, one of the most important ones, that it is a natural way of combining effects on different scales, are advantages of the energetic variational approach over the force-based approach (c.f. [EHL10]). This gets more important for systems which are not as easy as the Hookean spring.

Remark 14. *Equation* (3.9) *gives a good insight into how the dynamics of the system behave either near initial data, i.e., the short time behavior, or near equilibrium, i.e., the long time behavior.*
In Figure 3.2 one particular solution of the damped spring equation (3.9)*,*

$$x(t) = a \exp(bt) \cos(ct),$$

with $a > 0$, $b := -\frac{\gamma}{2m}$, $c := \sqrt{\frac{k}{m} - \frac{\gamma^2}{4m^2}}$, $x(0) = a$, *and the damping terms*

$$\pm a \exp(bt)$$

are sketched.
The long time behavior, this is when t is very large, is governed by the dissipative part: It is obvious that

$$\lim_{t\to\infty} |x(t) - a\exp(bt)| = 0,$$

so the solution $x(t)$ *behaves almost like* $a\exp(bt)$ *for large* t*, which is the damping from the dissipative part* $\gamma x_t = 0$ *(c.f.* (3.8)*), and the oscillations are approximately negligible.*
On the other hand, the short time is reflected by the Hamiltonian part, when the damping is negligible: For $t > 0$ *small, we have that* $\exp(bt) \approx 1$ *and thus*

$$x(t) \approx a\cos(\tilde{c}t),$$

with $\tilde{c} := \sqrt{\frac{k}{m}}$*, which is a solution of the Hamiltonian part* $-mx_{tt} - kx = 0$ *(c.f.* (3.7)*). So the damping is negligible near initial data in an approximation.*
This concept is again relevant later on when we talk about the micro-macro model in Section 4.2.

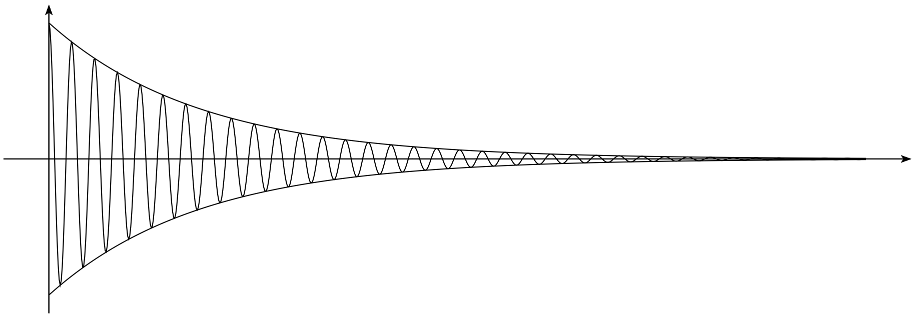

Figure 3.2: Near initial data vs. near equilibrium dynamics

3.2 Simple Solid Elasticity and Fluid Mechanics

In this section we derive the equation of motion for systems describing simple solid or fluid materials by a given energy law. Here *simple* refers to a system which is either a solid or a liquid.
The first example is a Hamiltonian system modeling an elastic solid material. We derive the equation of motion for the system.

Example 15. *Consider the energy law*

$$\frac{d}{dt}\left(\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 + \frac{1}{2}H\left|\frac{\partial x(X,t)}{\partial X}\right|^2 \, dX\right) = 0, \tag{3.10}$$

where $\rho_0(X)$ is the mass density in the Lagrangian coordinate system (note that the integral is taken over the reference configuration Ω_0^X) and H is a constant. The notion $|A|^2$ for $A \in \mathbb{R}^{n\times n}$ is defined as $|A|^2 := A : A$ with the double-dot product defined in Appendix A.1

Clearly, the first term is the kinetic energy, the second is the internal energy due to elastic effects where the deformation gradient is used.
Since the system is conservative (because the time-derivative of the total energy is zero, so energy is conserved), we only need to look at the least action principle. Therefore, we obtain the action for the system:

$$A(x(X,t)) = \int_0^{t^*}\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 - \frac{1}{2}H\left|\frac{\partial x(X,t)}{\partial X}\right|^2 \, dX \; dt.$$

Now we take the variation of the action with respect to x. Here, the energy has an integral form and the internal energy depends on the deformation gradient, too. The calculus of variations tells us that this leads to the Euler-Lagrange equation for the integrand of the action, $L(x, x_t, \frac{\partial x}{\partial X})$ (assuming L of class C^2, and bounded).
In addition to the dependence of the Lagrangian function on x and x_t, which leads to the Euler-Lagrange equation (3.6), we also consider the dependence on the deformation gradient $\frac{\partial x}{\partial X}$. The Euler-Lagrange equation is then given by

$$\frac{\partial L(x, x_t, \frac{\partial x}{\partial X})}{\partial x} - \frac{d}{dt}\left(\frac{\partial L(x, x_t, \frac{\partial x}{\partial X})}{\partial\,(x_t)}\right) - \nabla_X \cdot \left(\frac{\partial L(x, x_t, \frac{\partial x}{\partial X})}{\partial\left(\frac{\partial x}{\partial X}\right)}\right) = 0. \tag{3.11}$$

Since L does not depend on x itself in this particular example but only on the spatial and time derivatives of the flow map, the following equation is obtained:

$$\begin{aligned} -\rho_0(X)x_{tt}(X,t) + H\nabla_X \cdot \frac{\partial x(X,t)}{\partial X} &= 0 \\ \iff \rho_0(X)x_{tt}(X,t) &= H\nabla_X \cdot \nabla_X x(X,t). \end{aligned}$$

If we embrace a shorter notation and use the Laplacian of x as $\Delta_X x = \nabla_X \cdot \nabla_X x$, we obtain the wave equation

$$\rho_0(X)x_{tt} = H\Delta_X x. \tag{3.12}$$

Remark 16. *In the example we looked at a special case of elasticity,*

$$W(\widetilde{F}) = \frac{1}{2}H\left|\frac{\partial x(X,t)}{\partial X}\right|^2,$$

which is called the case of linear elasticity. If we consider the general case, equation (3.12) *changes to a nonlinear wave equation*

$$\rho_0(X)x_{tt} = \nabla_X \cdot W_{\widetilde{F}}(\widetilde{F}). \tag{3.13}$$

This equation is similar to (3.16) *where we consider a fluid material in the Lagrangian coordinate system.*

The second example is again a Hamiltonian system. This time, however, a fluid is described and the Eulerian description is used.

Example 17. *Consider the energy law*

$$\frac{d}{dt}\left(\int_{\Omega_t^x} \frac{1}{2}\rho(x,t)|u(x,t)|^2 + w(\rho(x,t))\ dx\right) = 0, \tag{3.14}$$

where $\rho(x,t)$ is the mass density in the Eulerian coordinate system (note that the integral here is taken over the deformed configuration Ω_t^x), u is the velocity and w is an internal energy density depending on the mass density.

Again, this system is conservative, so we only need to use the least action principle. However, the action functional incorporates an integral over the reference configuration $\int_{\Omega_0^X} \cdots dX$ since the variation is taken with respect to x.
Therefore, we need to write the energy law (3.14) in terms of the Lagrangian coordinate system first.
But, in addition to the simple coordinate change in the energy law, we also need information about how the mass density $\rho(x,t)$ changes under the transformation of the coordinate system. Thus, we have to consider Proposition 12.
Since we do not have any incompressibility condition, the general kinematic assumption of mass transport holds, this is

$$\rho_t + \nabla_x \cdot (u\rho) = 0$$

in the Eulerian coordinate system (as stated in equation (2.5)) or

$$\rho(x(X,t),t) = \frac{\rho_0(X)}{\det \widetilde{F}}$$

in the Lagrangian coordinate system (as stated in equation (2.6)). With this additional assumption we are able to transform the integral and set up the corresponding action functional (for brevity, we use $J = \det \widetilde{F}$):

$$\begin{aligned} A(x(X,t)) &= \int_0^{t^*}\int_{\Omega_0^X} \left(\frac{1}{2}\frac{\rho_0(X)}{J}|x_t(X,t)|^2 - w\left(\frac{\rho_0(X)}{J}\right)\right) J\ dX\ dt \\ &= \int_0^{t^*}\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 - w\left(\frac{\rho_0(X)}{J}\right) J\ dX\ dt. \end{aligned}$$

Thus, taking the variation (for any $y(X,t) = \tilde{y}(x(X,t),t)$ smooth with compact support) with respect to x yields

$$\begin{aligned}
0 =& \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} A(x(X,t)+\varepsilon y(X,t)) = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} A(x+\varepsilon y) \\
=& \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \int_0^{t^*}\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t+\varepsilon y_t|^2 \\
&\qquad\qquad - w\left(\frac{\rho_0(X)}{\det\frac{\partial(x+\varepsilon y)}{\partial X}}\right)\left(\det\frac{\partial(x+\varepsilon y)}{\partial X}\right)\, dX\ dt \\
=& \int_0^{t^*}\int_{\Omega_0^X} \rho_0(X)x_t\cdot y_t - \left(\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} w\left(\frac{\rho_0(X)}{\det\frac{\partial(x+\varepsilon y)}{\partial X}}\right)\right)\cdot\left(\det\frac{\partial x}{\partial X}\right) \\
&\qquad\qquad - w\left(\frac{\rho_0(X)}{\det\frac{\partial x}{\partial X}}\right)\cdot\frac{d}{d\varepsilon}\Big|_{\varepsilon=0}\left(\det\frac{\partial(x+\varepsilon y)}{\partial X}\right)\, dX\ dt \\
\overset{(*)}{=}& \int_0^{t^*}\int_{\Omega_0^X} \rho_0(X)x_t\cdot y_t - w_\rho\left(\frac{\rho_0(X)}{J}\right)\cdot\left(-\frac{\rho_0(X)}{J^2}\right)\cdot J\cdot\operatorname{tr}\left(\frac{\partial X}{\partial x}\frac{\partial y}{\partial X}\right)\cdot J \\
&\qquad\qquad - w\left(\frac{\rho_0(X)}{J}\right)\cdot J\cdot\operatorname{tr}\left(\frac{\partial X}{\partial x}\frac{\partial y}{\partial X}\right)\, dX\ dt,
\end{aligned}$$

where the formula for the derivative of the determinant from Lemma 9 is used at $(*)$. Next, we integrate by parts with respect to time which then yields

$$\begin{aligned}
0 =& \int_0^{t^*}\int_{\Omega_0^X} -\frac{\rho_0(X)}{J}x_{tt}\cdot y\cdot J \\
&\qquad + \left(w_\rho\left(\frac{\rho_0(X)}{J}\right)\cdot\frac{\rho_0(X)}{J} - w\left(\frac{\rho_0(X)}{J}\right)\right)\cdot\operatorname{tr}\left(\frac{\partial X}{\partial x}\frac{\partial y}{\partial X}\right)\cdot J\ dX\ dt \\
=& \int_0^{t^*}\int_{\Omega_t^x} -\rho(x,t)\left(\frac{d}{dt}u(x,t)\right)\cdot\tilde{y} \\
&\qquad + \left(w_\rho(\rho(x,t))\cdot\rho(x,t) - w(\rho(x,t))\right)\cdot\left(\nabla_x\cdot\tilde{y}\right)\ dx\ dt \\
=& \int_0^{t^*}\int_{\Omega_t^x} -\Big(\rho(x,t)\frac{d}{dt}u(x,t) + \nabla_x\big(w_\rho(\rho(x,t))\cdot\rho(x,t) - w(\rho(x,t))\big)\Big)\cdot\tilde{y}\ dx\ dt \\
=& \int_0^{t^*}\int_{\Omega_t^x} -\Big(\rho(x,t)(u_t + (u\cdot\nabla_x)\,u) + \nabla_x p(x,t)\Big)\cdot\tilde{y}\ dx\ dt,
\end{aligned}$$

where we integrate by parts with respect to x in the second to last step. Furthermore, the definition $p(x,t) := w_\rho(\rho(x,t))\cdot\rho(x,t) - w(\rho(x,t))$ for the pressure is used in the last step (equation of state). From the above calculation we get the equation of motion as $\rho(u_t + (u\cdot\nabla_x)u) + \nabla_x p = 0$ and thus we obtain the following system of equations:

$$\begin{cases}\rho_t + \nabla_x\cdot(u\rho) = 0 \\ \rho(u_t + (u\cdot\nabla_x)\,u) + \nabla_x p = 0 \\ p = w_\rho(\rho)\cdot\rho - w(\rho),\end{cases} \tag{3.15}$$

where the first equation is the Euler equation from the conservation of mass, the second equation is the equation of motion, and the last is the equation of state. System (3.15) describes an isentropic fluid, i.e., a fluid with constant entropy, if we assume, that there is no heat applied ($\frac{dQ}{dt} = 0$). Since the dissipation Δ is equal to zero in (3.14), from the second law of thermodynamics (3.3) follows that (assuming $T \neq 0$)

$$\frac{d\mathcal{S}}{dt} = 0,$$

so the entropy is constant.

Remark 18. *The kinetic energy has the same form in both Lagrangian and Eulerian description, in the sense that it is linear in the density and quadratic in the velocity. This can be easily seen from a straightforward calculation using Proposition 12:*

$$\begin{aligned}\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 \; dX &= \int_{\Omega_0^X} \frac{1}{2}\frac{\rho_0(X)}{\det \widetilde{F}}|x_t(X,t)|^2 \cdot \det \widetilde{F} \; dX \\ &= \int_{\Omega_t^x} \frac{1}{2}\frac{\rho_0(X)}{\det F}|u(x,t)|^2 \; dx \\ &= \int_{\Omega_t^x} \frac{1}{2}\rho(x,t)|u(x,t)|^2 \; dx,\end{aligned}$$

where we see that the determinants of the deformation gradient vanish when changing coordinates. However, this is not the case for the free energy in Example 17:

$$\int_{\Omega_t^x} w(\rho(x,t)) \; dx = \int_{\Omega_0^X} w\left(\frac{\rho_0(X)}{\det \widetilde{F}}\right) \det \widetilde{F} \; dX.$$

Remark 19. *In general, the free energy describing fluids only depends on the determinant of the deformation gradient* $\det \widetilde{F}$.
On the other hand, the free energy for solid materials can depend on the deformation gradient $\widetilde{F}$ *itself as seen in Example 15.*
One could say, the dependence on the deformation gradient $\widetilde{F}$ *itself reflects the fact that the atoms have less freedom to move within solid materials. On the other hand, the dependence only on* $\det \widetilde{F}$ *of a fluid's free energy corresponds to a higher degree of freedom to move.*

3.3 Change of Coordinate Systems

We considered solid materials and used the Lagrangian coordinate system, for fluid materials we used the Eulerian description. Now we take a look at how the formulae change when we use the description the other way round, i.e., Eulerian coordinates for solids and Lagrangian coordinates for fluids. This gives us the possibility to choose the best description for certain models which is useful, e.g., to combine frameworks that are a priori defined for different coordinate systems.

Since the kinetic energy takes the same form in both Lagrangian and Eulerian coordinate system (see Remark 18), we only consider the free energy density for a fluid material. We have

$$\int_{\Omega_t^x} w(\rho(x,t))\; dx = \int_{\Omega_0^X} \Phi(\widetilde{F})\; dX,$$

where we define $\Phi(\widetilde{F}) := \left(w\left(\frac{\rho_0(X)}{\det \widetilde{F}}\right) \det \widetilde{F} \right)$, and the least action principle (where we include the kinetic energy again, of course) yields the equation

$$\rho_0(X) x_{tt} = \nabla_X \cdot \Phi_{\widetilde{F}}(\widetilde{F}), \tag{3.16}$$

which is actually a nonlinear wave equation as in the solid case (also Lagrangian coordinate system) considered above where (3.13) is obtained.

To consider solid elastic materials in the Eulerian coordinate system, we first look at the variation of the action corresponding to

$$\frac{d}{dt}\left(\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 + W(\widetilde{F})\; dX \right) = 0, \tag{3.17}$$

which is the generalized version of the energy law (3.10) in Example 15. See Remark 16 for the Lagrangian description of the equation of motion of the generalized solid model. Now we calculate the variation of the action (for any $y(X,t) = \tilde{y}(x(X,t),t)$ smooth with compact support; for detailed calculations review Example 17) and, as within the fluid example, we transform into the

Eulerian coordinate system at a certain step:

$$
\begin{aligned}
0 =& \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x+\varepsilon y) \\
=& \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^{t^*} \int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t+\varepsilon y_t|^2 - W\left(\frac{\partial(x+\varepsilon y)}{\partial X}\right)\ dX\ dt \\
=& \int_0^{t^*} \int_{\Omega_0^X} \rho_0(X) x_t \cdot y_t - W_{\widetilde{F}}(\widetilde{F}) : \left(\frac{\partial y}{\partial X}\right)\ dX\ dt \\
=& \int_0^{t^*} \int_{\Omega_0^X} -\frac{\rho_0(X)}{J}\left(x_{tt}\cdot y\right) J - W_{\widetilde{F}}(\widetilde{F}) : (\nabla_X y)\ dX\ dt \\
=& \int_0^{t^*} \int_{\Omega_t^x} -\rho(x,t)(u_t + (u\cdot\nabla_x)\, u)\cdot\tilde{y} - \left(\frac{1}{J}\cdot W_F(F)\right) : (\nabla_x \tilde{y}\cdot F)\ dx\ dt \\
=& \int_0^{t^*} \int_{\Omega_t^x} -\rho(x,t)(u_t + (u\cdot\nabla_x)\, u)\cdot\tilde{y} - \left(\frac{1}{J}\cdot W_F(F)\cdot F^T\right) : (\nabla_x \tilde{y})\ dx\ dt \\
=& \int_0^{t^*} \int_{\Omega_t^x} -\rho(x,t)(u_t + (u\cdot\nabla_x)\, u)\cdot\tilde{y} + \nabla_x\cdot\left(\frac{1}{J}\cdot W_F(F)\cdot F^T\right)\cdot\tilde{y}\ dx\ dt \\
=& \int_0^{t^*} \int_{\Omega_t^x} -\left(\rho(x,t)(u_t + (u\cdot\nabla_x)\, u) - \nabla_x\cdot\left(\frac{1}{J}\cdot W_F(F)\cdot F^T\right)\right)\cdot\tilde{y}\ dx\ dt.
\end{aligned}
$$

Here we use the product $A : B$ from Appendix A.1 for $n \times n$-matrices and the fact that the derivative of the scalar-valued function $W(\widetilde{F})$ with respect to its argument $\widetilde{F}$ is again a matrix of dimension $n \times n$. For details concerning the derivative $\frac{d}{d\varepsilon}W\left(\frac{\partial(x+\varepsilon y)}{\partial X}\right)$ from above, see Appendix A.2.
The integration by parts in the second to last step is explained in detail in Appendix A.4.

Thus, we obtain the equation of motion for a solid material in the Eulerian description $\rho(x,t)(u_t+(u\cdot\nabla_x)\,u) = \nabla_x\cdot\left(\frac{1}{J}\cdot W_F(F)\cdot F^T\right)$. We add the kinematic assumptions and obtain the entire system

$$
\begin{cases}
\rho_t + \nabla_x\cdot(u\rho) = 0 \\
\frac{\partial F}{\partial t} + (u\cdot\nabla_x)\, F = \nabla_x u\cdot F \\
\rho(u_t + (u\cdot\nabla_x)\, u) = \nabla_x\cdot\left(\frac{1}{J}\cdot W_F(F)\cdot F^T\right),
\end{cases}
\tag{3.18}
$$

where the first equation is the general conservation of mass (c.f. (2.5)) and the second is the chain rule (2.3). The last equation is the wave equation in the Eulerian coordinate system.

Remark 20. *The quantity $W_{\widetilde{F}}(\widetilde{F})$ that comes up in Remark 16 is called the Piola-Kirchhoff stress (c.f. [TM11, Section 8.1.2]). The corresponding quantity in the Eulerian description is the so-called Cauchy-Green stress $\frac{1}{J}\cdot W_F(F)\cdot F^T$ from* (3.18) *(c.f. [TM11, Section 2.3.4]).*

3.4 Addition of Dissipation

In Sections 3.2 and 3.3 we considered only Hamiltonian systems of fluid and solid materials. Now we add dissipation terms to the fluid and solid models from above (c.f. energy dissipation law (3.1)). At first, we look at the energy law describing a solid material:

$$\frac{d}{dt}\left(\int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t(X,t)|^2 + W(\widetilde{F})\ dX\right) = -\int_{\Omega_0^X} \eta(x(X,t),t)|x_t(X,t)|^2\ dX,$$

where

$$\Delta = \int_{\Omega_0^X} \eta(x(X,t),t)|x_t(X,t)|^2\ dX \tag{3.19}$$

is the dissipation with a chosen dissipation coefficient η that depends on spatial and time variables.

This is one ansatz in modeling the dissipation functional. However, after the discussion of this particular dissipation in the Eulerian coordinate system for a fluid, we see another ansatz involving the spatial gradient and the divergence of the velocity u.

The dissipation is chosen to be quadratic in the rates, so the dissipative force that is derived from the dissipation by taking the variation of $\frac{1}{2}\Delta$ with respect to the velocity is linear in the rates. For the chosen dissipation Δ this yields

$$\text{force}_{dissipative} = \eta(x(X,t),t)x_t(X,t) = \eta x_t.$$

So, by Newton's force balance law, we can extend the equation of motion for the system (c.f. Remark 16) by a dissipative term, thus

$$\rho_0(X)x_{tt} = \nabla_X \cdot W_{\widetilde{F}}(\widetilde{F}) - \eta x_t.$$

This is a damped wave equation. If we look at the same system in the Eulerian coordinate system, we obtain by extending (3.18)

$$\begin{cases} \rho_t + \nabla_x \cdot (u\rho) = 0 \\ \frac{\partial F}{\partial t} + (u \cdot \nabla_x)\, F = \nabla_x u \cdot F \\ \rho(u_t + (u \cdot \nabla_x)\, u) = \nabla_x \cdot \left(\frac{1}{J} \cdot W_F(F) \cdot F^T\right) - \frac{1}{J}\eta u, \end{cases}$$

since we take the variation with respect to u of

$$\frac{1}{2}\Delta = \frac{1}{2}\int_{\Omega_0^X} \eta(x(X,t),t)|x_t(X,t)|^2\ dX = \frac{1}{2}\int_{\Omega_t^x} \frac{\eta(x,t)}{J}|u(x,t)|^2\ dx.$$

This can be done easily because we do not take the variation with respect to the flow map x (otherwise we would need to transform the integral into the Lagrangian coordinate system).

Remark 21. *The damping considered in* (3.19) *is called Darcy's damping.*

Concerning Example 17 for a fluid system, we can also add dissipation like Darcy's damping. This leads to the Euler-Darcy system

$$\begin{cases} \rho_t + \nabla_x \cdot (u\rho) = 0 \\ \rho(u_t + (u \cdot \nabla_x)\, u) + \nabla_x p = -\eta u \\ p = w_\rho(\rho) \cdot \rho - w(\rho), \end{cases}$$

which is extended from (3.15) using the dissipation $\Delta_1 = \int_{\Omega_t^x} \eta(x,t)|u(x,t)|^2 \; dx$, where we choose the dissipation coefficient $\eta(x,t)$ directly in the Eulerian coordinate system.

Moreover, we could also choose dissipation terms involving the spatial gradient and the divergence of u. This is used in modeling viscosity. We consider

$$\Delta_2 = \int_{\Omega_t^x} \mu_1(x,t)|\nabla_x u|^2 + \mu_2(x,t)|\nabla_x \cdot u|^2 \; dx, \tag{3.20}$$

where μ_1, μ_2 are viscosity constants. The name "constants" is due to the fact that they are constant for a particular material. However, they can depend on x and t (and are assumed to do so for now).
If we incorporate dissipation Δ_2, we can calculate the dissipative force through

$$\begin{aligned} 0 &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \frac{1}{2}\Delta_2\,(u + \varepsilon v) \\ &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{\Omega_t^x} \frac{1}{2}\mu_1(x,t)|\nabla_x u + \varepsilon \nabla_x v|^2 + \frac{1}{2}\mu_2(x,t)|\nabla_x \cdot u + \varepsilon \nabla_x \cdot v|^2 \; dx \\ &= \int_{\Omega_t^x} \mu_1(x,t)\nabla_x u : \nabla_x v + \mu_2(x,t)(\nabla_x \cdot u)(\nabla_x \cdot v) \; dx \\ &= \int_{\Omega_t^x} \Big(-\nabla_x \cdot (\mu_1(x,t)\nabla_x u) - \nabla_x(\mu_2(x,t)\nabla_x \cdot u) \Big) \cdot v \; dx, \end{aligned}$$

where v is any test function with compact support, and the system (3.15) becomes

$$\begin{cases} \rho_t + \nabla_x \cdot (u\rho) = 0 \\ \rho(u_t + (u \cdot \nabla_x)\, u) + \nabla_x p = \nabla_x \cdot (\mu_1 \nabla_x u) + \nabla_x\,(\mu_2 \nabla_x \cdot u) \\ p = w_\rho(\rho) \cdot \rho - w(\rho), \end{cases}$$

which describes a viscous fluid.

Now we have a look at the first viscosity term and transform the integral into the Lagrangian coordinate system. We get

$$\int_{\Omega_t^x} \mu_1(x,t)|\nabla_x u|^2 \; dx = \int_{\Omega_0^X} (J \cdot \mu_1(x(X,t),t))\, |\nabla_X x_t(X,t)\widetilde{F}^{-1}|^2 \; dX.$$

The transformation of the gradient can be easily seen by going a bit more into detail. For $1 \leq i, j \leq n$ we have that

$$\begin{aligned}(\nabla_X x_t(X,t))_{ij} &= \frac{\partial x_t^i(X,t)}{\partial X^j} = \frac{\partial u^i(x(X,t),t)}{\partial X^j} \\ &= \frac{\partial u^i(x(X,t),t)}{\partial x^k}\frac{\partial x^k}{\partial X^j} = \left((\nabla_x u)\,\widetilde{F}\right)_{ij}, \end{aligned} \tag{3.21}$$

where we use the Einstein summation convention and the chain rule. Hence

$$\nabla_x u = \nabla_X x_t(X,t)\widetilde{F}^{-1}. \tag{3.22}$$

From here we see that the expression gets much more complicated, since the deformation gradient comes into play, too, which yields the following remark.

Remark 22. *Viscosity is convenient to use with the Eulerian coordinate system.*

3.5 Consideration of Incompressibility Condition

From Definition 6 and Proposition 7 we recall the mathematical description of incompressibility. In the *Lagrangian coordinate system* it is

$$\det \widetilde{F} \equiv 1, \tag{3.23}$$

in the *Eulerian coordinate system* it is

$$\nabla_x \cdot u = 0. \tag{3.24}$$

Note that (3.23) is a nonlinear constraint for the flow map, while (3.24) is linear, so, if we do a variation with respect to the velocity u in the Eulerian coordinate system under incompressibility conditions, we can use functions $u + \varepsilon v$ which satisfy $\nabla_x \cdot (u + \varepsilon v) = 0$.
On the other hand, if we do a variation with respect to x, which is the case when applying the least action principle, the difficulty is that $\det\left(\frac{\partial x}{\partial X} + \varepsilon \frac{\partial y}{\partial X}\right) \equiv 1$ does not hold if $\det \frac{\partial x}{\partial X} \equiv 1$ holds.
In this case, we use volume preserving diffeomorphisms to perform the variation, i.e., functions x^ε such that

$$x^0 = x \quad \text{and} \quad \left.\frac{dx^\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} := y \quad \text{and} \quad \forall \varepsilon: \det \widetilde{F}^\varepsilon = \det \frac{\partial x^\varepsilon}{\partial X} \equiv 1. \tag{3.25}$$

The nonlinear constraint, however, leads to a divergence condition for $y(X,t) = \tilde{y}(x(X,t),t)$ similar to (3.24) in the Eulerian coordinate system. Indeed, from (3.25) we get

$$\begin{aligned}0 &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \det \frac{\partial x^\varepsilon}{\partial X} \\ &= \det \widetilde{F} \cdot \operatorname{tr}\left(\widetilde{F}^{-1} \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \frac{\partial x^\varepsilon}{\partial X}\right) = \operatorname{tr}\left(\sum_{k=1}^{n} \frac{\partial X^k}{\partial x^i}\frac{\partial y^j}{\partial X^k}\right) = \nabla_x \cdot \tilde{y}. \end{aligned} \tag{3.26}$$

Equation (3.26) provides us with a necessary condition which is crucial for calculating, e.g., first variations if incompressibility holds.

Now we look at a problem under incompressibility condition. We consider the energy law

$$\frac{d}{dt}\left(\int_{\Omega_t^x} \frac{1}{2}\rho(x,t)|u(x,t)|^2 \, dx\right) = -\int_{\Omega_t^x} \mu(x,t)|\nabla_x u|^2 \, dx, \tag{3.27}$$

which is a simple viscous fluid.
To put the simple part first, we start with the variation of the right-hand side. Here, we use $u+\varepsilon v$ since we are in the Eulerian coordinate system and $\nabla_x \cdot (u+\varepsilon v) = 0$ holds for any compactly supported and smooth test function v satisfying $\nabla_x \cdot v = 0$. The calculation is similar to the one using Δ_2 in the previous section; we obtain:

$$0 = \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \frac{1}{2}\Delta\left(u+\varepsilon v\right) = \int_{\Omega_t^x} \Big(-\nabla_x \cdot (\mu(x,t)\nabla_x u)\Big) \cdot v \, dx. \tag{3.28}$$

This is a crucial point: In the compressible case, the equation of motion is $-\nabla_x \cdot (\mu(x,t)\nabla_x u) = 0$ since the field v is arbitrary.
Now the field v is divergence free, hence we use *Weyl's decomposition* or *Helmholtz' decomposition* of a vector field (c.f. [DL00, Chapter IX, Section 1, Propostion 1]; we omit the proof for brevity):

Proposition 23. *If a vector field $w \in L^2(\Omega, \mathbb{R}^n)$ is orthogonal to all smooth divergence free vector fields with compact support, then w has gradient form, i.e., $w = \nabla p$ for some $p \in W^{1,2}(\Omega, \mathbb{R}^n)$.*

Thus, we obtain the following equation of motion for the dissipative part:

$$-\nabla_x \cdot (\mu \nabla_x u) = \nabla_x p_2 \tag{3.29}$$

with $p_2 \in W^{1,2}(\Omega, \mathbb{R}^n)$.
Now we turn to the Hamiltonian part. For the least action principle we use variations x^ε of x as described in (3.25) and (3.26) with y satisfying $y(X,0) = y(X,t^*) = 0$ for any $X \in \Omega_0^X$. Due to incompressibility, the mass density is constant, i.e., $\rho(x(X,t),t) = \rho_0(X)$, c.f. Proposition 11, and $J = \det \widetilde{F} \equiv 1$. So

we can calculate the variation of the action functional:

$$\begin{aligned} 0 = \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x^\varepsilon) &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^{t^*} \int_{\Omega_0^X} \frac{1}{2}\rho_0(X)|x_t^\varepsilon|^2 \; dX \; dt \\ &= \int_0^{t^*} \int_{\Omega_0^X} \rho_0(X) \left(x_t^\varepsilon\bigg|_{\varepsilon=0} \right) \cdot \left(\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} x_t^\varepsilon \right) \; dX \; dt \\ &= \int_0^{t^*} \int_{\Omega_0^X} \rho_0(X) x_t \cdot y_t \; dX \; dt \\ &= \int_0^{t^*} \int_{\Omega_0^X} -\rho_0(X) x_{tt} \cdot y \; dX \; dt \\ &= \int_0^{t^*} \int_{\Omega_t^x} -\rho(x,t)(u_t + (u \cdot \nabla_x)\, u) \cdot \tilde{y} \; dx \; dt, \end{aligned}$$

where the equality $y(X,t) = \tilde{y}(x(X,t),t)$ is used in the transformation of the integral in the last step. We can apply Proposition 23 again because $\tilde{y}$ is divergence free due to (3.26), hence, for some $p_1 \in W^{1,2}(\Omega, \mathbb{R}^n)$ we have

$$-\rho(x,t)(u_t + (u \cdot \nabla_x)\, u) = \nabla_x p_1. \tag{3.30}$$

Putting both results (3.29) and (3.30) together (where we make use of the force balance law: force$_{conservative}$ = force$_{dissipative}$) and adding also the kinematic assumptions of incompressibility (c.f. (3.24)) and conservation of mass (2.5), we obtain the following system

$$\begin{cases} \nabla_x \cdot u = 0 \\ \rho_t + (u \cdot \nabla_x)\, \rho = 0 \\ \rho(u_t + (u \cdot \nabla_x)\, u) + \nabla_x p = \nabla_x \cdot (\mu \nabla_x u)\, , \end{cases} \tag{3.31}$$

where we set $p = p_1 - p_2$. This is the Lagrange multiplier for the incompressibility constraint, reflecting both the Hamiltonian and the dissipative part of the system. This is a Navier-Stokes system for incompressible viscous fluids.

Now we can step into more complex examples in the next chapter and put the pieces together we learned so far.

4 Modeling of Complex Fluids

In this chapter we discuss exemplary models for complex fluids. We use the energetic variational approach and the mechanical tools explained in the previous chapters to derive differential equations from energy laws describing the phenomena within the materials.
Throughout this chapter we assume that the considered functions have enough regularity and the integrands are bounded, so the calculations are well-defined.
We start with a rather general model of incompressible viscoelastic materials such as biological materials (e.g. muscles) or rubbers. Here we put several concepts together in order to generate one modeling framework to incorporate solid and fluid properties. After that we go down on a smaller scale to see where these properties come from: We study polymeric fluids through a micro-macro analysis in Section 4.2 to analyze the effect of polymers, which are surrounded by a fluid, onto the (macroscopic) fluid flow. In Section 4.3 we consider liquid crystals and study coupling effects with a fluid.

4.1 Incompressible Viscoelasticity

As the title “Incompressible Viscoelasticity” implies, we have *incompressibility* first (c.f. (3.24)):

$$\nabla_x \cdot u = 0.$$

Secondly, there is some *visco* part, so we have viscosity (c.f. (3.20)), a property of fluid material, and something like

$$\int_{\Omega_t^x} \mu |\nabla_x u|^2 \, dx,$$

where $\mu > 0$ is a viscosity constant which is assumed to be constant in x and t.
Moreover, there is a third part, *elasticity*, so we need

$$\int_{\Omega_t^x} \lambda W(F) \, dx,$$

with an elasticity density $W(F)$ (c.f. (3.17)), incorporated with a relaxation parameter $\lambda > 0$.
As noted in Remark 22, viscosity is conveniently modeled in the Eulerian coordinate system, so we use the Eulerian description in this context.

In contrast to the previous chapter where we considered models for solid and fluid materials separately, we now take both fluid and solid properties together and create a unified *viscoelastic framework.*

This is also an approach to simplify the way we look at solid and fluid materials which is the idea of the viscoelastic model. However, special cases in terms of the choice of μ and λ lead to the model of (incompressible) solid elasticity and the model of (incompressible) viscous fluids, respectively.

We establish the energy law for this model of incompressible viscoelasticity as follows:

$$\frac{d}{dt}\int_{\Omega_t^x}\frac{1}{2}\rho|u|^2+\lambda W(F)\ dx=-\int_{\Omega_t^x}\mu|\nabla_x u|^2\ dx, \tag{4.1}$$

incorporating both solid (elasticity) and fluid (viscosity) properties. The action is given by

$$A(x)=\int_0^{t^*}\int_{\Omega_0^X}\frac{1}{2}\rho_0(X)|x_t(X,t)|^2-\lambda W(\widetilde{F})\ dX\ dt, \tag{4.2}$$

which is transformed into the Lagrangian coordinate system. Notice that $J=\det\widetilde{F}\equiv 1$ due to incompressibility.

Now we calculate the variation of the action (4.2), where we use volume preserving diffeomorphisms x^ε as characterized in (3.25) and (3.26) with y satisfying $y(X,0)=y(X,t^*)=0$ for any $X\in\Omega_0^X$, since we work under incompressibility conditions (compare also the variation of (3.17), where is, however, neither any relaxation nor incompressibility):

$$\begin{aligned}
0=&\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0}A(x+\varepsilon y)\\
=&\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0}\int_0^{t^*}\int_{\Omega_0^X}\frac{1}{2}\rho_0(X)|x_t+\varepsilon y_t|^2-\lambda W\left(\frac{\partial(x+\varepsilon y)}{\partial X}\right)\ dX\ dt\\
=&\int_0^{t^*}\int_{\Omega_0^X}\rho_0(X)x_t\cdot y_t-\lambda W_{\widetilde{F}}(\widetilde{F}):\left(\frac{\partial y}{\partial X}\right)\ dX\ dt\\
=&\int_0^{t^*}\int_{\Omega_0^X}-\rho_0(X)x_{tt}\cdot y-\lambda W_{\widetilde{F}}(\widetilde{F}):(\nabla_X y)\ dX\ dt\\
=&\int_0^{t^*}\int_{\Omega_t^x}-\rho(x,t)(u_t+(u\cdot\nabla_x)u)\cdot\tilde{y}-\lambda\left(W_F(F)\right):(\nabla_x\tilde{y}\cdot F)\ dx\ dt\\
=&\int_0^{t^*}\int_{\Omega_t^x}-\rho(x,t)(u_t+(u\cdot\nabla_x)u)\cdot\tilde{y}-\lambda\left(W_F(F)\cdot F^T\right):(\nabla_x\tilde{y})\ dx\ dt\\
=&\int_0^{t^*}\int_{\Omega_t^x}-\rho(x,t)(u_t+(u\cdot\nabla_x)u)\cdot\tilde{y}+\lambda\nabla_x\cdot\left(W_F(F)\cdot F^T\right)\cdot\tilde{y}\ dx\ dt\\
=&\int_0^{t^*}\int_{\Omega_t^x}-\Big(\rho(x,t)(u_t+(u\cdot\nabla_x)u)-\lambda\nabla_x\cdot\left(W_F(F)\cdot F^T\right)\Big)\cdot\tilde{y}\ dx\ dt,
\end{aligned}$$

where the product $A : B$ from Appendix A.1 is used. For details concerning the derivative $\frac{d}{d\varepsilon} W\left(\frac{\partial(x+\varepsilon y)}{\partial X}\right)$ from the calculation above, see Appendix A.2.
The integration by parts in the second to last step is explained in detail in Appendix A.4.

At this stage we apply Helmholtz' decomposition as in Proposition 23 and obtain for some $p_1 \in W^{1,2}(\Omega, \mathbb{R}^n)$

$$\rho(u_t + (u \cdot \nabla_x)\, u) - \lambda \nabla_x \cdot \left(W_F(F) \cdot F^T\right) = -\nabla_x p_1, \tag{4.3}$$

which yields the Hamiltonian part. For the dissipative part we look at the dissipation in the energy law (4.1):

$$\Delta = \int_{\Omega_t^x} \left(\mu |\nabla_x u|^2\right)\, dx,$$

where we perform the variation with respect to the velocity u. This variation, however, is the same as in (3.28). Again by Proposition 23, the calculations lead to the following equation of motion for the dissipative part (3.29):

$$-\nabla_x \cdot (\mu \nabla_x u) = \nabla_x p_2,$$

for $p_2 \in W^{1,2}(\Omega, \mathbb{R}^n)$, or equivalently, since μ is assumed to be constant in this model,

$$-\mu \Delta_x u = \nabla_x p_2. \tag{4.4}$$

Equations (4.3) and (4.4) are brought together by the force balance law force$_{conservative}$ = force$_{dissipative}$ which yields the entire equation of motion for the macroscopic scale

$$\rho(u_t + (u \cdot \nabla_x)\, u) + \nabla_x p = \mu \Delta_x u + \lambda \nabla_x \cdot \left(W_F(F) \cdot F^T\right). \tag{4.5}$$

where $p = p_1 - p_2$.

We now put the system's equations together. To this end, we state the kinematic assumptions of incompressibility (c.f. (3.24)), the chain rule for the deformation gradient (2.3) and conservation of mass (c.f. (2.5) and part 2 of Proposition 11), and the equation of motion (4.5). We obtain the following system:

$$\begin{cases} \nabla_x \cdot u = 0 \\ \frac{\partial F}{\partial t} + (u \cdot \nabla_x)\, F = \nabla_x u \cdot F \\ \rho_t + (u \cdot \nabla_x)\, \rho = 0 \\ \rho(u_t + (u \cdot \nabla_x)\, u) + \nabla_x p = \mu \Delta_x u + \lambda \nabla_x \cdot \left(W_F(F) \cdot F^T\right). \end{cases} \tag{4.6}$$

Notice that equation (4.5) consists of $(3.18)_3$ and $(3.31)_3$ with the viscosity and the elasticity part (notice the additional relaxation parameter $\lambda > 0$ here).

What can be easily seen in system (4.6) and in the corresponding energy law (4.1) is that we can use the parameters λ and μ to choose the influence of elasticity and viscosity, respectively, within the model.
If we set $\mu = 0$ and $\lambda > 0$, we get a model for incompressible solid elasticity as in (3.18). On the other hand, if we set $\lambda = 0$ and $\mu > 0$, the model is for incompressible viscous fluids. We obtained this earlier in (3.31). Basically, we tear the fluid and solid properties apart again.

Now it is interesting to ask where solid and fluid properties come from and where these properties have their seeds in. For a particular example of fluids, this is discussed in the following section.

4.2 Micro-Macro Models for Polymeric Fluids

This section deals with physical phenomena that happen on an atomistic scale. The question that came up in the last section, where do solid and fluid properties come from, shall be discussed to some extent.
What we do here, is the so-called multiscale modeling. This means, we look at phenomena occurring at different length and/or time scales [TM11, Chapter 10]. To make clear what is meant by different scales, we take a look at different length scales in some copper material like a coin (c.f. [TM11, Section 1.1]).
On the largest scale, i.e., what is visible to the naked eye at a 1mm scale, we see a solid coin made from hard material.
When we go down to finer scales at micrometers and nanometers, we can observe certain structures and patterns.
Down at the Ångstrom length scale, we see the individual positions of the atoms. Concerning time scales, we see that for the coin as a whole piece of copper at the largest scale, motion and deformation processes like creep and fatigue may take years. On the other hand, down at the finest scale, the vibration of atoms takes place on a femtosecond scale ($1\text{fs} = 0.000\ 000\ 000\ 000\ 001\text{s} = 10^{-15}\text{s}$).

In our modeling, however, we only use two scales: a macroscopic or "coarse" scale (largest) and a microscopic or "fine" scale. We assume that these scales communicate through averaging from micro to macro and through interpolation from macro to micro. Moreover, we assume separation of scales, i.e., if we know what happens on both the microscopic and the macroscopic scale, we know everything that happens in between.

We consider a domain $\Omega_t^x \subset \mathbb{R}^3$ in the Eulerian coordinate system on the macroscopic scale. On the fine scale we consider the configuration space $\mathbb{R}^3$, i.e., we look at the polymer molecules as end-to-end vectors $Q \in \mathbb{R}^3$. These polymers are modeled as small springs, see Figure 4.1. Additionally, we need a distribution function $f(Q,t)$ for the polymers satisfying $\int_{\mathbb{R}^3} f(Q,t)\ dQ = \text{const}$, and $\lim_{|Q|\to\infty} f(Q,t) = 0$ and $\lim_{|Q|\to\infty} \nabla_Q f(Q,t) = 0$ for all $t \geq 0$. Then we perform some averaging over the fine scale which leads to the effect onto the macroscopic scale. So, a point $x \in \Omega_t^x$ represents the properties of a bunch of polymers in the surroundings of x.

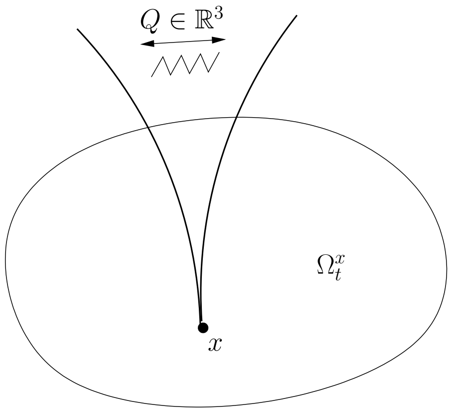

Figure 4.1: Microscopic vectors acting as springs in the fine scale, averaged to the macroscopic scale

4.2.1 Microscopic Scale

We start with the microscopic scale, where we look at the polymer end-to-end vectors $Q \in \mathbb{R}^3$ as springs. From previous chapters we know the equation of motion governing the spring (3.9). We use a general elastic potential $U(Q)$ (c.f. [LLZ07, Section 2]) and obtain

$$Q_{tt} + \gamma Q_t = -\nabla_Q U,$$

where $\gamma > 0$ is a damping constant. We consider situations where the motion on the fine scale is much faster than on the macroscopic scale. So for the microscopic behavior, we can say that we are only interested in the long time dynamics (c.f. Remark 14). Thus, we neglect the oscillation part Q_{tt} which yields

$$\gamma Q_t = -\nabla_Q U \tag{4.7}$$

as a governing equation. This dynamical behavior is called *gradient flow* or *near equilibrium dynamics.*

We consider now the distribution function $f(Q,t)$ from above. Like for the mass density or mass distribution function $\rho(x,t)$ considered in Section 2.4, we can establish the transport equation $f_t + \nabla_Q \cdot (Q_t \ f) = 0$ (c.f. equation (2.5)) since the number of particles is conserved over time.
With the gradient flow equation (4.7) the transport equation for f becomes

$$f_t - \nabla_Q \cdot \left(\frac{1}{\gamma} \nabla_Q U \ f \right) = 0.$$

Now we add thermal fluctuations to the gradient flow (4.7) by adding an isotropic Brownian motion and obtain

$$dQ = -\frac{1}{\gamma} \nabla_Q U \ dt + \sigma dW_t. \tag{4.8}$$

Here, W_t is a regular Wiener process representing the Brownian motion and $\sigma = kT$, where k is the Boltzmann constant and T is the temperature (c.f. [LLZ07]). When Itō's lemma from stochastic differential calculus is applied, we see that the distribution function $f(Q,t)$ satisfies

$$f_t = \nabla_Q \cdot \left(\frac{1}{\gamma}\nabla_Q U\ f\right) + \frac{\sigma^2}{2}\Delta_Q f, \tag{4.9}$$

which is the Fokker-Planck equation [PB99, Section 3.5]. Furthermore, it holds that $f \geq 0$ and the equilibrium distribution is given by $f = C\exp\left(-\frac{2}{\gamma\sigma^2}U\right)$ [LLZ07, Section 2].

We define the free energy $\int_{\mathbb{R}^3} A(f)\, dQ$ with the free energy density (c.f. [EHL10])

$$A(f) = \frac{\sigma^2}{2} f\ln f + \frac{1}{\gamma}U\ f.$$

The term $\frac{\sigma^2}{2} f\ln f$ is called Gibbs entropy and corresponds to the transport of the molecules through Brownian motion. The second term represents the elastic energy density due to the spring model of the polymers.
Now we can use (4.9) (in the third step) to derive the following dissipative energy law (we assume that f and U are chosen in the way that the boundary terms (as $|Q| \to \infty$) vanish in the integration by parts):

$$\begin{aligned}
&\frac{d}{dt}\int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2} f\ln f + \frac{1}{\gamma}U\ f\right)\, dQ \\
&= \int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2}(f_t\ln f + f_t) + \frac{1}{\gamma}U\ f_t\right)\, dQ \\
&= \int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right)\ f_t\ dQ \\
&= \int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right)\ \left(\nabla_Q \cdot \left(\frac{1}{\gamma}\nabla_Q U\ f\right) + \frac{\sigma^2}{2}\Delta_Q f\right)\, dQ \\
&= \int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right)\ \nabla_Q \cdot \left(\frac{1}{\gamma}\nabla_Q U\ f + \frac{\sigma^2}{2}\nabla_Q f\right)\, dQ \\
&= -\int_{\mathbb{R}^3} \nabla_Q\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right) \cdot \left(\frac{1}{\gamma}\nabla_Q U\ f + \frac{\sigma^2}{2}\nabla_Q f\right)\, dQ \\
&= -\int_{\mathbb{R}^3} \nabla_Q\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right) \cdot \left(\frac{1}{\gamma}\nabla_Q U + \frac{\sigma^2}{2}\frac{1}{f}\nabla_Q f\right)\ f\ dQ \\
&= -\int_{\mathbb{R}^3} f\nabla_Q\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right) \cdot \nabla_Q\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right)\, dQ \\
&= -\int_{\mathbb{R}^3} f\left|\nabla_Q\left(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U\right)\right|^2\, dQ,
\end{aligned}$$

so we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^3}\underbrace{\left(\frac{\sigma^2}{2}f\ln f+\frac{1}{\gamma}U\ f\right)}_{A(f)}\ dQ=-\int_{\mathbb{R}^3}f\left|\nabla_Q\underbrace{\left(\frac{\sigma^2}{2}(\ln f+1)+\frac{1}{\gamma}U\right)}_{\bar{\mu}}\right|^2\ dQ, \tag{4.10}$$

where it is obvious that $A_f(f)=\frac{\partial}{\partial f}A(f)=\bar{\mu}$, which is called chemical potential.

Now we couple (4.9) with the macroscopic variable x: We assume that the distribution function f also depends on the flow map $x(X,t)$, hence we write $f=f(x(X,t),Q,t)$. Moreover, we assume that the microscopic vector Q is also a deformed vector by the macroscopic motion. This is the Cauchy-Born relation (c.f. [TM11, Section 11.2.2])

$$Q=Fq, \tag{4.11}$$

where q is in the microscopic configuration of the reference configuration.
To establish the coupling with the macroscopic entities x and F, we exchange the partial derivative f_t in (4.9) by the total derivative

$$\frac{d}{dt}f(x(X,t),Fq,t).$$

To this end, we calculate

$$\begin{aligned}\frac{d}{dt}f(x(X,t),Fq,t)&=f_t+(\nabla_x f)\cdot u+(\nabla_Q f)\cdot\left(\left(\frac{d}{dt}F\right)q\right)\\&=f_t+(u\cdot\nabla_x)\,f+(\nabla_Q f)\cdot((\nabla_x u\ F)\,q)\\&=f_t+(u\cdot\nabla_x)\,f+(\nabla_x u\ Fq)\cdot\nabla_Q f\\&=f_t+(u\cdot\nabla_x)\,f+\nabla_x uQ\cdot\nabla_Q f,\end{aligned}$$

where we use Propostion 4 in the second and the Cauchy-Born relation (4.11) in the last step. Inserting this result into (4.9), we obtain the *microscopic force balance with coupling*:

$$f_t+(u\cdot\nabla_x)\,f+\nabla_x uQ\cdot\nabla_Q f=\nabla_Q\cdot\left(\frac{1}{\gamma}\nabla_Q U\ f\right)+\frac{\sigma^2}{2}\Delta_Q f, \tag{4.12}$$

where $((u\cdot\nabla_x)\,f+\nabla_x uQ\cdot\nabla_Q f)$ on the left-hand side is called *cross-scale interaction* term.

4.2.2 Macroscopic Scale

Now we turn to the macroscopic scale of the system. Here we consider an incompressible viscous fluid with constant mass density $\rho=1$ (c.f. (3.27)).
However, we couple the fluid with the polymers by adding the averaged free energy of the microscopic scale into the total energy of the macroscopic part.

Moreover, we add the dissipative part for the microscopic part into the dissipative part of the macroscopic scale.
To this end, we use a relaxation parameter $\lambda > 0$ to incorporate the free energy and dissipation terms from (4.10). We obtain the following dissipative energy law:

$$\begin{aligned}
&\frac{d}{dt}\int_{\Omega_t^x}\left(\frac{1}{2}|u|^2+\lambda\int_{\mathbb{R}^3}\left(\frac{\sigma^2}{2}f\ln f+\frac{1}{\gamma}U\ f\right)\ dQ\right)\ dx\\
&\qquad=-\int_{\Omega_t^x}\left(\mu|\nabla_x u|^2+\lambda\int_{\mathbb{R}^3}f\left|\nabla_Q\left(\frac{\sigma^2}{2}(\ln f+1)+\frac{1}{\gamma}U\right)\right|^2\ dQ\right)\ dx, \qquad (4.13)
\end{aligned}$$

where $\mu > 0$ is a viscosity constant and the distribution function takes the form $f = f(x(X,t), Fq, t)$, where we also assume that $f = 0$ on $\partial\Omega_t^x$.

We start with the least action principle and the variation of the action functional $A(x)$ with respect to x. The action is given by

$$\begin{aligned}
A(x)=\int_0^{t^*}\int_{\Omega_0^X}\Bigg(\frac{1}{2}|x_t|^2-\lambda\int_{\mathbb{R}^3}\bigg(&\frac{\sigma^2}{2}f(x(X,t),Fq,t)\ln f(x(X,t),Fq,t)\\
&+\frac{1}{\gamma}U(Q)\ f(x(X,t),Fq,t)\bigg)\ dQ\Bigg)\ dX\ dt.
\end{aligned}$$

Notice that there will be no variation in the elastic potential $U(Q)$ and in the volume element dQ.

In order to actually calculate the variation, we use volume preserving diffeomorphisms x^ε as characterized in (3.25) and (3.26) with y satisfying $y(X,0) = y(X,t^*) = 0$ for any $X \in \Omega_0^X$, since we work under incompressibility conditions:

$$\begin{aligned}
0&=\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0}A(x^\varepsilon)\\
&=\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0}\int_0^{t^*}\int_{\Omega_0^X}\Bigg(\frac{1}{2}|x_t^\varepsilon|^2-\lambda\int_{\mathbb{R}^3}\bigg(\frac{\sigma^2}{2}f(x^\varepsilon,(\nabla_X x^\varepsilon)q,t)\ \ln f(x^\varepsilon,(\nabla_X x^\varepsilon)q,t)\\
&\qquad\qquad+\frac{1}{\gamma}U(Q)\ f(x^\varepsilon,(\nabla_X x^\varepsilon)q,t)\bigg)\ dQ\Bigg)\ dX\ dt\\
&=\int_0^{t^*}\int_{\Omega_0^X}\Bigg(x_t\cdot y_t-\lambda\int_{\mathbb{R}^3}\bigg(\frac{\sigma^2}{2}(\nabla_x f\cdot y+\nabla_Q f\cdot(\nabla_X y)q)\ \ln f\\
&\qquad\qquad+\frac{\sigma^2}{2}f\ \frac{1}{f}\ (\nabla_x f\cdot y+\nabla_Q f\cdot(\nabla_X y)q)\\
&\qquad\qquad+\frac{1}{\gamma}U(Q)\ (\nabla_x f\cdot y+\nabla_Q f\cdot(\nabla_X y)q)\bigg)\ dQ\Bigg)\ dX\ dt\\
&=\int_0^{t^*}\int_{\Omega_0^X}\Bigg(-x_{tt}\cdot y-\lambda\int_{\mathbb{R}^3}\bigg(\left(\frac{\sigma^2}{2}(\ln f+1)+\frac{1}{\gamma}U(Q)\right)\nabla_Q f\cdot(\nabla_X y)q)\\
&\qquad\qquad+\left(\frac{\sigma^2}{2}(\ln f+1)+\frac{1}{\gamma}U(Q)\right)\nabla_x f\cdot y\bigg)\ dQ\Bigg)\ dX\ dt.
\end{aligned}$$

At this stage, we take care of the expression $(\nabla_X y)q$. It satisfies the following identity:

$$\begin{aligned}(\nabla_X y)q &= (\nabla_X y(X,t))q = (\nabla_X \tilde{y}(x(X,t),t))q \\ &= (\nabla_x \tilde{y}(x,t)\nabla_X x(X,t))q = (\nabla_x \tilde{y}(x,t))Fq = (\nabla_x \tilde{y}(x,t))Q = (\nabla_x \tilde{y})Q,\end{aligned}$$

where $Q = Fq$ is the Cauchy-Born relation. We plug this into the last result and continue the calculations:

$$\begin{aligned}0 &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x^\varepsilon) \\ &= \int_0^{t^*}\int_{\Omega_t^x}\Bigg(-(u_t + (u\cdot\nabla_x)u)\cdot\tilde{y} \\ &\qquad\qquad - \lambda\int_{\mathbb{R}^3}\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_Q f\cdot(\nabla_x\tilde{y})Q \\ &\qquad\qquad\qquad + \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_x f\cdot\tilde{y}\bigg)\,dQ\Bigg)\,dx\,dt,\end{aligned}$$

where we split this into three separate expressions:

$$0 = \int_0^{t^*}\int_{\Omega_t^x}\Big(-(u_t + (u\cdot\nabla_x)u)\cdot\tilde{y}\Big)\,dx\,dt \tag{4.14}$$

$$-\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_Q f\cdot(\nabla_x\tilde{y})Q\bigg)\,dQ\,dx\,dt \tag{4.15}$$

$$-\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_x f\cdot\tilde{y}\bigg)\,dQ\,dx\,dt. \tag{4.16}$$

In order to make the calculations a bit more well-arranged, we deal with each integral term (4.14)–(4.16) separately.

For (4.16) we obtain

$$\begin{aligned}&-\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_x f\cdot\tilde{y}\bigg)\,dQ\,dx\,dt \\ &= -\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\tilde{y}\bigg)\cdot\nabla_x f\,dQ\,dx\,dt \\ &= +\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\nabla_x\cdot\bigg(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\tilde{y}\bigg)f\,dQ\,dx\,dt \\ &= +\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\bigg(\nabla_x\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\cdot\tilde{y} \\ &\qquad\qquad + \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma}U(Q)\Big)\nabla_x\cdot\tilde{y}\bigg)f\,dQ\,dx\,dt.\end{aligned}$$

Here the incompressibility assumption $\nabla_x \cdot \tilde{y} = 0$ comes into play, so the second summand vanishes. We get

$$\begin{aligned}
&+\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} f \ \nabla_x \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) \cdot \tilde{y} \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \Big(\frac{\sigma^2}{2} \nabla_x f \Big) \cdot \tilde{y} \ dQ \ dx \ dt \\
&= -\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \frac{\sigma^2}{2} f \ \nabla_x \cdot \tilde{y} \ dQ \ dx \ dt = 0. \qquad (4.17)
\end{aligned}$$

Next, we turn to (4.15).

$$\begin{aligned}
&-\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \Big(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) \nabla_Q f \cdot (\nabla_x \tilde{y}) Q \Big) \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \nabla_Q \cdot \Big(\Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) (\nabla_x \tilde{y}) Q \Big) f \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \Big(\nabla_Q \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) \cdot (\nabla_x \tilde{y}) Q \\
&\qquad + \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) \nabla_Q \cdot ((\nabla_x \tilde{y}) Q) \Big) f \ dQ \ dx \ dt.
\end{aligned}$$

The second summand vanishes, since, by the following calculation, the expression $\nabla_Q \cdot ((\nabla_x \tilde{y}) Q)$ is equal to zero (remember the Einstein summation convention):

$$\begin{aligned}
\nabla_Q \cdot ((\nabla_x \tilde{y}) Q) &= \nabla_{Q_i} ((\nabla_x \tilde{y}) Q)_i = \nabla_{Q_i} ((\nabla_x \tilde{y})_{ij} Q_j) \\
&= \nabla_{Q_i} (\nabla_{x_j} \tilde{y}_i Q_j) = \delta_{ij} \nabla_{x_j} \tilde{y}_i = \nabla_{x_i} \tilde{y}_i = \nabla_x \cdot \tilde{y} = 0, \qquad (4.18)
\end{aligned}$$

where δ_{ij} is the Kronecker delta. We continue the treatment of (4.15):

$$\begin{aligned}
&+\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} f \ \nabla_Q \Big(\frac{\sigma^2}{2}(\ln f + 1) + \frac{1}{\gamma} U(Q) \Big) \cdot (\nabla_x \tilde{y}) Q \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \Big(\frac{\sigma^2}{2} \nabla_Q f + \frac{1}{\gamma} f \ \nabla_Q U(Q) \Big) \cdot (\nabla_x \tilde{y}) Q \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} \frac{\sigma^2}{2} \nabla_Q f \cdot (\nabla_x \tilde{y}) Q + \frac{1}{\gamma} f \ \nabla_Q U(Q) \cdot (\nabla_x \tilde{y}) Q \ dQ \ dx \ dt \\
&= +\lambda \int_0^{t^*} \int_{\Omega_t^x} \int_{\mathbb{R}^3} -\frac{\sigma^2}{2} f \ \nabla_Q \cdot ((\nabla_x \tilde{y}) Q) + \frac{1}{\gamma} f \ \nabla_Q U(Q) \cdot (\nabla_x \tilde{y}) Q \ dQ \ dx \ dt.
\end{aligned}$$

After integration by parts in the last step, we see that the first summand vanishes due to (4.18), so we go on with (4.15) and obtain using the Einstein summation convention

$$\begin{aligned}
&+\lambda\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}\frac{1}{\gamma}f\ \nabla_Q U(Q)\cdot(\nabla_x\tilde{y})Q\ dQ\ dx\ dt\\
&=+\frac{\lambda}{\gamma}\int_0^{t^*}\int_{\Omega_t^x}\int_{\mathbb{R}^3}f\ \nabla_{Q_i}U(Q)(\nabla_{x_j}\tilde{y}_i)Q_j\ dQ\ dx\ dt\\
&=+\frac{\lambda}{\gamma}\int_0^{t^*}\int_{\Omega_t^x}\nabla_{x_j}\tilde{y}_i\left(\int_{\mathbb{R}^3}f\ \nabla_{Q_i}U(Q)Q_j\ dQ\right)\ dx\ dt\\
&=-\frac{\lambda}{\gamma}\int_0^{t^*}\int_{\Omega_t^x}\nabla_{x_j}\left(\int_{\mathbb{R}^3}f\ \nabla_{Q_i}U(Q)Q_j\ dQ\right)\tilde{y}_i\ dx\ dt\\
&=-\frac{\lambda}{\gamma}\int_0^{t^*}\int_{\Omega_t^x}\nabla_x\cdot\left(\int_{\mathbb{R}^3}f\ \nabla_Q U(Q)\otimes Q\ dQ\right)\cdot\tilde{y}\ dx\ dt\\
&=-\int_0^{t^*}\int_{\Omega_t^x}(\nabla_x\cdot\tau_{ind})\cdot\tilde{y}\ dx\ dt. \qquad (4.19)
\end{aligned}$$

Here, we use the Kronecker product $(\nabla_Q U(Q)\otimes Q)_{ij}=\nabla_{Q_i}U(Q)Q_j$, $i,j=1,2,3$, and define

$$\tau_{ind}=\frac{\lambda}{\gamma}\int_{\mathbb{R}^3}f\ \nabla_Q U(Q)\otimes Q\ dQ,$$

which is called the induced stress from micro to macro. This is also a *cross-scale interaction* quantity.
Now we can bring (4.14), (4.17) and (4.19) together, which leads to

$$0=\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0}A(x^\varepsilon)=\int_0^{t^*}\int_{\Omega_t^x}\Big(-(u_t+(u\cdot\nabla_x)u)-\nabla_x\cdot\tau_{ind}\Big)\cdot\tilde{y}\ dx\ dt,$$

where we can apply Helmholtz' decomposition as in Proposition 23 and obtain for some $p_1\in W^{1,2}(\Omega,\mathbb{R}^3)$

$$-(u_t+(u\cdot\nabla_x)u)-\nabla_x\cdot\tau_{ind}=\nabla_x p_1. \qquad (4.20)$$

So far we considered the Hamiltonian part. For the dissipative part we look at the dissipation

$$\Delta=\int_{\Omega_t^x}\left(\mu|\nabla_x u|^2+\lambda\int_{\mathbb{R}^3}f\left|\nabla_Q\left(\frac{\sigma^2}{2}(\ln f+1)+\frac{1}{\gamma}U\right)\right|^2 dQ\right)\ dx$$

from (4.13) and perform the variation with respect to the velocity u. Since the microscopic part (which is the relaxed integral over the microscopic variable Q) does not contain the velocity u, this variation reduces to one as in (3.28). Again by Proposition 23, this leads to the equation of motion for the dissipative part (3.29):

$$-\nabla_x\cdot(\mu\nabla_x u)=\nabla_x p_2,$$

for $p_2 \in W^{1,2}(\Omega, \mathbb{R}^3)$, or equivalently, since μ is constant in this case,

$$-\mu \Delta_x u = \nabla_x p_2. \tag{4.21}$$

Equations (4.20) and (4.21) are brought together by the force balance law force$_{conservative}$ = force$_{dissipative}$ which yields the entire equation of motion for the macroscopic scale

$$u_t + (u \cdot \nabla_x)u + \nabla_x p = \mu \Delta_x u - \nabla_x \cdot \tau_{ind}.$$

where $p = p_1 - p_2$. Together with the incompressibility, the macroscopic scale system and force balance reads:

$$\begin{cases} \nabla_x \cdot u = 0 \\ u_t + (u \cdot \nabla_x)u + \nabla_x p = \mu \Delta_x u - \nabla_x \cdot \tau_{ind} \\ \tau_{ind} = \dfrac{\lambda}{\gamma} \displaystyle\int_{\mathbb{R}^3} f \ \nabla_Q U(Q) \otimes Q \ dQ. \end{cases} \tag{4.22}$$

4.2.3 Micro-Macro System

Now we summarize the calculations from the previous sections.
The first is the microscopic force balance (4.12). There we considered the influence from the macroscopic scale onto the microscopic scale through the Cauchy-Born relation and the additional dependence of the distribution function f on the macroscopic space variable x which lead to an extended Fokker-Planck equation. Secondly, we looked at the macroscopic scale. The influence of the microscopic scale onto the macroscopic is established by the incorporation of the microscopic energy and dissipation into the macroscopic energy law using a relaxation parameter. Again, Cauchy-Born and the dependence of f on both microscopic and macroscopic variables play important roles in the calculations to obtain the macroscopic system (4.22).
Finally, we obtain the entire coupled system from (4.12) and (4.22) as follows:

$$\begin{cases} \nabla_x \cdot u = 0 \\ u_t + (u \cdot \nabla_x)u + \nabla_x p = \mu \Delta_x u - \nabla_x \cdot \tau_{ind} \\ \tau_{ind} = \dfrac{\lambda}{\gamma} \displaystyle\int_{\mathbb{R}^3} f \ \nabla_Q U(Q) \otimes Q \ dQ \\ f_t + (u \cdot \nabla_x)f + \nabla_x u Q \cdot \nabla_Q f = \nabla_Q \cdot \left(\frac{1}{\gamma} \nabla_Q U \ f \right) + \frac{\sigma^2}{2} \Delta_Q f. \end{cases} \tag{4.23}$$

4.3 Liquid Crystalline Material

This section is dedicated to liquid crystals or liquid crystalline material (see, e.g., [dG79], [Col02], [JS10] for general theory, physical properties, and applications).

First of all, we explain what we understand by the term liquid crystals. As outlined in the introduction to this thesis, nematics are an example for liquid crystals which we consider in this section.

Nematics are like a bunch of molecules which are shaped like rods. They can move around but tend to align in one common direction. Nematic liquid crystals exhibit no positional, but orientational order. There are also liquid crystals which show partial positional order, they are called smectics. In fact they form layers where they exhibit nematic behavior inside these layers (c.f. [dG79, Section 1.4], [Col02, Chapter 1]).

4.3.1 Nematics Averaged from the Microscopic Scale

We are interested in a macroscopic description of the material coupled with an incompressible fluid. The molecules' structure is down on a microscopic scale. Figure 4.2 shows an exemplary configuration of rod shaped nematics. In order to describe liquid crystals on the macroscopic scale, we use a unit vector field

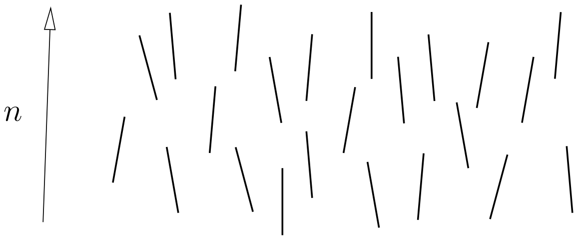

Figure 4.2: Nematic liquid crystals align along the director: microscopic scale

$$n : x \mapsto n(x,t), \quad \text{such that} \quad |n| = n \cdot n = 1,$$

assigned to any point $x \in \Omega_t^x \subset \mathbb{R}^3$ at time t. This is the macroscopic description and it is understood as an average direction of the molecules in the surroundings of x. We call this vector field the director field.
In addition to this, we introduce a scalar field

$$s : x \mapsto s(x,t),$$

which we call the degree of orientation or order parameter to describe the quality of the alignment along the director (c.f. [CL00, Section 1], [CGLL02]). Together with the director field, we obtain the orientation field

$$\mathbf{d} : x \mapsto \mathbf{d}(x,t) := s(x,t)n(x,t), \quad \text{with} \quad |n| = n \cdot n = 1.$$

In the following description we use $\mathbf{d}$ as the description of the liquid crystals instead of a more detailed analysis with the separate fields n and s.

It can be shown that the degree of orientation takes values in the interval $(-\frac{1}{2}, 1)$, where $s = 0$ represents an isotropic configuration, i.e., randomly oriented molecules, $s = -\frac{1}{2}$ stands for perfect alignment perpendicular to the director n, and $s = 1$ for perfect orientation along n, so perfect nematic configuration ([CGLL02]).

For this macroscopic vectorial description, which arises from coarse graining on the fine scale, we define a free energy which penalizes the states that are "less nematic" than a perfect nematic configuration, since through the variation of the energy we want to obtain equations that are necessary conditions for orientation fields which form a nematic state. We define

$$W(\mathbf{d}) := \int_{\Omega_t^x} \frac{k}{2} |\nabla_x \mathbf{d}|^2 + \frac{1}{4\eta} (|\mathbf{d}|^2 - 1)^2 \, dx, \tag{4.24}$$

where $k > 0$ is a material constant and η is a parameter assumed to depend on temperature.
The first summand accounts for the alignment. The smaller the gradient $\nabla_x \mathbf{d}$, i.e., the better the alignment of the molecules, the smaller this first summand. The second term describes the tendency to be away from isotropic. It gets smaller the closer s is to the value 1, which represents the perfect nematic phase. The higher the temperature, the less likely the system takes a nematic state, and the more likely the system is isotropic, thus, η increases with a temperature increase and the penalization of an isotropic configuration is lower.

Remark 24. *One could also include a term describing the response to an external electric field E. Such a term could look like $+\lambda |n \times E|^2$, so alignment that is not parallel to the electric field gets penalized. Modeling the response to an electric field is of particular interest in technical applications, to study the behavior within liquid crystal displays, for instance.*

Corresponding to the free energy we consider a dissipation term

$$\Delta \left(\frac{d}{dt} \mathbf{d} \right) = \int_{\Omega_t^x} \frac{1}{\gamma} \left| \frac{d}{dt} \mathbf{d} \right|^2 \, dx, \tag{4.25}$$

which incorporates the rate $\frac{d}{dt}\mathbf{d}$.

The free energy (4.24) and the corresponding dissipation (4.25) together yield an energy dissipation law (c.f. (3.1)) for the nematic configuration on the microscopic scale (remember that we use a macroscopic description for the microscopic scale!):

$$\frac{d}{dt} W(\mathbf{d}) = -\Delta \left(\frac{d}{dt} \mathbf{d} \right). \tag{4.26}$$

We can easily derive the microscopic force balance from this energy law. The Hamiltonian part follows from the Euler-Lagrange equation (3.11). Since we calculate the variation of the action $A(\mathbf{d}) = -W(\mathbf{d})$ with respect to the orientation field $\mathbf{d}$ and the spatial integration variable is x (notice that in (3.11) the spatial integration variable is X and the variation is taken with respect to x) we obtain

$$k\Delta_x \mathbf{d} - \frac{1}{\eta}(|\mathbf{d}|^2 - 1)^2 \mathbf{d} = 0. \tag{4.27}$$

Concerning the dissipative part, we calculate the variation of $\frac{1}{2}\Delta\left(\frac{d}{dt}\mathbf{d}\right)$ with respect to $\frac{d}{dt}\mathbf{d}$ and obtain

$$\frac{1}{\gamma}\frac{d}{dt}\mathbf{d} = 0. \tag{4.28}$$

The Hamiltonian equation (4.27) and the dissipative equation (4.29) are related by the force balance law force$_{conservative}$ = force$_{dissipative}$, which results in the microscopic force balance equation

$$k\Delta_x \mathbf{d} - \frac{1}{\eta}(|\mathbf{d}|^2 - 1)^2 \mathbf{d} = \frac{1}{\gamma}\frac{d}{dt}\mathbf{d}. \tag{4.29}$$

We now replace the rate $\frac{d}{dt}\mathbf{d}$ in (4.29) by the explicit formula for the total time-derivative of the orientation field and obtain as microscopic force balance:

$$k\Delta_x \mathbf{d} - \frac{1}{\eta}(|\mathbf{d}|^2 - 1)^2 \mathbf{d} = \frac{1}{\gamma}(\mathbf{d}_t + (u \cdot \nabla_x)\mathbf{d}). \tag{4.30}$$

Remark 25. *Rewriting* (4.29) *using a variational gradient notation*

$$\frac{\delta W(\mathbf{d})}{\delta \mathbf{d}} = k\Delta_x \mathbf{d} - \frac{1}{\eta}(|\mathbf{d}|^2 - 1)^2 \mathbf{d}$$

which is the Euler-Lagrange equation, we obtain a gradient flow form

$$\frac{d}{dt}\mathbf{d} = \gamma \frac{\delta W(\mathbf{d})}{\delta \mathbf{d}}.$$

This reflects the long time behavior of liquid crystals on the microscopic scale.

4.3.2 Macroscopic Scale and Kinematic Transport

Now we couple the nematics with a surrounding incompressible viscous fluid with constant density $\rho = 1$ (remember that $\det F = 1$ due to the incompressibility condition). Thus we get a combined dissipative energy law as follows from equations (3.27), (4.24), and (4.25):

$$\begin{aligned} \frac{d}{dt}\int_{\Omega_t^x} \left(\frac{1}{2}|u|^2 + \lambda\left(\frac{k}{2}|\nabla_x \mathbf{d}|^2 + \frac{1}{4\eta}(|\mathbf{d}|^2 - 1)^2\right)\right)\, dx & \\ = -\int_{\Omega_t^x} \left(\mu|\nabla_x u|^2 + \frac{\lambda}{\gamma}\left|\frac{d}{dt}\mathbf{d}\right|^2\right)\, dx, & \qquad (4.31) \end{aligned}$$

where $\mu > 0$ is a viscosity constant and $\lambda > 0$ is a relaxation parameter. Note that the energy law does not include an integration over Q as in (4.13) since it is phrased using the orientation field $\mathbf{d}$ which is already a macroscopic description. We also replace the rate $\frac{d}{dt}\mathbf{d}$ in (4.31) by the explicit formula for the total time-derivative of the orientation field and obtain

$$\frac{d}{dt}\int_{\Omega_t^x}\left(\frac{1}{2}|u|^2+\lambda\left(\frac{k}{2}|\nabla_x\mathbf{d}|^2+\frac{1}{4\eta}(|\mathbf{d}|^2-1)^2\right)\right)\,dx \\ = -\int_{\Omega_t^x}\left(\mu|\nabla_x u|^2+\frac{\lambda}{\gamma}\left|\mathbf{d}_t+(u\cdot\nabla_x)\mathbf{d}\right|^2\right)\,dx. \tag{4.32}$$

In order to establish the equation of motion on the macroscopic scale, we need certain kinematic assumptions, in particular, how the orientation field $\mathbf{d}$ is transported. Since we consider rod-shaped molecules, the following assumption is reasonable (c.f. [SL09, WXL12])

$$\mathbf{d}(x(X,t),t) = F\mathbf{d}_0(X), \tag{4.33}$$

where $\mathbf{d}_0(X)$ represents the initial condition at time $t = 0$. This transport includes the transport of the center of mass and the stretching of the director. We take the (total) derivative with respect to time on both sides of (4.33) which yields

$$\begin{aligned}\mathbf{d}_t+(u\cdot\nabla_x)\mathbf{d} &= \frac{d}{dt}F\mathbf{d}_0\\ &= (\nabla_x u)F\mathbf{d}_0 = (\nabla_x u)\mathbf{d} = (\mathbf{d}\cdot\nabla_x)u,\end{aligned}$$

or equivalently

$$\mathbf{d}_t+(u\cdot\nabla_x)\mathbf{d}-(\mathbf{d}\cdot\nabla_x)u = 0. \tag{4.34}$$

Remark 26. *For different shapes of molecules one can find different transport equations. In the case of general ellipsoidal shapes we can define*

$$\mathbf{d}(x(X,t),t) = \mathcal{E}\mathbf{d}_0(X), \tag{4.35}$$

where $\mathcal{E} = \mathcal{E}(x(X,t),t)$ *satisfies the differential equation*

$$\dot{\mathcal{E}} = \Omega_u\mathcal{E} + (2\alpha-1)A_u\mathcal{E}$$

with $A_u = \frac{\nabla_x u+(\nabla_x u)^T}{2}$ *the symmetric part and* $\Omega_u = \frac{\nabla_x u-(\nabla_x u)^T}{2}$ *the skew symmetric part of* $\nabla_x u$. *Here* $2\alpha - 1 = \frac{r^2-1}{r^2+1}$ *and* r *is the aspect ratio of the ellipsoids ([SL09, WXL12]). The general transport equation then becomes*

$$\mathbf{d}_t+(u\cdot\nabla_x)\mathbf{d}-\Omega_u\mathbf{d}-(2\alpha-1)A_u\mathbf{d} = 0$$

which is established in the same way as (4.34) *by taking the derivative with respect to time on both sides of* (4.35).

Next we look at the least action principle applied to the total energy in (4.32).

Notice that the orientation field $\mathbf{d}$ transforms into the Lagrangian coordinate system according to the considered transport rule (4.33). However, for the transformation of $\nabla_x \mathbf{d}$ we do the same calculation as in (3.21) and (3.22), respectively, so we get in total

$$\nabla_x \mathbf{d} = \nabla_X (F\mathbf{d}_0(X))F^{-1}$$

as the transformation rule for the gradient of $\mathbf{d}$.

The action is then given by

$$A(x) = \int_0^{t^*} \int_{\Omega_0^X} \left(\frac{1}{2}|x_t|^2 - \lambda \left(\frac{k}{2} |\nabla_X (F\mathbf{d}_0(X))F^{-1}|^2 + \frac{1}{4\eta}(|(F\mathbf{d}_0(X))|^2 - 1)^2 \right) \right) dX\ dt. \tag{4.36}$$

To perform the variation with respect to the flow map, we consider volume preserving diffeomorphisms x^ε as characterized in (3.25) and (3.26) with $\tilde{y}$ and its gradient satisfying zero boundary condition. We use these volume preserving diffeomorphisms due to the incompressibility condition. Notice that the deformation gradient $F = \frac{\partial x}{\partial X}$ depends on x and thus on the variation.

$$\begin{aligned}
0 &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x^\varepsilon) \\
&= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^{t^*} \int_{\Omega_0^X} \left(\frac{1}{2}|x_t^\varepsilon|^2 - \lambda \left(\frac{k}{2} |\nabla_X ((\nabla_X x^\varepsilon)\mathbf{d}_0(X))(\nabla_X x^\varepsilon)^{-1}|^2 \right.\right. \\
&\qquad\qquad \left.\left. + \frac{1}{4\eta}(|((\nabla_X x^\varepsilon)\mathbf{d}_0(X))|^2 - 1)^2 \right) \right) dX\ dt \\
&= \int_0^{t^*} \int_{\Omega_0^X} \Bigg(x_t \cdot y_t \\
&\qquad - \lambda k \Bigg(\left(\nabla_X (F\mathbf{d}_0(X))F^{-1} \right) : \Bigg(\nabla_X (F\mathbf{d}_0(X)) \underbrace{\left(\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} (\nabla_X x^\varepsilon)^{-1} \right)}_{=-F^{-1}(\nabla_X y)F^{-1}} \\
&\qquad\qquad + \nabla_X \underbrace{\left(\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} (\nabla_X x^\varepsilon)\mathbf{d}_0(X) \right)}_{=(\nabla_X y)\mathbf{d}_0(X)} F^{-1} \Bigg) \Bigg) \\
&\qquad + \frac{\lambda}{\eta}(|F\mathbf{d}_0(X)|^2 - 1)(F\mathbf{d}_0(X)) \cdot \left(\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} ((\nabla_X x^\varepsilon)\mathbf{d}_0(X)) \right) \Bigg) dX\ dt.
\end{aligned}$$

For the identity $\frac{d}{d\varepsilon}\big|_{\varepsilon=0}(\nabla_X x^\varepsilon)^{-1} = -F^{-1}(\nabla_X y)F^{-1}$ more detailed calculations are carried out in Appendix A.5. We continue the calculation:

$$
\begin{aligned}
0 = \int_0^{t^*} \int_{\Omega_0^X} \Big(& x_t \cdot y_t \\
& - \lambda k \Big(\big(\nabla_X (F\mathbf{d}_0(X)) F^{-1}\big) : \Big(-\nabla_X (F\mathbf{d}_0(X)) F^{-1} (\nabla_X y) F^{-1} \\
& \qquad + \nabla_X \big(\underbrace{(\nabla_X y)\mathbf{d}_0(X)}_{=(\nabla_X y)F^{-1}F\mathbf{d}_0(X)} \big) F^{-1} \Big) \Big) \\
& + \frac{\lambda}{\eta} (|F\mathbf{d}_0(X)|^2 - 1)(F\mathbf{d}_0(X)) \cdot \Big(\underbrace{(\nabla_X y)\mathbf{d}_0(X)}_{=(\nabla_X y)F^{-1}F\mathbf{d}_0(X)} \Big) \Big) \, dX \; dt.
\end{aligned}
$$

Now we transform the integral back into the Eulerian coordinate system:

$$
\begin{aligned}
0 = \int_0^{t^*} \int_{\Omega_t^x} \Big(& -\frac{d}{dt} u \cdot \tilde{y} \\
& - \lambda k \Big((\nabla_x \mathbf{d}(x,t)) : \Big(-\nabla_x \mathbf{d}(x,t)(\nabla_x \tilde{y}) \\
& \qquad + \nabla_x ((\nabla_x \tilde{y})\mathbf{d}(x,t)) \Big) \Big) \\
& + \frac{\lambda}{\eta} (|\mathbf{d}(x,t)|^2 - 1)\mathbf{d}(x,t) \cdot (\nabla_x \tilde{y})\mathbf{d}(x,t) \Big) \, dx \; dt.
\end{aligned}
$$

We rewrite this expression and obtain

$$
\begin{align*}
0 = & \int_0^{t^*} \int_{\Omega_t^x} \Big(-(u_t + (u \cdot \nabla_x) u) \cdot \tilde{y} \Big) \, dx \; dt \tag{4.37} \\
& - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big((\nabla_x \mathbf{d}(x,t)) : \Big(-\nabla_x \mathbf{d}(x,t)(\nabla_x \tilde{y}) \Big) \Big) \, dx \; dt \tag{4.38} \\
& - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big((\nabla_x \mathbf{d}(x,t)) : \Big(\nabla_x ((\nabla_x \tilde{y})\mathbf{d}(x,t)) \Big) \Big) \, dx \; dt \tag{4.39} \\
& + \frac{\lambda}{\eta} \int_0^{t^*} \int_{\Omega_t^x} \Big((|\mathbf{d}(x,t)|^2 - 1)\mathbf{d}(x,t) \cdot (\nabla_x \tilde{y})\mathbf{d}(x,t) \Big) \, dx \; dt. \tag{4.40}
\end{align*}
$$

For the following calculations we make use of the simplified notation $\nabla_j := \frac{\partial}{\partial x^j}$ and the Einstein summation convention.

For (4.38) we get

$$
\begin{aligned}
& - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big((\nabla_x \mathbf{d}) : \Big(-\nabla_x \mathbf{d} (\nabla_x \tilde{y}) \Big) \Big) \, dx \; dt \\
= & + \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_j \mathbf{d}_i \nabla_l \mathbf{d}_i \nabla_j \tilde{y}_l \Big) \, dx \; dt \\
= & - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_j (\nabla_j \mathbf{d}_i \nabla_l \mathbf{d}_i) \tilde{y}_l \Big) \, dx \; dt,
\end{aligned}
$$

where integration by parts is used. We define the product $(\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d})_{lj} := \nabla_j \mathbf{d}_i \nabla_l \mathbf{d}_i$, $l, j = 1, 2, 3$ (since we consider liquid crystals in $\mathbb{R}^3$), which is obviously a symmetric 3×3-matrix (at least in this case, where the factors are the same, namely $\nabla_x \mathbf{d}$). Then we obtain the following expression for (4.38):

$$-\lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_x \cdot (\nabla_x \mathbf{d} \odot \nabla_x \mathbf{d}) \Big) \cdot \tilde{y} \; dx \; dt. \tag{4.41}$$

Next we consider equation (4.39):

$$\begin{aligned} & - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big((\nabla_x \mathbf{d}) : \Big(\nabla_x ((\nabla_x \tilde{y}) \mathbf{d}) \Big) \Big) \; dx \; dt \\ = & - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_j \mathbf{d}_i \nabla_j (\nabla_l \tilde{y}_i \mathbf{d}_l) \Big) \; dx \; dt \\ = & + \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\underbrace{\nabla_j (\nabla_j \mathbf{d}_i)}_{=(\Delta \mathbf{d})_i} \mathbf{d}_l \nabla_l \tilde{y}_i \Big) \; dx \; dt \\ = & - \lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_l (\underbrace{\nabla_j (\nabla_j \mathbf{d}_i)}_{=(\Delta \mathbf{d})_i} \mathbf{d}_l) \tilde{y}_i \Big) \; dx \; dt, \end{aligned}$$

where integration by parts is used twice in the last steps. Now we use the Kronecker product $(\Delta \mathbf{d} \otimes \mathbf{d})_{il} = \nabla_j (\nabla_j \mathbf{d}_i) \mathbf{d}_l$, $i, l = 1, 2, 3$, and obtain for (4.39):

$$-\lambda k \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_x \cdot (\Delta \mathbf{d} \otimes \mathbf{d}) \Big) \cdot \tilde{y} \; dx \; dt. \tag{4.42}$$

Now we turn to equation (4.40):

$$\begin{aligned} & + \frac{\lambda}{\eta} \int_0^{t^*} \int_{\Omega_t^x} \Big((|\mathbf{d}|^2 - 1) \mathbf{d} \cdot (\nabla_x \tilde{y}) \mathbf{d} \Big) \; dx \; dt \\ = & + \frac{\lambda}{\eta} \int_0^{t^*} \int_{\Omega_t^x} \Big((\mathbf{d}_l \mathbf{d}_l - 1) \mathbf{d}_i \nabla_j \tilde{y}_i \mathbf{d}_j \Big) \; dx \; dt \\ = & - \frac{\lambda}{\eta} \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_j ((\mathbf{d}_l \mathbf{d}_l - 1) \mathbf{d}_i \mathbf{d}_j) \tilde{y}_i \Big) \; dx \; dt, \end{aligned}$$

where integration by parts is used in the last step. We use again a Kronecker product $((|\mathbf{d}|^2 - 1) \mathbf{d} \otimes \mathbf{d})_{ij} = (\mathbf{d}_l \mathbf{d}_l - 1) \mathbf{d}_i \mathbf{d}_j$, $i, j = 1, 2, 3$, and obtain for (4.40):

$$-\frac{\lambda}{\eta} \int_0^{t^*} \int_{\Omega_t^x} \Big(\nabla_x \cdot ((|\mathbf{d}|^2 - 1) \mathbf{d} \otimes \mathbf{d}) \Big) \cdot \tilde{y} \; dx \; dt. \tag{4.43}$$

Equations (4.37) and (4.41)–(4.43) are put together in the following result for the variation of the action functional (4.36):

$$\begin{aligned}
0 &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} A(x^\varepsilon) \\
&= \int_0^{t^*}\int_{\Omega_t^x} \Big(-(u_t+(u\cdot\nabla_x)u)\Big)\cdot\tilde{y} - \lambda k\Big(\nabla_x\cdot(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d})\Big)\cdot\tilde{y} \\
&\qquad\qquad - \lambda k\Big(\nabla_x\cdot(\Delta\mathbf{d}\otimes\mathbf{d})\Big)\cdot\tilde{y} - \frac{\lambda}{\eta}\Big(\nabla_x\cdot(((|\mathbf{d}|^2-1)\mathbf{d}\otimes\mathbf{d})\Big)\cdot\tilde{y}\;dx\;dt \\
&= \int_0^{t^*}\int_{\Omega_t^x} -\Big((u_t+(u\cdot\nabla_x)u) + \lambda k\Big(\nabla_x\cdot(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d})\Big) \\
&\qquad\qquad + \lambda k\Big(\nabla_x\cdot(\Delta\mathbf{d}\otimes\mathbf{d})\Big) + \frac{\lambda}{\eta}\Big(\nabla_x\cdot(((|\mathbf{d}|^2-1)\mathbf{d}\otimes\mathbf{d})\Big)\Big)\cdot\tilde{y}\;dx\;dt \\
&= \int_0^{t^*}\int_{\Omega_t^x} -\Big(u_t+(u\cdot\nabla_x)u \\
&\qquad\qquad + \lambda\nabla_x\cdot\Big(k(\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}) + k(\Delta\mathbf{d}\otimes\mathbf{d}) \\
&\qquad\qquad\qquad + \frac{1}{\eta}((|\mathbf{d}|^2-1)\mathbf{d}\otimes\mathbf{d})\Big)\Big)\cdot\tilde{y}\;dx\;dt.
\end{aligned}$$

We can rearrange this in a convenient way as follows:

$$\begin{aligned}
0 = \int_0^{t^*}\int_{\Omega_t^x} &-\Big(u_t+(u\cdot\nabla_x)u \\
&+ \lambda\nabla_x\cdot\Big(k\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d} + \Big(k\Delta\mathbf{d}+\frac{1}{\eta}(|\mathbf{d}|^2-1)\mathbf{d}\Big)\otimes\mathbf{d}\Big)\Big)\cdot\tilde{y}\;dx\;dt.
\end{aligned}$$

Next we apply Helmholtz' decomposition as in Proposition 23 and obtain for some $p_1\in W^{1,2}(\Omega,\mathbb{R}^3)$:

$$u_t+(u\cdot\nabla_x)u+\lambda\nabla_x\cdot\Big(k\nabla_x\mathbf{d}\odot\nabla_x\mathbf{d}+\Big(k\Delta\mathbf{d}+\frac{1}{\eta}(|\mathbf{d}|^2-1)\mathbf{d}\Big)\otimes\mathbf{d}\Big) = -\nabla_x p_1, \tag{4.44}$$

which is the Hamiltonian force balance on the macroscopic scale.

Now we turn to the dissipative part of the energy law (4.32):

$$\int_{\Omega_t^x}\Big(\mu|\nabla_x u|^2+\frac{\lambda}{\gamma}\left|\mathbf{d}_t+(u\cdot\nabla_x)\mathbf{d}\right|^2\Big)\;dx.$$

However, due to the microscopic force balance (4.30) we can rewrite this expression and obtain:

$$\int_{\Omega_t^x}\left(\mu|\nabla_x u|^2+\frac{\lambda}{\gamma}\left|k\Delta_x\mathbf{d}-\frac{1}{\eta}(|\mathbf{d}|^2-1)^2\mathbf{d}\right|^2\right)\;dx,$$

where the second part does not depend on the macroscopic velocity u. So the variation of the dissipative part yields just a viscosity term as in (4.21). Since the macroscopic fluid is assumed to be incompressible, we obtain for $p_2 \in W^{1,2}(\Omega, \mathbb{R}^3)$:

$$-\mu \Delta_x u = \nabla_x p_2. \tag{4.45}$$

Equations (4.44) and (4.45) are connected by the force balance law $\text{force}_{conservative} = \text{force}_{dissipative}$ which yields the entire equation of motion for the macroscopic scale

$$\begin{aligned} &u_t + (u \cdot \nabla_x) u + \nabla_x p \\ &\quad = \mu \Delta_x u - \lambda \nabla_x \cdot \left(k \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \left(k \Delta \mathbf{d} + \frac{1}{\eta}(|\mathbf{d}|^2 - 1)\mathbf{d} \right) \otimes \mathbf{d} \right), \end{aligned} \tag{4.46}$$

where $p = p_1 - p_2$.

4.3.3 Micro-Macro System for Nematic Liquid Crystals

Finally, we can bring all the equations from the two scales together to obtain the entire system for the considered model of nematic liquid crystals. With the incompressibility (3.24), the microscopic force balance (4.30), the transport equation for the orientation field (4.34), and the macroscopic force balance (4.46), we obtain the entire system as follows:

$$\begin{cases} \nabla_x \cdot u = 0 \\ k \Delta_x \mathbf{d} - \frac{1}{\eta}(|\mathbf{d}|^2 - 1)^2 \mathbf{d} = \frac{1}{\gamma} \mathbf{d}_t + (u \cdot \nabla_x) \mathbf{d} \\ \mathbf{d}_t + (u \cdot \nabla_x) \mathbf{d} - (\mathbf{d} \cdot \nabla_x) u = 0 \\ u_t + (u \cdot \nabla_x) u + \nabla_x p \\ \quad = \mu \Delta_x u - \lambda \nabla_x \cdot \left(k \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \left(k \Delta \mathbf{d} + \frac{1}{\eta}(|\mathbf{d}|^2 - 1)\mathbf{d} \right) \otimes \mathbf{d} \right). \end{cases} \tag{4.47}$$

The cross-scale coupling, which is the effect from the microscopic scale onto the macroscopic scale and vice versa, is represented by the transport equation and a coupling term in the macroscopic force balance.

The transport equation $(4.47)_3$ reflects one way of coupling, which is the effect from macro onto micro: The equation states how the molecules move along with the macroscopic fluid.

On the other hand, the coupling term

$$k \nabla_x \mathbf{d} \odot \nabla_x \mathbf{d} + \left(k \Delta \mathbf{d} + \frac{1}{\eta}(|\mathbf{d}|^2 - 1)\mathbf{d} \right) \otimes \mathbf{d}$$

in the macroscopic force balance $(4.47)_4$ reflects the other way of coupling, this is the effect from micro onto macro: The included liquid crystal molecules directly influence the macroscopic flow behavior.

This model is a good example to highlight the convenience of the energetic variational approach. It is relatively easy to establish the energy terms, even to couple different scales. However, to use a force-based approach could be frustrating since especially the coupling-term is not an entity that is easy to set up.

5 Conclusion

In the preceding work we saw that the energetic variational approach gives us the opportunity to study relatively complex physical systems and to set up corresponding partial differential equations in a convenient way. Several examples of complex fluids which are diverse and important for many technological fields were treated, namely the incompressible viscoelasticity, the polymeric fluids and the nematic liquid crystals.

Considering liquid crystals, smectic liquid crystals, for instance, which additionally exhibit partial positional order can also be treated through an energetic variational approach using a distance function to model their layering order structure (see, e.g., [CLV98], [Liu00], [CLV01]).

Further areas of research, where these methods can be applied, are in cell biology: Cell membranes consist of layer forming lipids with amphiphilic structure, similar to liquid crystals (see, e.g., [JS10]). As already mentioned in the introduction, ionic solutions which run through our body can be treated as complex fluids since they consist of charged particles within a surrounding fluid (see, e.g., [EHL10]). Thus the treatment of transport and osmosis through the membranes in the energetic variational approach leads to a system of partial differential equations that allow to model, for instance, a safe prediction of chemicals' impact onto the human body.

Other examples are interface models which are employed to study, e.g., the motion of droplets of fluid A within fluid B (see, e.g., [Ryh06], [RLZ07]), and the motion of interfaces in two-phase fluid materials (see, e.g., [YFLS04], [HKL10]), and to analyze mixtures with charged particles or magnetic fluids (see, e.g., [EHL10], [RLZ07]).

The models considered throughout this work raise further mathematical considerations and problems. We derived systems of partial differential equations under the assumptions that we have enough regularity. A next step would be to weaken these regularity assumptions and to study existence and uniqueness of solutions. We remark that if we consider systems that contain the Navier-Stokes system (3.31), we cannot expect better results than from the Navier-Stokes system itself (c.f., [LL95, Section 1], [LL00, Section 4]). In fact, this is the case for all the models considered in Chapter 4, since these complex fluids are coupled with an incompressible viscous fluid (which results in the Navier-Stokes system as a subsystem).

Finally, the established models can be used to simulate the behavior of the physical phenomena numerically (see, e.g., [Ryh06], [EHL10]) with the help of certain discretization methods such as finite element or finite volume methods.

A Remarks on Matrix Calculus

A.1 Matrix Double-Dot Product

The double-dot product for matrices is important for calculations in this thesis. For $A, B \in \mathbb{R}^{n \times n}$ we define

$$A : B := \operatorname{tr}(A^T B) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij} \in \mathbb{R}.$$

Due to the properties of the trace of a matrix, the following identities hold for any $A, B, C \in \mathbb{R}^{n \times n}$:

$$A : B = \operatorname{tr}(AB^T) = \operatorname{tr}(B^T A) = \operatorname{tr}(BA^T) = B : A$$

and

$$A : (BC) = \operatorname{tr}(AC^T B^T) = (AC^T) : B.$$

A.2 Chain Rule

For $\varepsilon_0 > 0$ let $F : (-\varepsilon_0, \varepsilon_0) \to \mathbb{R}^{n \times n},\ \varepsilon \mapsto F(\varepsilon)$ be a differentiable matrix-valued function defined on an interval in the reals, let $W : \mathbb{R}^{n \times n} \to \mathbb{R},\ E \mapsto W(E)$ be a differentiable real-valued function defined on $n \times n$-matrices.
We calculate the derivative of $W \circ F : (-\varepsilon_0, \varepsilon_0) \to \mathbb{R},\ \varepsilon \mapsto W(F(\varepsilon))$ with respect to ε. To this end, we use the chain rule from multi-variable real calculus [Kna05, Theorem 3.10]. But since this rule is only defined for vector-valued functions and functions defined on vectors, we use a little trick.
Define the following diffeomorphism with its inverse

$$\Phi : \mathbb{R}^{n \times n} \to \mathbb{R}^{nn},\ F \mapsto f := (F_1^T, \dots, F_n^T)^T,$$

$$\Phi^{-1} : \mathbb{R}^{nn} \to \mathbb{R}^{n \times n},\ f = (f_1, \dots, f_{nn}) \mapsto F = \begin{pmatrix} f_1 & f_{n+1} & \cdots & f_{n^2-n+1} \\ f_2 & f_{n+2} & \cdots & f_{n^2-n+2} \\ \vdots & \vdots & \ddots & \vdots \\ f_n & f_{2n} & \cdots & f_{n^2} \end{pmatrix},$$

where $F_1, \dots, F_n$ are the columns of F. So, Φ takes the columns of F and writes them into a vector with n^2 lines. Φ^{-1} easily does the inverse process.

Notice that Φ and Φ^{-1} is nothing but a different labeling: F_{ij} in the matrix is equal to $f_k = f_{(j-1)n+i}$ in the vector (this is what Φ does). The reverse (i.e., what Φ^{-1} does) is done by setting $F_{ij} = f_k$ with $j = \frac{k-k \mod n}{n} + 1$ and $i = k \mod n$ which is the remainder after division by n.

From here, we can define new functions:

$$\begin{aligned}
F^* &:= \Phi \circ F : \mathbb{R} \to \mathbb{R}^{nn},\ \varepsilon \mapsto F^*(\varepsilon) = \Phi(F(\varepsilon)) = f(\varepsilon), \\
W^* &:= W \circ \Phi^{-1} : \mathbb{R}^{nn} \to \mathbb{R},\ f \mapsto W^*(f) = W(\Phi^{-1}(f)).
\end{aligned}$$

Consequently, we have that

$$W^* \circ F^* = W \circ \Phi^{-1} \circ \Phi \circ F = W \circ F,$$

so we calculate

$$\begin{aligned}
\frac{d}{d\varepsilon}\big(W \circ F\big)(\varepsilon) &= \frac{d}{d\varepsilon}\big(W^* \circ F^*\big)(\varepsilon) = D(W^*)(f(\varepsilon)) \cdot \left(\frac{d}{d\varepsilon}F^*(\varepsilon)\right) \\
&= \sum_{k=1}^{n^2} \frac{\partial W^*}{\partial f_k}(f(\varepsilon))\frac{df_k(\varepsilon)}{d\varepsilon} = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial W}{\partial F_{ij}}(F(\varepsilon))\frac{dF_{ij}(\varepsilon)}{d\varepsilon} \\
&= W_F(F(\varepsilon)) : \left(\frac{d}{d\varepsilon}F(\varepsilon)\right).
\end{aligned}$$

The second to last step is clear with Φ described as a labeling. So the derivative of $\big(W \circ F\big)(\varepsilon)$ with respect to ε is given by the formula

$$\frac{d}{d\varepsilon}\big(W \circ F\big)(\varepsilon) = W_F(F(\varepsilon)) : \left(\frac{d}{d\varepsilon}F(\varepsilon)\right).$$

A.3 Derivative of the Determinant

Let $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$ be the determinant defined on invertible matrices $A \in \mathrm{GL}(n,\mathbb{R}) \subset \mathbb{R}^{n\times n}$. We calculate the derivative of the determinant $\det A$ with respect to the matrix A. This we denote by $\frac{\partial(\det A)}{\partial A}$.
At first, we use the Laplace expansion for the determinant along the j-th column [Brö04, Chapter III, (2.6)]:

$$\det A = \sum_{i=1}^{n} (-1)^{i+j} a_{ij} \det A_{ij},$$

where a_{ij} is the matrix element at position ij and A_{ij} is the $(n-1)\times(n-1)$-matrix which results from A by removing the i-th row and j-th column.
From here we take the derivative of the determinant with respect to the element a_{kj}. Since $\det A_{ij}$ does not depend on a_{kj} for all $k = 1, \dots, n$ (since the j-th column is removed), we obtain

$$\begin{aligned}
\frac{\partial}{\partial a_{kj}} \det A &= \frac{\partial}{\partial a_{kj}} \sum_{i=1}^{n} (-1)^{i+j} a_{ij} \det A_{ij} \\
&= \sum_{i=1}^{n} (-1)^{i+j} \delta_{ik} \det A_{ij} = (-1)^{k+j} \det A_{kj},
\end{aligned}$$

where δ_{ik} is the Kronecker delta. By definition of the adjugate matrix $\operatorname{adj}(A)$ corresponding to A [Brö04, Chapter III, (3.3)], we have that

$$\frac{\partial}{\partial a_{kj}} \det A = (-1)^{k+j} \det A_{kj} =: \operatorname{adj}(A)_{jk},$$

hence,

$$\frac{\partial(\det A)}{\partial A} = \left(\frac{\partial}{\partial a_{kj}} \det A\right)_{kj} = \left(\operatorname{adj}(A)_{jk}\right)_{kj} = \operatorname{adj}(A)^T.$$

Finally, by Cramer's rule [Brö04, Chapter III, (3.4)], we obtain

$$\frac{\partial(\det A)}{\partial A} = \operatorname{adj}(A)^T = A^{-T} \det A.$$

A.4 Integration by Parts for the Matrix Double-Dot Product

Let $b(x) \in \mathbb{R}^n$ on $\Omega \subset \mathbb{R}^n$ be a continuously differentiable vector field with $b = 0$ on $\partial\Omega$ and let $A(x) \in \mathbb{R}^{n\times n}$ be a continuously differentiable matrix field on Ω. We consider the scalar field $A : \nabla_x b$ involving the double-dot product defined in Appendix A.1 and the integral

$$\int_\Omega A : \nabla_x b \; dx.$$

For this we derive a formula for integration by parts as follows:

$$\begin{aligned}
\int_\Omega A : \nabla_x b \; dx &= \int_\Omega \sum_{i,j} A_{ij} (\nabla_x b)_{ij} \; dx \\
&= \sum_{i,j} \int_\Omega A_{ij} \nabla_j b_i \; dx \\
&= \sum_{i,j} \left(- \int_\Omega (\nabla_j A_{ij}) b_i \; dx \right) = - \int_\Omega (\nabla_x \cdot A) \cdot b \; dx,
\end{aligned}$$

which follows by integration by parts for real valued functions [Eva10] and Definition 5 on the divergence of a matrix field.

A.5 Derivative of an Inverse Matrix Field

For $\varepsilon_0 > 0$ let $F : (-\varepsilon_0, \varepsilon_0) \to \mathrm{GL}(n, \mathbb{R}) \subset \mathbb{R}^{n\times n}$, $\varepsilon \mapsto F(\varepsilon)$ be a differentiable function with values in the invertible matrices and defined on an interval in the reals. We calculate the derivative

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(\varepsilon)^{-1}.$$

To this end, we use that for any ε the identity $I = F(\varepsilon)F(\varepsilon)^{-1}$ holds. Consequently, by the chain rule

$$\begin{aligned} 0 = \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} I &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \big(F(\varepsilon)F(\varepsilon)^{-1}\big) \\ &= \left(\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(\varepsilon)\right) F(0)^{-1} + F(0) \left(\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(\varepsilon)^{-1}\right). \end{aligned}$$

Thus, we obtain for the derivative of the inverse

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(\varepsilon)^{-1} = -F(0)^{-1} \left(\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(\varepsilon)\right) F(0)^{-1}.$$

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Declaration

Erklärung

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