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Irreversible thermodynamical study of elastic, thermal expansion, rheological and heat conduction processes in solids

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Declaration

Undersigned, Mátyás Szücs, author of this Thesis, hereby, I declare that I prepared this Thesis myself, and I used only the referred sources. All parts of the Thesis, which are either cited verbatim or with the same content but rephrased as in the original source, are referred unambiguously and with providing the sources used.

Budapest, on the 28th of January, 2022

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Abstract

Advances in modern engineering technology pointed out that description and modeling of some phenomena have to go beyond the usual and well-known models applied in engineering for heat conduction and solid mechanics, namely, Fourier's law and Hooke's law. The development of such models, which give insight and calculation opportunities for these phenomena, began as early as the middle of the 20th century but the elaboration of the details is still in progress today.

This dissertation focuses on models of non-Fourier heat conduction and of rheology of solids.

Regarding heat conduction beyond Fourier's law, several experiments were performed to justify it and, accordingly, various theoretical models and explanations have been born. Until recently, corresponding engineering applications covered only a narrow range of special areas, such as extreme conditions (*e.g.*, low temperature), micro and nano scales and high-frequency processes. However, nowadays it is known that a relatively simple description of heat conduction in heterogeneous materials as rocks, layered structures, foams and 3D printed samples can be achieved by heat conduction models beyond Fourier's law. If the newly introduced heat conduction parameters of such structures can be controlled via the production technology then a new level of thermal design can be reached.

Rheology is well-known in the context of non-Newtonian fluids, where nontrivial internal friction effects are manifest. In parallel, similar behaviors can be observed for various solid materials, *e.g.*, polymers, biomaterials, rocks and in long-term measurements of steels operated at high temperature (*e.g.*, power plant steam pipes). Additionally, modeling and simulation of the rheology of solids gain a new potential application area for the design of gravitational wave detectors. Currently, gravitational waves are detected from displacement signals, thus distinguishing and separating all the noises (*e.g.*, the vibrations caused by transport, industry and seismic wave propagation) is a key concept. Since several rock materials show rheological behavior, wave propagation in the rock block, into which an underground gravitational wave detector (*e.g.*, the Einstein Telescope proposed by the European Union) will be established, has to be calculated via rheological models.

Irreversible thermodynamics ensures a common general framework to investigate all these mentioned phenomena. During the 20th century, several different theories of irreversible thermodynamics have been born. However, the emergence of these branches have led not only to understanding of dissipative and irreversible processes but also to the disintegration of the unified science of thermodynamics. Nowadays the endeavor to unification can be observed in irreversible thermodynamics.

This dissertation investigates non-Fourier heat conduction and rheology of solids in two frameworks of irreversible thermodynamics, namely, Internal Variable Methodology and the GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) formulation. Regarding heat conduction, the effect of thermal expansion on heat conduction, as well as the physical interpretation of entropy current multipliers are analyzed. Concerning rheology, the generalization of the Kluitenberg–Verhás rheology of solids to include thermal expansion is derived in the GENERIC framework, and is compared to the results of derivation with internal variables. Based on the obtained GENERIC equation, a staggered finite-difference solution method is investigated: stability of the scheme is analyzed, requirements on the parameters to eliminate the numerically originated dispersive and dissipation errors are estimated, and the scheme is demonstrated to numerically ensure the conservation of total energy. Finally, analytical solutions for three spatial dimensional rheological problems of solids in the force equilibrial approximation are provided. These results can be applied for validating numerical methods, they highlight that rheology results in a more complex mechanical behavior than damped and delayed elasticity, and help in interpreting observed phenomena in plastics (*e.g.*, thick-walled tubes) and around underground tunnels.

Szilárd közegek rugalmas, hőtágulási, reológiai és hővezetési folyamatainak irreverzibilis termodinamikai vizsgálata – Kivonat

A modern mérnöki technológia fejlődése rámutatott, hogy egyes jelenségek leírása és modellezése túlmutat a mérnöki gyakorlatban szokásos és jól ismert hővezetési és szilárdtest-mechanikai modelleken, nevezetesen a Fourier-törvényen és a Hooke-törvényen. Már a 20. század közepén elkezdődött olyan modellek fejlesztése, amelyek betekintést és számítási lehetőséget nyújtanak ezen jelenségekhez, azonban a részletek kidolgozása még ma is tart.

Jelen PhD-dolgozat középpontjában a nem-Fourier-típusú hővezetési, illetve a szilárd közegek reológiájának leírására szolgáló modellek állnak.

A Fourier-féle hővezetéstől eltérő viselkedés már számos kísérletben igazolást nyert, ennek megfelelően több elméleti modell és magyarázat született a leírására. A jelenség mérnöki alkalmazásai azonban csak speciális területek szűk körére terjednek ki, mint például extrém körülmények mellett (pl. alacsony hőmérsékleten), mikro- és nanoskálákon lejátszódó, illetve nagyfrekvenciás folyamatok esetén, de ma már ismert, hogy a heterogén anyagok, mint a kőzetek, réteges szerkezetek, habok vagy 3D nyomtatott minták hővezetésének viszonylag egyszerű leírása nyerhető a Fourier-törvényen túlmutató hővezetési modellekkel. Ha az ilyen szerkezetek újonnan bevezetett hővezetési paraméterei a gyártástechnológián keresztül szabályozhatók, akkor a termikus tervezés új szintjére léphetünk.

A reológia jól ismert nem-newtoni folyadékok kapcsán, ahol a folyadék belső súrlódásának hatásait írja le. Hasonló viselkedés számos szilárd anyagnál is megfigyelhető, pl. polimerek, bioanyagok, kőzetek vagy magas hőmérsékleten üzemeltetett acélok hosszú ideig tartó folyamatai esetén (pl. erőművi gőz fővezetékek ún. tartós folyása). A szilárdtest-reológiai modellezés és szimuláció új és potenciális alkalmazási területet nyerhet a gravitációshullám-detektorok tervezésekor. Jelenleg a gravitációs hullámokat az elmozdulásjelekből érzékelik, így az összes zaj (pl. közlekedés, ipar és szeizmikus hullámterjedés okozta rezgések) megkülönböztetése és elkülönítése kulcsfontosságú. Mivel számos kőzetfajta reológiai viselkedést mutat, a hullámterjedést a kőzettömbben, amelybe egy földalatti gravitációshullám-detektort (pl. az Einstein-teleszkópot) létesítenek, reológiai modellekkel kell modellezni.

Az irreverzibilis termodinamika egy közös általános keretet biztosít ezen két jelenség vizsgálatához. A 20. század folyamán a tudományág keretén belül számos különböző irányzat született, melyek megjelenése nem pusztán a disszipatív és irreverzibilis folyamatok mélyebb megértéséhez vezetett, hanem egyben a termodinamika egységes tudományának széttagolódásához is. Jelenleg a tudományág művelőinek köre erősen törekszik ezen irányzatokat és a belőlük nyert tanulságokat egységesíteni.

A dolgozat szilárd közegek nem-Fourier-típusú hővezetését és reológiáját vizsgálja az irreverzibilis termodinamika belső változós módszertana és a GENERIC (General Equation for the Non-Equilibrium Reversible–Ireversible Coupling) formalizmus segítségével. Elemezzük a hőtágulás hővezetésre gyakorolt hatását, valamint az entrópiaáram-szorzók egyfajta tartalmi interpretációját adjuk meg. Levezetjük a hőtágulással általánosított Kluitenberg–Verhás-féle szilárdtest-reológiai modellcsaládot a GENERIC keretrendszerben, majd összehasonlítjuk a belső változós módszertannal nyert eredménnyel. Ezután egy, az előzőleg levezetett, GENERIC-ben reprezentált egyenletrendszer alapján felállított eltolt mezős végesdifferencia-alapú numerikus megoldási módszert vizsgálunk, amely numerikusan is biztosítja az összenergia megmaradását. Elemezzük a séma stabilitását, valamint meghatározzuk a numerikus eredetű diszperziós és disszipációs hibák kiküszöböléséhez a séma paramétereivel szemben támasztott követelményeket. Végezetül szilárd közegek három térdimenziós reológiai feladataihoz adunk analitikus megoldásokat az erőegyensúlyi közelítésben. Ezen eredmények használhatók numerikus módszerek validálására, sőt, rávilágítanak arra, hogy a reológia összetettebb mechanikai viselkedést is eredményez, mint pusztán csillapított és késleltetett rugalmasságot.

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Frequently used notations

Latin letters

$\mathbf{C},\ \mathbb{c}$	entropy current multipliers second and higher order, respectively
c_{ϵ}	constant-strain specific heat capacity
c_{σ}	constant-stress specific heat capacity
c_{\parallel}	longitudinal elastic wave propagation velocity
Ë	energyfunctional / Young's modulus
$E^{d} = 2G$	deviatoric elasticity modulus, G is the shear modulus
$E^{\rm s} = 3K$	spherical elasticity modulus, K is the bulk modulus
E_0, E_1, E_2	longitudinal rheological coefficients
$E_0^{\rm d}, E_1^{\rm d}, E_2^{\rm d}$	deviatoric rheological coefficients
$E_0^{s}, E_1^{s}, E_2^{s}$	spherical rheological coefficients
e	(mass) specific internal energy
j	numerical time index
\mathbf{j}_E	heat current density/heat flux
\mathbf{j}_S	entropy current density/entropy flux
k, K, l, L	Onsagerian coefficients
l, m, n	numerical space indices
\mathbf{L}	reversible operator matrix
M	irreversible operator matrix
S	entropyfunctional
s	(mass) specific entropy
t	time coordinate
Δt	numerical time step
T	temperature
V	volume
V	velocity field
x, y, z	spatial coordinates
$\Delta x, \ \Delta y, \ \Delta z$	numerical space steps
X	vector collecting the state variables
\mathbf{x}^*	vector collecting the entropy-conjugated state variables
$\dot{\mathbf{x}}_{\mathrm{rev}}, \dot{\mathbf{x}}_{\mathrm{irr}}$	reversible and irreversible contribution to dynamics

Greek letters

α	(linear) thermal expansion coefficient
ε	"small" strain
λ	thermal conductivity
$\xi, \boldsymbol{\xi}$	internal variables
Ξ	dissipation potential
π_S	entropy production rate density
au	longitudinal stress relaxation coefficient
$ au^{\mathrm{d}}$	deviatoric stress relaxation coefficient
$ au^{\mathrm{s}}$	spherical stress relaxation coefficient
Q	(mass) density
σ	stress tensor

Mathematical symbols

d	differential
$\frac{\partial f}{\partial r}\Big _{\mathcal{H}}$	partial derivative of the function $f(x, y, z)$ w.r.t. the variable x while the
0	variables y and z are kept constant
∂_a	partial derivative w.r.t. the variable of ath index
∂_t	partial time derivative
$D_{\mathbf{v}}$	comoving/substantial/material time derivative
$\frac{\delta A}{\delta x}$	functional derivative of the functional $A[x]$ w.r.t. the function x
Σ	nabla operator
$\overline{\mathbf{\nabla}}$	nabla operator acts on the quantity standing on its left side
∇	nabla operator acts on the quantity standing on its right side
Δ	Laplace operator
d, s	deviatoric and spherical parts of a tensor, respectively
det	determinant
s, A	symmetric and antisymmetric parts of a tensor, respectively
Т	transpose of a tensor
tr	trace of a tensor
•	scalar product, also applied for full contraction of type $A_{abcde}B_{de}$
\otimes	dyadic product
×	cross/vector product
$\{ullet,ullet\}$	Poisson bracket
[ullet,ullet]	dissipative bracket
1	identity tensor
0	zero vector/tensor

Chapter I

Introduction

Our world is too large and complicated to be understood via a single universal discipline so, historically, different modelling approaches have been born around more-or-less different areas of phenomena. However, processes described in different scientific fields go hand in hand in reality, thus, for example, mechanical and thermal processes are inseparable from each other. Pure mechanical, as well as pure thermal, processes are approximations of coupled thermomechanical processes. Let us consider, for example, elastic wave propagation in a solid. At first sight, this phenomenon appears reversible. However, spatial domains that are "pushed" or "pulled" by the wave, get warmer and cooler, respectively, which results in an instantaneously inhomogeneous temperature distribution, which induces heat conduction in the body. After a long time, heat conduction—induced by the wave propagation itself—attenuates the process via the emerging additional thermal stress, and the kinetic and elastic energy transported by the wave is transformed to thermal (internal) energy. Frequently, these temperature differences are negligibly small, and then heat conduction can be ignored when modeling such phenomena. A crucial and fundamental issue in engineering modeling is to distinguish between important and insignificant effects.

However, engineering applications also require the treatment of such phenomena where the thermal and mechanical processes cannot be separated of each other.

Several well-known theories of coupled thermal and mechanical processes are known, such as convective heat transfer, gas dynamics or thermoelasticity. These formulations have a wide range of engineering applications, *e.g.*, in the design of internal combustion engines, turbines, heat exchangers, power plant pipeline systems, jet engines and air brake systems.

The importance of thermodynamics also shows up for processes that appear to be purely mechanical. As an evidence, Figure I.1 presents the temperature distribution of a polymeric sample during a uniaxial rupture test. Usually, in such experiments only the mechanical quantities (*e.g.*, stress and strain) are investigated, however, thermal quantities like temperature) have their own stories.



Figure I.1: Snapshots about the temperature distribution of a polymeric sample, taken by thermal camera during a uniaxial rupture test [1]. The first image presents the approximately homogeneous initial temperature distribution before the start of the measurement. On the second one, the Joule–Thomson cooling due to elastic deformations can be obtained. The third and fourth images show temperature increase during dissipative processes, namely rheological and plastic—permanent deformation involved—changes. Finally, the last one illustrates the strongly increased temperature at the time instant of failure.

The message of Figure I.1 is that mechanical processes—even the *reversible*¹ elastic ones—are always accompanied by thermal processes, which are observable through the temperature change of the sample. This coupled mechanical and thermal behavior is more conspicuous in case of *irreversible*² and *dissipative*³ processes, *e.g.*, in rheology or plasticity.

Nevertheless, thermodynamics and mechanics are usually treated almost fully independently, thus a goal of this dissertation is to present this interdisciplinary field as a complete unit. This kind of formulation is not foreign to engineers skilled in applied mechanics—especially if skilled in continuum mechanics—and, hopefully, it can support and deepen the knowledge and understanding of engineers working in the fields of heat conduction, thermo-hydraulics and simulation of coupled thermo-mechanical problems.

I.1 Motivation

The dissertation focuses on two topics, heat conduction beyond Fourier's law and rheology of solids (linear solid mechanics beyond Hooke's law). Both phenomena have been known for a long time, several experiments and measurements justify them, however, their engineering applications are limited only to certain specific problems. Moreover, several different theories have been born to explain and model them, but there is no uniformly accepted and distinguished explanation about them.

The focus on these effects is twofold; first, the rapid development of technology has necessitated the description of fast and high-frequency processes, heterogeneous materials and micro- and nanosystems, requiring the knowledge of non-Fourier heat conduction as well as rheology. At first sight, there is no connection between these phenomena, however, both can be investigated within the framework of irreversible thermodynamics. Several different branches of irreversible thermodynamics were born during the 20th century; in this work, Internal Variable Methodology and GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling)⁴ formulation are applied. Hence, the second reason is to compare these two frameworks through examples, which contributes to the unification of methodologies of irreversible thermodynamics.

Now, a short historical review and a summary of the possible engineering application opportunities of these phenomena are presented.

I.1.1 From the exotic behavior of superfluids to engineering applications of beyond-Fourier heat conduction

Usually, heat conduction is described via the well-known Fourier law, which gives a linear relationship between the heat current density and the temperature gradient. This model is applied for calculations in the engineering praxis.

However, during the 20th century, several experiments proved that there exist such heat conduction phenomena that are inexplicable with Fourier's law. First, these phenomena are observed at extreme conditions. In the first part of the 20th century, a number of hitherto unseen phenomena (such as superconductivity) had been discovered during investigations of liquid helium near its lambda transition (≈ 2.2 K), in the so-called helium II phase [2]. Tisza and Landau predicted such a heat conduction behavior in helium II, in which temperature shows a dissipative yet wavy nature of propagation, which can not be explained via Fourier's law [3, 4]. This phenomenon, called second sound, was experimentally justified by Peshkov [5] applying heat pulse excitation. This kind of non-Fourier like behavior were investigated later in several experiments (see *e.g.*, [6, 7]).

¹Capable of being turned back, here: after unloading the sample regains its original shape and size.

²Incapable of being turned back.

³Energy dispersive.

⁴Basic ideas and details of these frameworks are given in Chapter II.



Figure I.2: *Left:* A simplified schematic picture about Peshkov's experiment [2]. In a glass tube (G), heat pulse signals are generated by the heater (H), and temperature is measured by the thermometer (T). A and B denote tubes with adjustable positions, which ensured better observability of the temperature waves. *Right:* A screenshot from Alfred Leitner's video⁵ demonstrating wave-like propagation of temperature in helium II from 1963.

The research for non-Fourier heat conduction behavior had been continued. Guyer and Krumhansl have derived a non-Fourier like heat conduction equation via linearizing the Boltzmann equation [8, 9], thus microscopic and statistical considerations are in the background. This equation can also describe the second sound phenomenon, and according to Guyer and Krumhansl, nonmetallic crystal as lithium fluoride (LiF) or solid He⁴ are the prime subject of investigations. The so-called ballistic-type heat propagation was showed in sodium fluoride (NaF) crystals by Jackson, Walker and McNelly [10, 11, 12]. This latter type of heat conduction also deviates strongly from Fourier heat conduction (see Figure I.3).



Figure I.3: *Left:* Result of the NaF experiments [11, 12]. L and T denote the time instants of arrivals of longitudinal and transversal signals.

⁵Source of the picture: https://www.youtube.com/watch?v=NjPFfT2EyxQ, accessed: 2022-01-31.

An independent direction of investigations of beyond-Fourier heat conduction theory is hyperbolization of thermoelasticity, a brief review of which is given in [13], and corresponding Hungarian researches are published in [14, 15, 16, 17, 18]. However, this topic is out of the scope of the present thesis.

It looked like that beyond-Fourier heat conduction theories can explain such exotic heat conduction behaviors, nevertheless, they have not yet taken a root in engineering applications. There are two reasons for this; first, the materials investigated in such experiments were so "perfect" (*e.g.*, for the NaF experiments monocrystallines were grown), which do not typically exist in nature; second, such extreme conditions (*e.g.*, low temperature), which were applied during the experiments, occur rarely in praxis.

However, targeted experiments at the Department of Energy Engineering at Budapest University of Technology and Economics have shown that deviation from Fourier-like heat conduction can be observed on several samples at room temperature, too. These deviations are not as conspicuous as second sound phenomena, however, their measured behavior can not be explained and fitted by Fourier's law.

These measurements are performed via heat-pulse experiments (see Figure I.4). Usually, in the engineering praxis, this method is applied to determine the thermal diffusivity of a sample (see *e.g.*, [19, 20]). However, for the first time [21] published such measurement results at room temperature that cannot be correctly fitted by Fourier's law. Moreover, this article highlighted that, although there is no known microsopic background information, modeling heat conduction and fitting two extra parameters via the Guyer–Krumhansl equation follows the measured temperature signal properly.



Figure I.4: Arrangement of the heat-pulse experiment. The front face of the specimen is excited by a heat pulse and rear-side temperature is measured [21].

This recognition led to a series of experiments, which were performed on heterogeneous samples like rocks and layered structures (Figure I.5 presents some of them), which also show non-Fourier like behavior [22, 23, 24]. More and more materials turn out to show beyond-Fourier heat conduction behavior, including rocks, 3D printed polymers and metals, and metal and carbon foams.



Figure I.5: Heterogeneous samples that show non-Fourier heat conduction behavior. *From left to right:* 3D printed metal, 3D printed concrete, carbon foam applied for CERN experiments and metal foam. Photos taken by Róbert Kovács (Department of Energy Engineering at Budapest University of Technology and Economics).

Naturally, a question arises whether it is measurement errors that are considered as non-Fourier effects in these experiments? However, Figure I.6 presents that the difference between the measured signal and the Fourier-model prediction tends to exceed the measurement errors, while the Guyer–Krumhansl prediction follows the measured signal appropriately.



Figure I.6: Result of a heat-pulse experiment: measured and fitted rear-side temperature of carbon foam samples. The Fourier fit strongly deviates from the measured data, while the Guyer–Krumhansl-fit follows the measured signal well. The deviation of the Fourier fit is considerably larger than the measurement error. The measurement and fitting procedure have been performed by Anna Fehér and Róbert Kovács (both are staff members of Department of Energy Engineering at Budapest University of Technology and Economics).

Unfortunately, there exists no general physical picture about the phenomenon that causes such a deviation from Fourier's law at room temperature. For example, in the case of heterogeneous materials, the varied composition of the material, the porosity properties, and even the cracks and discontinuities can strongly modify the nature of the heat conduction phenomenon, since then several parallel heat transfer mechanisms exist, *e.g.*, heat conduction in the bulk material, and convective heat transfer between the bulk material and inclusions. Fortunately, Internal Variable Methodology of irreversible thermodynamics offers a general formulation of such problems, where no physical background is known. Since one concludes from measurement results that a beyond-Fourier model of heat conduction is required, and from the measurement the newly introduced parameters are determined, thus engineering calculations can also be performed on these materials. In contrast, for modeling crystal lattices around 10 K, a specific microscopic background is known, which can be explained via averaging the phonon-Boltzmann equations in the framework of extended thermodynamics⁶. However, a systematic series expansion requiring at least 30 degrees of freedom is needed for a prediction consistent with the measurement results [25]. Such a model is not applicable in engineering practice. As conclusion, beyond-Fourier heat conduction equations derived via the Internal Variable methodology provide an efficient and easy-to-use model analogous to Fourier's law rather than a tool to explore the detailed physical mechanism. Development of the corresponding analytical and numerical techniques has already begun (see *e.g.*, [26, 27]) and is still in progress.

In nutshell, this is our knowledge about non-Fourier heat conduction today.

A possible next step is to transfer this knowledge into engineering applications. It has become clear that thermal properties depend not only on the material but on its internal structure. Modern technologies make it possible to manufacture objects with well-designed internal structure (*e.g.*, 3D printing) for specific tasks. Nowadays, thermal investigation of metamaterials⁷ is also in progress [28]; here, a promising field of application is thermal cloaking. Since metamaterials also are usually layered structures, transfering the experiences and conclusions reached in non-Fourier behavior can contribute to such researches. It means that if the relationships among the internal structure and thermal properties—including non-Fourier effects—are identified, then a higher level of thermal design methodology can be developed.

It is now obvious that several challenges and promises stand before engineering regarding non-Fourier heat conduction. At the same time, neither physical explanations nor modeling techniques or computational methods are fully developed, thus further theoretical investigations are also required, which are still in progress.

I.1.2 How does rheology of solids contribute to design of gravitational wave detectors?



Figure I.7: "Panta rhei – everything flows". La persistència de la memòria (The persistence of memory)⁸ by Salvador Dalí from 1931.

⁶A branch of irreversible thermodynamics, for details see Chapter II.

⁷The term metamaterial is originated from the Greek words meta (beyond) and materia (matter). In fact, metamaterials are not materials but structures. These are designed to have such properties that are not found in pure materials.

⁸Source of the picture: https://en.wikipedia.org/wiki/The_Persistence_of_Memory, accessed: 2022-01-07.

Rheology is a well-known phenomenon in fluid dynamics, it models the fluid's internal friction and describes its effects on the dynamics. The term rheology is created by Eugene C. Bingham from the Greek words rheo (flow) and logia (study of). The simplest and most commonly used rheological model for fluids is Newton's viscosity law (*e.g.*, usually water is modeled as a Newtonian fluid), however, several other more complicated rheological models existing, these are summarized under the name non-Newtonian fluids, such materials are for example paints and honey.

Most solids from the point of view of common engineering applications (*e.g.*, steel) can be modeled via elastic material laws, which neglect the internal friction of the material. Naturally, internal friction can also play important role in processes of solids, thus it is not a suprise that a large variety of technically important solid materials possess rheological characteristics. To be specific, hereafter, in this dissertation, rheology is restricted to linear viscoelasticity of the form where the material is described by a linear relationship among stress, strain and their time derivatives, up to some finite order of derivatives, and the small-strain approximation is assumed. Correspondingly, under rheological change/process/behavior, such time dependence of stress and strain are understood that are not in an elastic stress–strain relationship, the contribution of the mentioned time derivative terms being manifest.

Importance of rheological behavior of solids is well-known in mechanical engineering, too, *e.g.*, in polymer technique, as well as in thermal engineering – for example, turbine blades or power plant steam pipes have to be verified for creep (sometimes called cold flow); furthermore, many biology-originated objects and protheses used in medical technology also show rheological properties – for instance, rheological behavior of knee ligaments is apparent. Accordingly, rheological behavior must be taken into account when designing technical devices and facilities, which require the characterization of the materials and reliable calculation methods. Nevertheless, rheology means not only disadvantages and problems but also benefits. For example, one can rely on its effect of damping and absorbing vibrations [29].

Modeling and simulation of rheology of solids may gain a new and potential application area by the design of new generation *underground* gravitational wave detectors.

Existence of gravitational waves had already been conceived by Henri Poincaré in 1905 [30], but first Albert Einstein had predicted them on theoretical basics in 1916 [31, 32]. For a long time, only indirect evidences supported Einstein's prediction. Until 2015 had to be waited for the first direct observation of gravitational waves, when a signal generated by merging of two black holes was recognized by the gravitational wave detector LIGO (Laser Interferometer Gravitational-Wave Observator). In 2017, the Nobel Prize in Physics was awarded for this discovery. Naturally, more gravitational wave detectors were existing worldwide before this breakthrough but the first direct detectation has motivated the development of the existing and new detectors.

Signals emitted by different gravitational wave sources can be detected at different frequency ranges. Three major groups of detectors can be distinguished: pulsar timing telescopes (*e.g.*, IPTA, SKA) for very low frequency sources, space-based telescopes (*e.g.*, LISA, DECIGO proposals) for low frequency sources and ground-based telescopes (*e.g.*, LIGO, VIRGO, KAGRA, Einstein Telescope proposal) for high-frequency sources [33]. Visualization of the previous together with sensitivities of the detectors are presented on Figure I.8. Hereinafter, the focus is on ground-based telescopes.

The common principle of operation of ground-based detectors is interferometry. Already existing gravitational wave detectors has two arms. For simplicity, let us explain the operation of LIGO. A coherent laser beam is splittered by a beamsplitter in two beams, which are reflected on mirrors placed at the end of the arms. The reflected beams recombine and an interference pattern can be detected. When a gravitational wave passes through, then "spacetime curves" locally, which causes a relative change of the length of the arms. Due to this length change, the reflected beams, which have been in phase so far, become slightly out of phase, which modify the interference pattern, which leads to a measurable signal. Other existing detectors operate similarly with minor modifications, *e.g.*, VIRGO operates in vacuum. KAGRA has to be emphasized here, since it is the first underground operating detector, moreover, it is the first one where cryogenic mirrors are applied, however, certain problems occured during the operation (*e.g.*, soaking).

Nowadays, the biggest challenge is to increase the sensitivity and to widen the frequency range. The



Figure I.8: Characteristic strain – frequency diagram of different gravitational wave sources and sensitivity of different gravitational wave detectors [34].

proposed Cosmic Explorer (CE) is based on the technology of LIGO, however, with longer arms-while the arms of LIGO are 10 km long, the arms of CE are designed to be 40 km long. Another, proposed detector is the Einstein Telescope (ET), which became a project of ESFRI (European Strategy Forum on Research Infrastructures) in 2020. About 700 collaborators joined to the ET project, including Wigner Research Centre for Physics, ATOMKI (Institute for Nuclear Research) and Budapest University of Technology and Economics from Hungary. ET is based on a quite new conception. In contrast to other gravitaional wave telescopes, ET has three arms with low-frequency and high-frequency instrumentation in all arms, furthermore, similarly to KAGRA, ET also applies cryogenic mirrors. CE and ET are third-generation detectors with increased sensitivity compared to the existing ones (see Figure I.8). CE has the greater sensitivity beyond 10 Hz, however, under 10 Hz ET is more sensitive, which opens the opportunity to detect gravitational waves emitted by lower-frequency sources. Importance of this possibility lies in the fact that low-frequency sources are planned to be observed via space-based detectors, however, at present, these space-based detectors are still proposals, the first missions being expected in the 2030's years. Since space-based detectors are untested so far, the success of the missions are questionable. These space-based detectors may need further development. Until the first success of these space missions, hopefully, ET also may offer evaluable observations about low-frequency sources.



Figure I.9: Artist's impression of ET and its schematic arrangement [35].

			* Tentative schedule
2021	2022 2024 2025	2026 2028 2030	2035
\diamond \diamond	ESFRI status		
CDR ESFRI prop 2011 2020	ocsal		1
Enabling technolo	gies development		I
Sites qualification	Site dec	cision	I.
Cost evaluation			1
Building governar	ic <mark>e</mark>		1
Raising initial fund	ds		1
Raising	g construction funds		i
	Committing c	onstruction funds	
Pre-engineering s	studies		1
	RI operative TD	ET RI construction	1
	Detector operative TD	ET ITFs construction	
		ET installation	n í
		Commiss	ioning 🚫 Science
ESFRI Phases: Des	ign Preparatory	Implementation	Operation

Figure I.10: Investment and construction schedule of Einstein telescope [36].

Figure I.10 presents the milestones of the planned construction of ET proposal. The project has already begun, now, choosing the right location is the most important task. Currently, gravitational waves are detected from diplacement signals. Naturally, deformations and displacements of the detectors are originated not only by "curvature of spacetime", but mechanical processes of the surronding soil and rocks also affect the motion of the detector. It means that the measured signals also contain such mechanical effects, thus distinguishing and separating all noises (*e.g.*, the vibrations caused by transport, industry or seismic wave propagtion) is a key to recognize gravitational waves. It means that the possible site of ET has to be seismically and geologically stable enough. Planned operation of ET is expected to start in 2035. Hence, the next more than 10 years is about development and design of ancillary facilities and instrumentations. In this time period several opporunities and challenges stand before engineering, where new ideas and new models can be testified.

But how does rheology of solids contribute to design of gravitational wave detectors?

Time-dependent mechanical behavior of rocks is an old-known fact in civil engineering, mine industry and tunneling, for example, time dependence with a time scale of years may be measured in the soil or rock around an opened tunnel (see Figure I.11).

As opposed to prompt elastic response, the neighborhood of the tunnel typically exhibits delayed and damped behavior, which can originated from a number of reasons. Nevertheless, linear rheological constitutive equations offer a frequently usable tool to model such phenomena.

The above figures speak for themselves: the knowledge of the initial underground *in situ* stress state is a key step, since motion of the surrounding rock as well as forces acting on the support of the tunnel strongly depend on the initial stress state. However, measuring *in situ* stress directly, especially all components of the stress tensor, is infeasible, thus indirect methods are required. Nowadays, the most promising technique is the ASR (Anelastic Strain Recovery) method [40, 41, 42], in which the temporal changes of the strain field in different directions are measured on the surface of a freshly obtained rock core sample in its already stress-free state, and via backwards extrapolation in time, the initial strain state corresponding to the initial *in situ* stress can be determined, from which the initial stress state itself is calculated. The reliability of the extrapolation depends on the knowledge of material parameters, which are usually determined via fitting. However, a sufficiently accurate evaluation can only be performed via material models that go beyond the commonly known simplest rheological models (Kelvin–Voigt, Maxwell, Poynting–Thomson–Zener): more closely, stress and its time derivative, and strain and its first and second time derivative all have to be taken into account. In 2015, within the framework of internal variable methodology, this experimentally distinguished rheological model family for solids was also



Figure I.11: Illustrative examples for time dependent processes around bores are observed in tunneling. *Top line:* Significant examples on well-known phenomena in tunneling: squeezing and convergence [37, 38]. *Bottom line:* Measured (and fitted) exponential-like displacement history of tunnel walls at the National Radioactive Waste Repository, Bátaapáti, Hungary, with characteristic times of 3–10 years [39] (different colors mean different directions at a given cross-section of the tunnel).

theoretically found distinguished, and was termed the Kluitenberg-Verhás model family [43].

In rock engineering, several experimental methods exist to evaluate the material—including both elastic and rheological—parameters. One of the simplest experiments is the creep test (see Figure I.12). Here, after loading, the force—thereby approximately (apart from the change of cross-section area) the stress—is kept constant, and strain is measured in various directions along the surface of the sample via strain gauges. Usually, longitudinal and transversal strains are measured, however, direct use of them in parameter fitting proves problematic. Instead, assuming isotropic material structure and corresponding constitutive equations, the deviatoric–spherical decomposition can facilitate the parameter fitting



Figure I.12: A standardized rock sample for determination of its rheological properties, and visualized measurement results. The diagrams show the results of a creep test. The left one presents the constant axial stress (red) and the longitudinal (green) and transversal (blue) strains. The right one presents the strain in the deivatoric (green)–spherical (blue) decomposition. The small oscillations are caused by thermal expansion, which are in relationship with the measured temperature signal (not displayed here).

procedure, and in parallel, it can shed light on important facts. For example, small oscillations can be seen both on the longitudinal and on transversal strain components (left diagram of Figure I.12), while these oscillations appear only on the spherical strain component (right diagram of Figure I.12). Comparing these strain signals to the recorded time dependence of temperature of the laboratory where the measurements were performed, the mechanical effect of thermal expansion can be recognized. Since thermal expansion does not affect deviatoric stress and strain in isotropic materials, this behavior is self-evident.

Several known phenomena can be explained by rheological models. For example, "dynamic" elasticity parameters (*e.g.*, Young modulus, bulk modulus, shear modulus, *etc.*) of rocks are always larger than their "static" ones. Here, dynamic and static refer to the rapidity of the measurement. When loading is fast enough then the dynamic elasticity parameters, and when loading is slow enough (theoretically, when the measurement is performed with zero velocity) then the static elasticity parameters are determined. This recognation is visualized on Figure I.13, where measured dynamic and static bulk moduli for different rocks are presented. This behavior can be explained via thermodynamical requirements on the so-called Poynting–Thomson–Zener model [43, 44].



Figure I.13: Relationship among the dynamic and static bulk moduli for various types of rocks [45].

This behavior affects wave propagation, too. Purely elastic materials are so-called non-dispersive media, thus phase⁹ and group¹⁰ velocities are equal. When phase and group velocities differ from each other then wave packets are broadening during propagation. This is called dispersion. In rheological media, dispersion should also be taken into account. Since dynamical elasticity parameters are larger than the static ones, wave propagation velocity at high frequency are larger than at low frequency [46]. The so-called dilatation resonance frequency method is based on wave propagation (see Figure I.14) [47]. Evaluation of the measurement is performed via elastic material models and the dynamic elasticity parameters are determined via the method.

It is now self-evident that detection and analysis of gravitational waves with ET depends strongly on the knowledge of the motion of surrounding rock formations. Since the detector is quite sensitive, in addition to purely elastic processes, the rheological behavior, as well as thermal expansion, have to be taken into account. These processes may cause strains comparable with the strains caused by gravitational waves. All these need reliable calculations of complex wave propagation phenomena.

⁹Phase velocity of a wave is the velocity of a single plane wave.

¹⁰Group velocity of a wave is the velocity with which the overall envelope shape of the amplitudes of the wave moves.



Figure I.14: *Left:* Dilatation resonancy frequency test device in uniaxial (*top*) and triaxial (*bottom*) setup. *Right:* Evaluation of the measurement, peaks in the gain at certain frequencies correspond to resonances, from which material coefficients are determined. Current evaluation protocoll based on purely elastic material model [47].

However, effective numerical simulation of dynamical phenomena is still in its infancy. Calculated solutions of elastic—thus reversible—wave propagation even just in one spatial dimension via commercial finite element softwares depend strongly on the settings of the applied method in the software and, frequently, numerics-originated instabilities¹¹, dissipation errors¹² and dispersion errors¹³ occur [44] (for details, see Chapter V). When such numerical phenomena appear, then distinguishing between the real physical and the artificial numerical behavior is difficult, or maybe impossible. The question arises how one can trust numerical simulations of more complex situations—such as wave propagation in rheological continua or higher spatial dimensional problems—when the reliability of the solutions for even simpler problems raises so many questions.

As illustration and to support the previous statements, let us consider the wave equation in two spatial dimensions, for a single scalar degree of freedom u = u(t, x, y), with constant (unit) coefficients and no source term in the equation, *i.e.*,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}.$$
 (I.1)

A rectangular sample is taken with 'flux' (Neumann) boundary condition (normal spatial derivative component is prescribed): on one of the edges, one cosine-type pulse is applied [for details see (V.94) in Chapter V], while the other edges are kept 'free' (zero normal derivative). Initially, both u and $\partial u/\partial t$ are set to zero ('relaxed initial state'). The numerical calculations are shown in Figure I.15; a 50 × 50 spatial grid is taken. The pulse duration is 0.3 time unit. All calculations are presented with the above-defined parameters, only the time-integration method is modified and its effect is investigated.

One can see that the solution depends on the choice of time-integration very seriously. There are large-scale differences and fine-structured irregularities both. Moreover, one has no means of validation which outcome is correct to what extent. Although the software offers plenty of options for implementing user-defined material models, the reliability of the solution of such a well-known classical problem is also questionable.

¹¹Exponential blow-up of the solution.

¹²Artificial damping in the solution.

¹³Artificial oscillation of the solution.



Figure I.15: u(2, x, y) with various COMSOL settings [48]. Left column, from top to bottom: BDF Max. order 5 & min. order 2, BDF Max. order 3 & min. order 2, BDF Max. order 1 & min. order 1, BDF Max. order 5 & min. order 3 Strict time stepping, RK34 Default. Right column, from top to bottom: DP5 PI-Smooth, DP5 PI-Standard, DP5 PI-Quick, Generalized- α (GA), GA Predictor Constant. Not shown (failed like DP5 PI-Standard or GA Predictor Constant): DP5 Pi-Off, RK34 Manual, Cash-Karp 5 Free or Strict (Manual with a small time step gives a result similar to that of RK Default).

Fortunately, the situation is not so desperate. In addition to commercial finite element softwares, some have been developed to treat specific problems. One of such programs is SPECFEM3D Cartesian, via which simulations of acoustic, elastic, coupled acoustic–elastic, poroelastic or seismic wave propagation are feasible in complex geometries (Figure I.16 illustrates simulation results obtained via the software) [49]. This software have been already applied to characterize a potential site for ET [36].



Figure I.16: Elastic wave propagation in complex geometry simulated via SPECFEM3D Cartesian [36].

The results are seemingly correct and free from strong numerical originated errors, which can be expected from a program specified for wave propagation. However, something is missing. Although the software is constantly evolving, modeling of complex dissipative behavior (such as rheology) has so far been omitted.

Nowadays, a promising, also engineeringly important field of irreversible thermodynamics is numerics. In the last decade reliable, thermodynamically motivated numerical methods have been published, which techniques try to reproduce physical principles and experiences, such as numerical conservation of linear momentum and total energy or the increase of entropy [50, 51, 52, 53, 54, 55, 56, 57]. Hopefully, implementing such methods into already existing softwares, the opportunity of reliable solution to complex dissipative dynamical problems may become available to a wide range of engineering society.

Regarding numerical solutions, one more important point has to be addressed. Namely, numerical solutions have to be validated and verified for numerical artefacts (*e.g.*, dependence on the applied number of space cells, ...). However, since experiments and measurements can be performed only for a narrow range of problems—or often an experiment or measurement is designed based on the results of numerical simulations—, other opportunities have to be found. A possibility is to produce numerical solutions for problems, for which corresponding (exact) analytical solution is known. Although solution of complex tasks with the help of computers has become available, importance of analytical solutions remains eternal.

These all support that development of methodology as well as of calculation techniques—both analytical and numerical ones—are required, which have to be tested and demonstrated on real technical problems with corresponding boundary and initial conditions, which ensure the possibility of comparison with experimental data.

I.2 An overview of the dissertation

This work is strongly based on the irreversible thermodynamical methodologies of internal variables and GENERIC so Chapter II gives a literature review on both these frameworks and a short historical summary of the evolution of irreversible thermodynamics.

Chapters III-VI communicate the author's own scientific results.

In Chapter III, theoretical investigations are carried out according to beyond-Fourier heat conduction. First, room-temperature flash experiments come under scrutiny. A possible and *known* physical source of the measured non-Fourier-like behavior is investigated, namely, the effect of thermal expansion on heat conduction. This most fundamental issue has not yet been addressed and analyzed. Based on the basic equations of thermoelasticity, a non-Fourier-like heat conduction equation on temperature can be derived. Parameter testing of this equation corresponding to the flash experiment is executed for several technically important materials. This investigation supports that *the deviation from Fourier's law measured in flash experiments can not be originated from thermal expansion*. This observation highlights that further investigations and analyses of non-Fourier phenomena are required.

Since the observed and measured non-Fourier behavior can not or just partly be interpreted as an interplay of coupled phenomena, different branches of irreversible thermodynamics have their own methodologies to derive equations that describe beyond-Fourier heat conduction. These theories lead to the same or similar equations, but the thermodynamical background is variably developed and their physical explanations and interpretations are insufficient. For example, internal variable methodology is a strong tool of modeling. Physical interpretation of internal variables as well as of entropy current multipliers¹⁴ is usually not necessary, only some physical principles (as balance laws and the second law of thermodynamics) have to be respected. The derived thermodynamically compatible equations enable the investigation of the problems. However, the physical origin of the phenomena usually remains hidden and such coefficients appear that can only be determined in well-designed measurements. In parallel, GENERIC as a microscopic-motivated framework is strongly based on statistical considerations, from which macroscopic behavior cannot always be interpreted. A further investigation in Chapter III connects to entropy current multipliers. Namely, *applying simultaneously the internal variable methodology and the framework of GENERIC, entropy current multipliers—at least in heat conduction theory—can be interpreted as irreversible generalizations of reduced higher-order state variables.*

In chapters IV–VI, rheology of solids is in focus.

Motivated by the wide applicability of the GENERIC formalism, Section IV presents and discusses how the internal variable formulation of the Kluitenberg–Verhás model family can be implemented in GENERIC. This work does not just compare the frameworks of internal variable methodology and GENERIC but ensures such a representation of the system of describing equations that suggests thermodynamics-based numerical solution methods. The results are reported both via using specific entropy and temperature as independent state variables, the former one fitting better to theoretical investigations, while the latter one to applications. The derivation is generalized by thermal expansion, which has been ignored beforehand. It is shown and proved here that, for constant material coefficients—which is well-applicable from the point of view of engineering—the symplectic structure of the describing equations can be expanded by the antisymmetric part of the Onsagerian equations, which provides further numerical benefits.

Solutions of rheological problems in the force-equilibrial and space-independent limit have proved successful in explaining experimental results [1]. The next level of understanding is the investigation of solutions in the space-dependent—but still force-equilibrial—treatment (thus, for example, rheological processes caused by drilling can be modeled). Then, leaving the force-equilibrial approximation, wave propagation in rheological media can also be analyzed.

In this thesis, these results are presented in a different order because Chapter V, presenting a numerical solution method for determining wave propagation in rheological solids, is strongly based on the results of Chapter IV.

¹⁴Another opportunity to enlarge the degrees of freedom of modeling, for details see Chapter II.

Chapter V presents a finite-difference based method with half space and time shifts, which is applicable for reversible–non-dissipative, as well for irreversible–dissipative systems, and can be considered as a second-order generalization of the symplectic Euler method. Applicability and reliability of the method are demonstrated on wave propagation in elastic and rheological solids, presented first in one spatial dimensional problems, which is followed by a more general three spatial dimensional treatment. *Stability conditions of the one spatial dimensional scheme are determined via von Neumann analysis. It is found that, by choosing the Courant number appropriately, numerics-originated dispersion errors vanish and numerics-originated dissipation errors are weakly proportional to the size of the time step. Numerical simulations demonstrate that the scheme preserves total energy numerically, also in the three spatial dimensional case.*

This significant part of the dissertation improves the reliability and accuracy of numerical calculations. Moreover, this chapter is the foundation of a long-term research, too. Further development of the method is currently ongoing, generalization of the scheme also is applied to curved geometries (cylinders and spheres), and hopefully, thermohydraulic phenomena and thermomechanical problems of solids may be invesigated via the method. An extra advantage of this method is its simplicity, since it also runs quite quickly on personal computers, in the future it may be used for parameter testing, parameter optimization, and even for control, too.

In Chapter VI, exact analytical solutions are presented for processes in rheological solids in the space-dependent but force-equilibrial framework. In the investigated examples, the process is induced by temporal change in boundary conditions, hence, modeling of drilling processes and pressurizing/depressurizing of pipes and tanks can be obtained. Albeit the scope of analytical solutions is limited, analytical solution of a simplified version of the problem may provide a reasonable first approximation and give useful insight; moreover, analytical solutions can also be utilized for validating numerical methods. *The presented solutions demonstrate that rheology is more than damped and delayed elastic behavior: unexpected direction dependent and temporary counter-intuitive motions can also be observed. The results also illustrate well-known phenomena in tunneling: convergence, tunnel squeezing, and rotation of the cross section.*

The parts that present the author's own scientific results are highlighted in the margins between the
 « symbols » and «, as shown here.

Chapter II

Overview of the applied irreversible thermodynamical methodologies

Thermodynamics is usually defined as the discipline that deals with the different forms of energy (*e.g.*, thermal, mechanical, ...) and how these forms of energy can be converted to each other.

Similarly to mechanics, thermodynamics is also such an area of phenomena that can be experienced easily in our every day life. Then it is not a surprise that it was already a known fact by the ancient Alexandrians that air expands under the influence of heat. The great Italian polymath Leonardo da Vinci constructed a simple steam-powered device in the 15th century and, based on Watt's steam engine, the first industrial revolution swept across Europe in the 18th and 19th centuries. At the end of the 19th century, internal combustion engines appeared, then in the 20th century gas turbines, jet engines, refrigerators and power plants became the part of everyday life, the development of which is ongoing in the present, too [58].

During the 18th and 19th centuries, the theoretical foundations of thermodynamics were also laid down. Usually, it is called equilibrium thermodynamics, since investigations focus on an unchanged, equilibrium state, which is independent of time. The denomination classical thermodynamics is also frequently used. The subjects of thermodynamical investigation are the states and state changes—otherwise the processes—of the so-called thermodynamical system. The question may arise how processes can be treated when the investigations are independent of time. The basic concept of most branches of physics—*e.g.*, classical mechanics, electrodynamics or quantum mechanics—is the process, which is the solution of a temporal differential equation. Nevertheless, in classical thermodynamics, time as an independent variable never appears. From a mathematical point of view, equilibrium is a special process, namely, a process that does not change in time. Based on these, classical thermodynamics can be called more appropriately thermostatics. Nevertheless, classical thermodynamics is more than mere statics; by analogy with mechanics, if the process is known, then works and heats can be calculated, thus it can be concluded that classical thermodynamics describes the *statics and kinematics* of thermal processes.

The most important principles of classical thermodynamics are the first and second laws. The first law provides and ensures the experimental observation of conservation of *total energy*, however, the other conservation laws—such as conservation of mass, linear and angular momenta—are treated mostly indirectly. Since thermal and mechanical processes usually take place simultaneously, thus description of macroscopic behavior of systems also requires these principles. *Entropy*—as a basic concept of thermodynamics and of the second law—can be interpreted in several ways, *e.g.*, as a statistical measure of "disorder", or as a potential, which ensures that the thermodynamical state space is free of vortices. Apart from these interpretations, entropy is a useful theoretical—but unmeasurable—thermodynamical quantity, which favors the description of *irreversible* and *dissipative* processes through the second law. Understanding the second law—ergo, the direction of *processes*—in a time-independent—ergo in a

¹The origin of the term thermodynamics are the Greek words therme (heat) and dynamis (power). However, in this dissertation, dynamics is used as a mathematical concept, namely, the description of time dependency.

process-free—treatment is quite difficult, hence, the second law was formulated in various ways in the 19th century, which formulations were treated as equivalent for a long time. However, it has been proven that different, individual parts of the law are captured by these phrasings. Furthermore, the mathematically precise formulation of classical thermodynamics is missing², which caused that classical thermodynamics is infected by plenty of implicit agreements. These facts cause a lot of misunderstanding and complication.

From a more philosophical point of view, thermodynamics was always the stepchild of physics. In the 19th century, classical mechanics became the cornerstone of physics and a model for new theories. By this time, based on the experimental observations—such as Newton's law of motion, the principles of action–reaction and of superposition, *etc.* —most results of analytical mechanics had been obtained. Calculus of variations has to be emphasized, since for a long time physicists thought of it as the only universal method to derive dynamical equations. At the end of the 19th century, electrodynamics came into the focus of physics and, at the turn of the century, modern physics—relativity and quantum mechanics—was born. Since thermodynamics can not be understood in the classical mechanical way of thinking, and its equations can not or can just partly be derived by calculus of variations, it has drifted further and further from the construction system proposed by classical mechanics. The advent of statistical physics (founded by Boltzmann, Maxwell and Gibbs) and the belief that irreversible macroscopic phenomena can be explained via reversible microscopic mechanics has pushed thermodynamics further towards the periphery of physics.

It is already obvious from the former statements that thermodynamics holds interesting challenges from the point of view of both applications and theory. However, thermodynamics is much more than the physics of heat and its technical applications: thermodynamics can be classified as a framework of macroscopic physics. Since mechanics and electrodynamics deal with *possible but ideal* processes, irreversibility and dissipation are discussed by thermodynamics, thus thermodynamics describes *feasible* processes through the second law and entropy production.

Deeper understanding and mathematical formulations of process-oriented thermodynamics have been built in the 20th century, collectively called *irreversible thermodynamics*³. The birth of irreversible thermodynamics can be attributed to the publication of the famous articles by Onsager [60, 61] in 1931. The theory of Classical Irreversible Thermodynamics-which grew mainly out of Onsager's workexplained the experienced transport laws (such as Fourier heat conduction), however, the non-Fourier like heat conduction behavior, which was observed and widely studied at this time, was out of its scope. To explain this behavior (and much more), several different theories of irreversible thermodynamics have been born (see Chapter II for details). However, the emergence of these branches of irreversible thermodynamics have led not only to deeper understanding of physics of irreversible processes, but because of the above mentioned difficulties and ambiguous formulations, have led to the disintegration of the unified science of thermodynamics. Nowadays the endeavor to unification can be observed in irreversible thermodynamics. Several works compare different frameworks to each other (e.g., [62, 63]) and the Theme issue of The Royal Society Fundamental aspects of non-equilibrium thermodynamics communicates the articles from the most authentic scientists of several branches of irreversible thermodynamics. As written in the editorial [64], this issue tries to find and understand the connections between the different methodologies.

This section lays down the theoretical foundations of the methods applied in the dissertation. First, Classical Irreversible Thermodynamics is shortly revised, presenting the concepts and equations—which also form the basics for other branches of irreversible thermodynamics—, as well as the limitations of the theory. Then, the tools of Internal Variable Methodology and the GENERIC framework are described.

²The mathematical formulation of thermodynamics is given by Matolcsi in [59], however, this has not yet been built into the scientific consciousness.

³Frequently called *non-equilibrium thermodynamics*, too, however, this denomination also includes a statistical background, which is not necessary for the phenomenological description of irreversibilities and dissipations.

II.1 Classical irreversible thermodynamics

The two famous articles of the Nobel laureate Norwegian-born physical chemist and theoretical physicist Lars Onsager, published in 1931 and entitled *Reciprocal relations in irreversible processes* [60, 61] laid down the concept of irreversible thermodynamics and appointed the directions of future researches. These works built on microscopic and statistical observations. The first macroscopic consideration of irreversible thermodynamics is published in 1940 by Carl Eckart, in three parts entitled *The thermodynamics of irreversible processes* [65, 66, 67], which discuss the derivation of entropy production from the balance equations and the relationships between thermodynamic forces and fluxes for continua. The first part treats simple fluids, the second the mixtures of fluids, while the third one considers the relativistic theory of fluids. This series of articles is extended with a fourth part in 1948, which treats elastic and inelastic solids [68]. The main results and several applications based mostly on these mentioned six works is called *Classical Irreversible Thermodynamics*⁴ (CIT) and are summarized in several monographs like [69, 70, 71].

CIT is strongly based on classical (equilibrium) thermodynamics, however, it is formulated locally (at a given spatial point) and, in addition, time-dependence of state variables is also allowed and required. The localizability condition is given by the *hypothesis of local* or *cellular equilibrium*, which implicitly expresses that the Gibbs relation remains valid out of homogeneous and time-independent equilibrium. In other words, the same—equilibrium—state variables can be used to characterize both equilibrium states and the process. The aim of CIT is three-folded [72]:

- 1. Ensuring a unified background to derive the equations of classical transport processes, *e.g.*, mass transport by Fick diffusion, transport of linear momentum by Newton's and Stokes' viscosity laws, transport of internal energy—heat transport—by Fourier heat conduction and transport of electric charge by Ohm's law;
- 2. Discussing systematically the different cross-effects⁵; and
- 3. Investigating the stationary but non-homogeneous processes.

Let us restrict our treatment to non-polar continua with only one single component, thus mass diffusion processes are out of scope; furthermore, only mechanical and thermodynamical phenomena are investigated. CIT deals mostly with fluids and gases so, first, this is presented in a nutshell, then short remarks are given for the treatment of solids in the small-strain regime.

A thermodynamical body or system can be identified by the so-called state variables. State variables are a set of independent physical quantities, which obviously describe the behavior of the system. In the sense of classical thermodynamics, state variables are interpreted only in time-independent equilibrium state but, through the Gibbs relation (see later) this assumption can be weakened. The thermodynamical body can be uniquely described by *N* extensive state variables X_a , $a \in 1, ..., N$ and the Cartesian product of all X_a spans the thermodynamical state space. So-called *intensive state functions* Y_a , $a \in 1, ..., N$ belong to the extensive state variables, which depend on X_a s. Considering fluids and gases, the extensive state variables are the mass m, the volume V and the internal energy E, while the corresponding intensive state functions are the chemical potential μ , the pressure p and the temperature T, respectively.

Entropy is a key concept of thermodynamics. Here, following Matolcsi [59] and Ván [73], the most important properties of entropy are collected:

1. The thermodynamical body is entropic if a potential function S of the vector field spanned by the intensive thermodynamical functions Y_a , $a \in 1, ..., N$ exists; this property is expressed by the

⁴Several branches of irreversible thermodynamics emerged during the 20th century. In order to distinguish and highlight the foundation of all the subsequent theories, the name Classical Irreversible Thermodynamics was given by the successors.

⁵For example electric field strength caused by temperature difference and vice versa; diffusion caused by temperature difference and vice versa; diffusion caused by electric field strength and vice versa; that is, e.g. the Seebeck and Peltier effects; Soret and Dufour thermodiffusion; electrolysis and sedimentation.

well-known Gibbs relation in differential form as

$$dS(X_1, \dots, X_N) = \sum_{a=1}^N Y_a dX_a.$$
 (II.1)

It means that the intensive state functions are the partial derivatives of entropy, *i.e.*,

$$Y_a(X_1, \dots, X_N) = \left. \frac{\partial S}{\partial X_a} \right|_{X_b, \ a \neq b}, \qquad a \in 1, \dots, N.$$
(II.2)

For single-component fluids and gases, the Gibbs relation is

$$dS(E, V, m) = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{T}dm,$$
(II.3)

and correspondingly the intensive state functions are

$$\frac{1}{T}(E,V,m) = \left. \frac{\partial S}{\partial E} \right|_{V,m}, \quad \left. \frac{p}{T}(E,V,m) = \left. \frac{\partial S}{\partial V} \right|_{E,m}, \quad \left. -\frac{\mu}{T}(E,V,m) = \left. \frac{\partial S}{\partial m} \right|_{E,V}. \quad \text{(II.4)}$$

These relations are usually called state equations. More precisely, these are the equilibrium or reversible parts of the constitutive equations, which preserve entropy.

- 2. Entropy is an extensive thermodynamical state function, which is the key to localize the theory. More precisely:
 - (a) Entropy is an Euler homogeneous function of its variables, *i.e.*,

$$S(bX_1, \dots, bX_N) = bS(X_1, \dots, X_N), \qquad b \in \mathbb{R}^+.$$
(II.5)

(b) For any scalar extensive X_A, the X_A-specific entropy can be introduced, which is the function of the corresponding X_A-specific state variables x_a := X_a/X_A, a ∈ 1,..., N (x_A = X_A/X_A ≡ 1), e.g., the X₁-specific entropy s_{X₁} is defined via the relationship

$$S(X_1, \dots, X_N) = X_1 s_{X_1}(x_2, \dots, x_N).$$
 (II.6)

Usually, under the term of specific entropy the mass-specific entropy $s_m \equiv s = \frac{S}{m}$ is understood, which is the function of the (mass) specific internal energy $e = \frac{E}{m}$ and specific volume $v = \frac{V}{m}$. Furthermore, the volume specific entropy, usually called entropy density, $s_V \equiv \rho_S = \frac{S}{V}$ is also applied, which is the function of (mass) density $\rho_m \equiv \rho = \frac{m}{V}$ and of internal energy density $\rho_E = \frac{E}{V}$.

(c) The Euler relation for entropy reads

$$S(X_1, \dots, X_N) = \sum_{a=1}^{N} Y_a(X_1, \dots, X_N) X_a,$$
 (II.7)

which, for fluids and gases is

$$S(E, V, m) = \frac{1}{T}E + \frac{p}{T}V - \frac{\mu}{T}m$$
(II.8)

and, in the light of (II.6) and (II.7), this can be given as

$$S(E,V,m) = ms(e,v) = m\left(\frac{1}{T}e + \frac{p}{T}v - \frac{\mu}{T}\right),$$
(II.9)

where the expression in the bracket is mass-specific entropy. As a consequence of the previous statements, the Gibbs relation on the specific entropy can be derived. First, based on the specific quantities, equation (II.3) can be reformulated as

$$dS(E, V, m) = d[ms(e, v)] = \frac{1}{T}d(me) + \frac{p}{T}d(mv) - \frac{\mu}{T}dm,$$
 (II.10)

then the product rule for differentials implies

$$mds(e,v) + s(e,v)dm = \left(\frac{1}{T}e + \frac{p}{T}dv - \frac{\mu}{T}\right)dm + m\left(\frac{1}{T}de + \frac{p}{T}dv\right).$$
 (II.11)

The first bracket of the RHS of (II.11) is exactly the specific entropy defined in (II.9). Since $m \neq 0$ (if m = 0 then there is no material and the derivation is meaningless), the specific Gibbs relation is

$$ds(e,v) = \frac{1}{T}de + \frac{p}{T}dv.$$
 (II.12)

Equations (II.3) and (II.12) highlight that a distinction has to be made between the body and its material. While materials have only states, bodies also have an extent, which requires more variables to the description.

3. The X_1 -specific entropy is a concave function of its variables, *i.e.*,

$$\det\left\{\frac{\partial^2 s_{X_1}(x_2,\ldots,x_N)}{\partial x_a \partial x_b}\right\}_{a,b=2,\ldots M;\ M \le N} < 0.$$
(II.13)

This statement ensures the internal or material stability criteria. For fluids and gases, these criteria result in the inequalities

$$c_v := \left. \frac{\partial e}{\partial T} \right|_v > 0, \qquad \qquad \chi_T := -\frac{1}{v} \left. \frac{\partial v}{\partial p} \right|_T > 0, \qquad (\text{II.14})$$

where c_v is isochoric specific heat capacity and χ_T is isothermal compressibility.

Based on [59], the Gibbs relation does not describe dynamics but is just a relationship among the state variables, which remains valid from time instant to time instant during a whole process, hence,

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{1}{T}\frac{\mathrm{d}e}{\mathrm{d}t} + \frac{p}{T}\frac{\mathrm{d}v}{\mathrm{d}t},\tag{II.15}$$

where t is time, which parametrizes the process. Based on the previous statements, the thermodynamical potentials and the relationships among the material properties (like specific heat capacities, heat expansion coefficient, compressibility coefficient, ...) and state variables remain valid along the process.

Irreversible thermodynamics of continua requires the generalization of the concept of state variables, thus such quantities that are not observable in equilibrium (*e.g.*, linear and angular momenta and the corresponding linear and angular velocities), but also characterize the body or the material, have to be investigated, too.

A process of the system is the temporal change of the state variables, which is determined as the solution of the balance equations. The temporal change of a quantity at a fixed *material* point moving with velocity v is described via the operator combination

$$D_{\mathbf{v}} \bullet := \underbrace{\partial_t \bullet}_{\text{local}} + \underbrace{\left(\bullet \otimes \overleftarrow{\nabla} \right) \cdot \mathbf{v}}_{\text{convective}}, \tag{II.16}$$

which is called the comoving/substantial/material time derivative⁶. Its first term characterizes the *local*⁷ changes, while the second one the *convective*⁸ ones. Here and in what follows, ∂_t denotes the partial time derivative and, considering spatial derivatives and tensor operations, ∇ and ∇ are the nabla operators, which act on the quantity standing on their left and right side, respectively. Furthermore, \cdot denotes the full contraction of type $A_{abcde}B_{de}$, *e.g.*, for the arbitrary vectors **a**, **b** and arbitrary second-order tensors **A**, **B**, in index notation,

$$\mathbf{a} \cdot \mathbf{b} = a_i b_i,$$
 $(\mathbf{A} \cdot \mathbf{a})_i = A_{ij} a_j,$ $\mathbf{A} \cdot \mathbf{B} = A_{ij} B_{ij},$ (II.17)

here and later on the Einstein summation convention is applied. Furthermore, \otimes is the dyadic product, thus the right and left gradients and divergences of the arbitrary field f of arbitrary tensorial order are

$$\left(f \otimes \overleftarrow{\nabla}\right)_{abc...xyz} = \partial_z f_{abc...xy}, \qquad \left(\overrightarrow{\nabla} \otimes f\right)_{abc...xyz} = \partial_a f_{bc...xyz}, \qquad (II.18)$$

$$\left(f\cdot \stackrel{\leftarrow}{\nabla}\right)_{abc\ldots x} = \partial_y f_{abc\ldots xy}, \qquad \left(\stackrel{\rightarrow}{\nabla} \cdot f\right)_{bc\ldots xy} = \partial_a f_{abc\ldots xy}. \tag{II.19}$$

This acting direction of the nabla operator does not play a role for the gradient of a scalar and for the divergence of a vector, hence, in these cases, the notation ∇ will be used, *e.g.*, the gradient of the scalar field *T* is denoted by ∇T , while the divergence of the vector field **v** is $\nabla \cdot \mathbf{v}$.

Following Gyarmati [71], the following substantial balance equations can be derived for thermomechanical processes of non-polar⁹ continua:

1. Conservation of mass implies the continuity equation

$$\mathbf{D}_{\mathbf{v}}\varrho + \varrho\nabla \cdot \mathbf{v} = 0. \tag{II.20}$$

2. Cauchy's first equation of motion

$$\rho \mathbf{D}_{\mathbf{v}} \mathbf{v} = \boldsymbol{\sigma} \cdot \overleftarrow{\nabla} + \rho \mathbf{g} \tag{II.21}$$

ensures the conservation of linear momentum. Here σ denotes the Cauchy stress tensor—which is the negative of the often-applied pressure tensor P—and g is the external field strength.

3. The consequence of the conservation of angular momentum on non-polar continua is the symmetricity of the Cauchy stress tensor, *i.e.*,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}},\tag{II.22}$$

which is usually called *Cauchy's second equation of motion*. Here ^T denotes the transpose of a tensor; in index notation, $(\sigma^{T})_{jk} = \sigma_{kj}$. More precisely, (II.22) is merely a sufficient condition of conservation of angular momentum but not a necessary one—for details, see [74]. Hereafter, this condition will be assumed as a constraint on the balance equations.

4. Conservation of total energy implies the *balance of internal energy* or the *first law of thermodynamics*, which reads

$$\rho \mathbf{D}_{\mathbf{v}} e = -\nabla \cdot \mathbf{j}_E + \overset{*}{q}_V + \mathrm{tr} \Big[\boldsymbol{\sigma} \Big(\mathbf{v} \otimes \overleftarrow{\nabla} \Big) \Big], \qquad (\text{II.23})$$

⁶For an arbitrary field f of arbitrary tensorial order, the time derivative is $\frac{df(t, \mathbf{r}(t))}{dt} = \partial_t f + (f \otimes \overleftarrow{\nabla}) \cdot \frac{d\mathbf{r}}{dt}$, where \mathbf{r} denotes the spatial coordinate of an investigated material point and the kinematical relation is $\mathbf{v} = \frac{d\mathbf{r}}{dt}$. Consequently, $\frac{d}{dt} \equiv D_{\mathbf{v}}$. ⁷Temporal change at a fixed spatial point.

⁸Temporal change caused by the drift of the material from a spatial point to an other one.

⁹Most materials in the engineering praxis can be modeled as non-polar continua, *e.g.*, most of the metals, water or air. Examples for polar continua are liquid crystals.
where \mathbf{j}_E denotes the conductive current of internal energy—usually called heat current density or heat flux—and $\overset{*}{q}_V$ is the volumetric heat source density. The term $\operatorname{tr}\left[\boldsymbol{\sigma}\left(\mathbf{v}\otimes\overset{\leftarrow}{\nabla}\right)\right]$ is the mechanical power, for which $\operatorname{tr}\left[\boldsymbol{\sigma}\left(\mathbf{v}\otimes\overset{\leftarrow}{\nabla}\right)\right] = \operatorname{tr}\left[\boldsymbol{\sigma}\left(\mathbf{v}\otimes\overset{\leftarrow}{\nabla}\right)^{\mathrm{s}}\right]$ holds in the light of (II.22); here, tr denotes the trace operation, and $^{\mathrm{s}}$ is the symmetric part of a second-order tensor, *i.e.*, for an arbitrary second-order tensor \mathbf{A} is $\mathbf{A}^{\mathrm{s}} = \frac{1}{2}(\mathbf{A} + \mathbf{A}^{\mathrm{T}})$, in parallel, the antisymmetric part will be denoted by $^{\mathrm{A}}$, that is, $\mathbf{A}^{\mathrm{A}} = \frac{1}{2}(\mathbf{A} - \mathbf{A}^{\mathrm{T}})$.

The balance equations of conservative quantities are accompanied by the *balance of entropy*, which is

$$\rho \mathbf{D}_{\mathbf{v}} s = -\nabla \cdot \mathbf{j}_S + \pi_S \tag{II.24}$$

in substantial form, where \mathbf{j}_S is the entropy current density or entropy flux and π_S denotes the entropy production rate density, which measures the dissipation along a process, thus it is non-negative and it is zero for reversible non-dissipative processes. The concavity of entropy described by equation (II.13) ensures the *internal stability* of the material, while the non-negativity of π_S ensures the *stability of the interactions*, thus (II.24) together with (II.13) formulates the *second law of thermodynamics* in continuum physics.

The second law of thermodynamics has a crucial role: namely, thermodynamically consistent constitutive equations can be derived with the help of (II.24). The reversible—thus entropy preserving contribution of the constitutive equations are embedded in the entropy function [see (II.1)], while the irreversible or dissipative contribution—which increases entropy—can be derived via evaluating the entropy production rate density. For this, various mathematically systematic techniques are known in the literature (*e.g.*, the Coleman–Noll method [75] and the Liu procedure [76]), nevertheless, in what follows, a much simpler (though less general) method, the separation of divergences will be applied in the studied concrete examples.

From a mathematical point of view, the derived equations within the framework of CIT are parabolic partial differential equations, which enable processes with infinitely large speed of signal propagation, which is in contradiction with physical observations. In the first half of the 20th century, the investigation of a number of previously unknown phenomena became possible, such as the superconductivity of helium II [3, 4]. In parallel, a non-Fourier-like heat conduction behavior was experimentally justified in superfluid helium by Peshkov [5]. In the subsequent years, several experiments performed in supefluid helium [6, 7] and in sodium fluoride (NaF) crystals [10, 11, 12] confirmed such deviations from Fourier heat conduction, which can not be interpreted by the theory of CIT. Considering solids, the rheological/viscoelastic behavior can just partly be explained by CIT. The rapid development of technology has necessitated the description of fast and high-frequency processes, heterogeneous materials, and micro-and nanosystems. These phenomena are out of the scope of the local equilibrium hypothesis, therefore, they are out of the scope of CIT. This means that CIT has only a limited region of validity, which implied the birth of other theories, which can explain the above-mentioned phenomena as well.

II.1.1 Solids in the small-strain regime

This thesis considers solids in the small-strain approximation. It means that the strain ε is "small", *i.e.*, $|\varepsilon| \ll 1$, thus there is no need to distinguish material (Lagrangian) and spatial (Eulerian) variables and vectors/tensors, the mass density ρ can be treated as constant, the substantial and partial time derivatives can be identified, *i.e.*, $D_v \equiv \partial_t$, furthermore, the kinematic equation

$$\partial_t \boldsymbol{\varepsilon} = \left(\mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathrm{S}} \tag{II.25}$$

connects strain and velocity fields to each other.

Strain—since it measures the *change* of shape of a body—is not a state variable, nevertheless, in the continuum thermodynamics of solids, strain is treated as a state variable (which requires special initial conditions). Based on [77], the energetic representation¹⁰ of the Gibbs relation for solids is

$$de = Tds + \frac{1}{\varrho} \operatorname{tr}(\boldsymbol{\sigma} d\boldsymbol{\varepsilon}) \tag{II.26}$$

Second-order symmetric tensors can be given in the isotropic decomposition, e.g., for the strain as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{d} + \boldsymbol{\varepsilon}^{s}, \qquad \boldsymbol{\varepsilon}^{s} = \frac{1}{3} (\operatorname{tr} \boldsymbol{\varepsilon}) \mathbf{1}, \qquad \boldsymbol{\varepsilon}^{d} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{s}, \qquad (II.27)$$

with ^d and ^s denoting the deviatoric and spherical parts of the tensors, respectively, and 1 is the identity tensor. The deviatoric and spherical parts are isotropically independent $[tr(\mathbf{A}^{d}\mathbf{B}^{s}) = 0 \text{ for any } \mathbf{A}, \mathbf{B}]$ so (II.26) can be given as

$$de = Tds + \frac{1}{\varrho} \operatorname{tr}(\boldsymbol{\sigma}^{d} d\boldsymbol{\varepsilon}^{d}) + \frac{1}{\varrho} \operatorname{tr}(\boldsymbol{\sigma}^{s} d\boldsymbol{\varepsilon}^{s}), \qquad (II.28)$$

where the term $tr(\sigma^{d}\varepsilon^{d})$ is related to the energy density contribution of distortion.

Summarizing, thermomechanical processes of solids in the small-strain approximation are described by

- the kinematic equation (II.25),
- the balance of linear momentum (II.21) and internal energy (II.23),
- constitutive equations compatible with the Gibbs relation (II.26) and the balance of entropy (II.24), and
- initial and boundary conditions.

II.2 Internal Variable Methodology

The demand to generalize constitutive equations arose as early as in the 19th century, including but not limited to the work by James Clerk Maxwell, who introduced time-derivative terms into constitutive equations [78]. A similar technique appeared later in the works by Onsager and Machlup [79, 80], though only for homogeneous systems.

In the 1960s, more important works have been born, which promoted the development of such a theory, via which generalized constitutive equations can be derived.

Internal variables with thermodynamical constraints are introduced in [81] by Bernard D. Coleman and Morton E. Gurtin¹¹. Their derivation of constitutive equations applying internal variables allows not only functional relationships among the variables but temporal differential equations can also connect them, which describe memory effects, *e.g.*, in case of rheology. Although [81] was a strict mathematical achievement, it halted the development process of internal variable methodology for a long time because the applied framework derived *ordinary* differential equations on the internal variables, which meant only *homogeneous* and *temporal* extensions of the classical constitutive equations, while *non-local* effects—described by gradient terms—were not realized in this approach.

At the same time, Ingo Müller explained signal propagation with finite speed observed in thermodynamics by introducing a "non-equilibrial" specific entropy with inertial terms based on the structure of

¹⁰By the expressions energetic and entropic representation one means that internal energy is treated as a function of entropy and other state variables, and that entropy is treated as a function of internal energy and other state variables, respectively.

¹¹Although internal variables have been known for a long time, thermodynamic conditions have not been prescribed for them beforehand. Internal variables also appear in the works of Duhem, Mandelstam and Leontovich, and are also mentioned by the famous ten-part theoretical physics textbook by Landau and Lifshitz [73].

kinetic theory [82, 83, 84]. This work gave birth to *extended thermodynamics*. This kind of description is extended in the sense that current densities can also be state variables. Simultaneously with the birth of extended thermodynamics, Müller realized that the usual and accepted entropy current – heat current relationship can also be generalized, and he introduced an additional term in this relationship, which is called the K vector [84, 85].

Müller's works [82, 83, 84, 86, 85] can be considered as the forerunner of *Rational Extended Thermodynamics* (RET) [87, 88]. The approach of RET is based on principles inherited from kinetic theory and, because of the structure of kinetic theory, the newly introduced non-equilibrium state variables can only be the current densities of the extensive quantities.

In the same decade, the school of Hungarian thermodynamics led by István Gyarmati started operating. Gyarmati, the most prominent figure of Hungarian non-equilibrium thermodynamics, dealt with irreversible processes and the field theoretical approach of thermodynamics. He gained international glory with his thermodynamical variational principle named after him, which he developed based on Onsager's and Prigogine's results on dissipative systems, and on the Gauss principle of least constraint in classical mechanics. Gyarmati's principle seemed to be a general technique to derive the equations of non-ideal physics from so-called dissipation potentials, however, only the irreversible part of the evolution equations can be generated by the method. One of his faded, but more important, result is the so-called *Wave approach of thermodynamics* [89]. This work proposed to assume the thermodynamical currents as non-equilibrium state variables in specific entropy, with the benefit that generalized, beyond-Fourier, heat conduction equations can be obtained.

Gyarmati's wave approach motivated the birth of *Extended Irreversible Thermodynamics* (EIT) [90, 91, 92, 93]. In constrast to RET, EIT generalizes the Gibbs relation via quadratic terms of dissipative current densities independently of kinetic theory.

Extended theories can describe memory (*e.g.*, rheology), non-local (*e.g.*, in micro or nanomaterials) and nonlinear (*e.g.*, shock waves) effects as well. Furthermore, the obtained description is hyperbolic so finite signal propagation speed is ensured. These theories apply the current densities as additional non-equilibrium state variables. These variables have clear physical meaning and interpretation.

Internal variable methodology (IVM) ensures a more general framework of modeling, since the additional state variables are not necessarily connected to current densities and, in fact, nothing has to be assumed about the physical meaning of the internal variables, they only have to fulfil some physical principles. IVM has a long history (started with [81]) with strong Hungarian traditions.

József Verhás, Gyarmati's most famous pupil and colleague, investigated the applications of irreversible thermodynamics to fluids and solids. His monograph *Thermodynamics and rheology* [94] studies the relationship between thermodynamics and non-ideal mechanical behaviors—for solids, rheology and plasticity while, for fluids, Newtonian and non-Newtonian rheology—based on internal variables, which Verhás called *dynamical degrees of freedom*. Dynamical degrees of freedom in the sense of Verhás are non-equilibrium state variables, which vanish in equilibrium, however, in entropy production, a relevant contribution of dynamical degrees of freedom appear.

Balázs Nyíri, another member of Gyarmati's school, introduced the method of current multipliers [95], with which the thermodynamically derived constitutive equations can be further generalized. This technique has a long history. Müller's works [84, 85] together with the corresponding work by Verhás [96] pointed out that the usual entropy current – heat current relationship applied in rational mechanics is excessively restrictive, hence, entropy current should also be obtained as a constitutive quantity. To exploit this fact, Nyíri's method proved to be constructive: the entropy current – heat current relationship is generalized via unknown constitutive tensors, which are determined from the entropy production rate density. Assuming simultaneously the existence of internal variables and Nyíri multipliers, a more general level of thermodynamical modeling can be reached, which includes memory as well as non-local effects.

Further contributions and generalizations to the internal variable methodology are given in [97, 98, 99, 100, 101]; nevertheless, the present dissertation relies mostly on the works by Verhás and Nyíri.

Similarly to the methodology of CIT, in IVM, the balances of mass, linear momentum, angular

momentum and internal energy are used as constraints to evaluate the entropy production rate density from the balance of entropy, whose positive semi-definiteness is ensured via Onsagerian equations.

IVM assumes that the thermodynamical state space—which is spanned by N independent extensive state variables X_j , $j \in 1, ..., N$ (see in Section II.1), among which we fix $X_1 \equiv S$ because entropy S (and specific entropy s) plays an important role—is extended by one or more—so-called internal variables. In contrast to the methodology of EIT, they are not given any physical interpretation. Usually (see *e.g.*, in [94]), it is assumed that entropy is shifted by a concave expression of the internal variables; the simplest choice (supported by the Morse lemma) being a quadratic function. Let ξ_k , $k \in 1, ..., M$ denote M internal variables with arbitrary tensorial orders and characters; then the extended specific entropy can be given as

$$\tilde{s}\left(e, x_{j}, \xi_{k}\right) = s\left(e, x_{j}\right) - \sum_{k=1}^{M} \left(\frac{m_{k}}{2} \cdot \xi_{k}\right) \cdot \xi_{k},\tag{II.29}$$

where, in general, m_k , $k \in 1, ..., M$ are coefficient functions of appropriate tensorial orders, which, for simplicity, are treated as constants hereafter. More general quadratic extensions could also be applied but such extensions can result in nonlinear expressions so here we restrict ourselves to the simplest form provided by (II.29). Forming the total differential of (II.29) and applying the generalization of (II.12), we obtain the extended Gibbs relation in the entropic representation, *viz.*,

$$d\tilde{s} = ds - \sum_{k=1}^{M} (m_k \cdot \xi_k) \cdot d\xi_k = \frac{1}{T} de - \sum_{j=2}^{N} \frac{Y_j}{T} dx_j - \sum_{k=1}^{M} (m_k \cdot \xi_k) \cdot d\xi_k,$$
(II.30)

from which the energetic representation of this extended Gibbs relation is

$$de = Td\tilde{s} + \sum_{j=2}^{N} Y_j dx_j + \sum_{k=1}^{M} T\left(m_k \cdot \xi_k\right) \cdot d\xi_k.$$
(II.31)

This shows that introducing new variables in the entropy also generates new terms in the internal energy.

The entropy production rate density is calculated using this newly-defined extended entropy \tilde{s} , where the internal variables and their time derivatives also appear. Therefore, the generated constitutive relations also contain their time derivatives, and the methodology yields time evolution equations on the internal variables. Since one may have no physical interpretation for the internal variables, application of the generated equations may be problematic and, consequently, the internal variables are usually eliminated, yielding extended equations for the usual physical quantities. Furthermore, since nothing is assumed about the behavior of the internal variables (as in works like [101, 43, 102]), time-reversal parity properties of internal variables and internal variable related forces and fluxes are not known a priori. The knowledge of parity is necessary when employing the Onsager–Casimir reciprocal relations, see *e.g.*, [103], but if no thermodynamic coupling terms are present then that knowledge is not necessary.

Another opportunity in IVM is the assumption of a generalized heat current density – entropy current density relationship. This means that, instead of the usual relationship

$$\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E,\tag{II.32}$$

the expression

$$\mathbf{j}_{S} = \left(\frac{1}{T}\mathbf{1} + \mathbf{C}\right) \cdot \mathbf{j}_{E} + \sum_{k=1}^{M} \varepsilon_{k} \cdot \xi_{k}$$
(II.33)

is assumed, where C and c_k , $k \in 1, ..., M$ are constitutive tensors of second¹² and appropriate orders, respectively, and are often called Nyíri multipliers [95]. Substituting expression (II.33) into the balance of entropy, other, non-usual, terms are generated in the entropy production rate density.

¹²In Nyíri's original article [95], the form $\mathbf{j}_S = \mathbf{B}\mathbf{j}_E$ is used, however, the term $\frac{1}{T}\mathbf{1}$ always gets separated from the tensor **B** so the convention given in (II.33) proves simpler to use.

II.3 The GENERIC framework

In the middle of the 20th century, the American mathematician Clifford Truesdell started to reform classical continuum mechanics in the name of *Rational Mechanics*. The name suggests that mechanics was considered as a part of mathematics by the practitioners of this trend. The main aims were to simplify and unify the theory, and to implement rheology into the framework with a more accurate understanding of the basic principles. The second law was also investigated in detail, and thermodynamically compatible constitutive laws also are essential parts of the theory.

The demand to discuss the theory of mechanics and thermodynamics in a unified framework has already appeared in the Truesdellian school but the framework of rational mechanics proved to be too limited for this purpose. The same motivation gave birth to the GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) framework, which looks back on a larger past. The essence of the method is to find the dynamics as a sum of a reversible and an irreversible contribution. On one side, the reversible part is originated from mechanics, therefore, it is considered to be a Hamiltonian system while irreversibilities and dissipation are described by thermodynamics so they are connected to entropy and entropy production. The pioneering work by the Russian physicists Dzyaloshinkii and Volovick [104] derived dynamical equations in a similar way, *i.e.*, the reversible contribution is generated from a Hamiltonian, while dissipations are derived from a dissipation potential.

A more general treatment and the denomination *GENERIC* was born in [105, 106] by Miroslav Grmela and Hans Christian Öttinger. The framework was originally developed for the treatment of complex and rheological fluids, but it can be applied fruitfully for relativistic fluids, for dissipative processes of solids, for statistical considerations; furthermore, it allows to investigate multilevel description of processes (microscopic \rightarrow macroscopic transitions). The methodology of GENERIC and its several applications are summarized in [107, 103]. An additional strength of the framework is that it suggests novel numerical solution ideas [108, 56, 109].

In contrast to other branches of non-equilibrium thermodynamics, the GENERIC framework is highly motivated by geometric mechanics [105, 106, 107, 103]. The basic idea behind GENERIC is the separation of the reversible and irreversible contributions to dynamics. Collecting the state variables in the vector \mathbf{x} , time evolution is looked for in the sum of two state-space vector fields, *i.e.*,

$$\partial_t \mathbf{x} = \overset{\diamond}{\mathbf{x}}_{\text{rev}} + \overset{\diamond}{\mathbf{x}}_{\text{irr}},\tag{II.34}$$

where $\hat{\mathbf{x}}_{rev}$ and $\hat{\mathbf{x}}_{irr}$ denote the reversible and irreversible contributions to time evolution, respectively, which can be uniquely distinguished by means of the time-reversal transformation [110].

The object of geometric mechanics is the description of dynamics without dissipation, and Hamiltonian mechanics gives a canonical description. The first term on the right hand side of (II.34) provides the reversible part of the time evolution of state variables, and it is generated by a Poisson bracket and a Hamiltonian. The Hamiltonian plays the role of total energy, more closely, the volumetric integral of the sum of kinetic and internal energy densities, $\rho_{kin} = \frac{\rho}{2} \mathbf{v} \cdot \mathbf{v}$ and $\rho_E = \rho e$, respectively, *i.e.*,

$$E = \int_{V} \left(\varrho_{\rm kin} + \varrho_E \right) \mathrm{d}V. \tag{II.35}$$

Then, in the GENERIC framework,

$$\partial_t \mathbf{x}|_{\text{rev}} = \hat{\mathbf{x}}_{\text{rev}} \equiv \mathbf{L}(\mathbf{x}) \frac{\delta E}{\delta \mathbf{x}},$$
 (II.36)

where L is the reversible operator matrix or Poisson bivector (satisfying the Jacobi identity and thus generating the Poisson bracket), *i.e.*, $\mathbf{L} = -\mathbf{L}^{\mathrm{T}}$, with ^T denoting transposition, which, for operators, means not merely matrix index transposition but also includes operator adjoint, and $\frac{\delta}{\delta \mathbf{x}}$ denotes the functional derivative w.r.t. \mathbf{x} . More specifically, the time evolution of an arbitrary functional A on the state space restricted to reversible dynamics is

$$\left. \frac{\mathrm{d}A}{\mathrm{d}t} \right|_{\mathrm{rev}} = \int_{V} \left(\frac{\delta A}{\delta \mathbf{x}} \partial_{t} \mathbf{x} \right|_{\mathrm{rev}} \right) \mathrm{d}V = \int_{V} \left[\frac{\delta A}{\delta \mathbf{x}} \mathbf{L}(\mathbf{x}) \frac{\delta E}{\delta \mathbf{x}} \right] \mathrm{d}V, \tag{II.37}$$

and the RHS of (II.37) is interpreted as a Poisson bracket,

$$\{A, B\} := \int_{V} \left[\frac{\delta A}{\delta \mathbf{x}} \mathbf{L}(\mathbf{x}) \frac{\delta B}{\delta \mathbf{x}} \right] \mathrm{d}V, \tag{II.38}$$

where A and B are arbitrary functionals of the state variables [107].

The Poisson bracket satisfies the following criteria, where c_1 , c_2 are any real constants and A, B, C arbitrary functionals:

- antisymmetry, *i.e.*, $\{A, B\} = -\{B, A\}$; especially, $\{A, A\} = 0$;
- bilinearity, *i.e.*, $\{A, c_1B + c_2B\} = c_1\{A, B\} + c_2\{A, C\};$
- Leibniz rule, *i.e.*, $\{A, B \cdot C\} = \{A, B\} C + \{A, C\} B$;
- Jacobi identity, *i.e.*, $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$.

Thanks to the last property, invariance of the Poisson bracket under time evolution can be shown, see e.g. [103].

Irreversible evolution and dissipation are connected to the growth of entropy, which is the volume integral of entropy density ρ_S , *i.e.*,

$$S = \int_{V} \varrho_S \mathrm{d}V. \tag{II.39}$$

Inspired by Gyarmati [71] and following [111], the irreversible evolution is generated by a convex dissipation potential Ξ ,

$$\partial_t \mathbf{x}|_{\mathrm{irr}} = \overset{\diamond}{\mathbf{x}}_{\mathrm{irr}} \equiv \left. \frac{\delta \Xi}{\delta \mathbf{x}^*} \right|_{\mathbf{x}^* = \frac{\delta S}{\delta \mathbf{x}}}.$$
 (II.40)

Now, adding (II.36) and (II.40), we obtain the GENERIC time evolution of the state variables:

$$\partial_t \mathbf{x} = \mathbf{L}(\mathbf{x}) \frac{\delta E}{\delta \mathbf{x}} + \left. \frac{\delta \Xi}{\delta \mathbf{x}^*} \right|_{\mathbf{x}^* = \frac{\delta S}{\delta \mathbf{x}}}.$$
 (II.41)

By calculating the second functional derivative of a quadratic dissipation potential, one can introduce a symmetric and positive semi-definite operator called the irreversible or dissipative operator matrix,

$$\mathbf{M}(\mathbf{x}) := \frac{\delta^2 \Xi}{\delta(\mathbf{x}^*)^2}, \qquad \mathbf{M} = \mathbf{M}^{\mathrm{T}}, \qquad (II.42)$$

with which time evolution equation (II.41) can be reformulated in the GENERIC [107] form as

$$\partial_t \mathbf{x} = \mathbf{L}(\mathbf{x}) \frac{\delta E}{\delta \mathbf{x}} + \mathbf{M}(\mathbf{x}) \frac{\delta S}{\delta \mathbf{x}}.$$
 (II.43)

Thanks to the antisymmetry of L and to the imposed degeneracy requirement

$$\mathbf{M}\frac{\delta E}{\delta \mathbf{x}} = \mathbf{0},\tag{II.44}$$

energy is conserved, *i.e.*, $\frac{dE}{dt} = 0$. In parallel, the symmetry of M and the other required degeneracy condition

$$\mathbf{L}\frac{\delta S}{\delta \mathbf{x}} = \mathbf{0} \tag{II.45}$$

together ensure that the total entropy does not decrease. This is how the first and second laws of thermodynamics are embedded in the GENERIC framework.

Time evolution of an arbitrary functional A under irreversible dynamics is formulated, in the case of a quadratic dissipation potential, as

$$\frac{\mathrm{d}A}{\mathrm{d}t}\Big|_{\mathrm{irr}} = \int_{V} \left(\frac{\delta A}{\delta \mathbf{x}} \partial_{t} \mathbf{x}\Big|_{\mathrm{irr}}\right) \mathrm{d}V = \int_{V} \left[\frac{\delta A}{\delta \mathbf{x}} \mathbf{M}(\mathbf{x}) \frac{\delta S}{\delta \mathbf{x}}\right] \mathrm{d}V.$$
(II.46)

Analogously to the Poisson bracket, the RHS of (II.46) can be interpreted as a bilinear product of arbitrary functionals A and B

$$[A, B] := \int_{V} \left[\frac{\delta A}{\delta \mathbf{x}} \mathbf{M}(\mathbf{x}) \frac{\delta B}{\delta \mathbf{x}} \right] \mathrm{d}V, \tag{II.47}$$

which is symmetric and positive semi-definite—induced by symmetry and positive semi-definiteness of \mathbf{M} —, *i.e.*, [A, B] = [B, A] and $[A, A] \ge 0$, called the dissipative bracket. Time evolution of an arbitrary functional A can be then given in the bracket formulation as

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{A, E\} + [A, S]. \tag{II.48}$$

The famous work by Hendrik Brugt Gerhard Casimir entitled *On Onsager's principle of microscopic reversibility* [112] showed that antisymmetric phenomenological matrices can also appear in the force–flux relations, which leads to entropy preserving though irreversible processes. Along the lines of this work and based on dissipative brackets without a dissipation potential, the so-called quasilinear formulation of GENERIC is also generally accepted [107, 113]. This also allows such irreversible terms that do not dissipate and, accordingly, such an irreversible operator matrix can be given that is not necessarily symmetric, while it is necessarily positive semidefinite. This thesis applies both formulations: in Chapter III the dissipation potential based formulation is applied, while in Chapter IV the quasilinear one is utilized.

Since entropy is conserved by the reversible dynamics, *i.e.*, $\{S, E\} = 0$, and because of the symmetry and positive semi-definiteness of the dissipative bracket defined (II.47), time evolution of entropy is

$$\frac{\mathrm{d}S}{\mathrm{d}t} = [S,S] \ge 0,\tag{II.49}$$

which is the global balance of entropy, hence, [S, S] is the entropy production rate. In the case of a non-quadratic dissipation potential, the growth of entropy is obtained from the convexity of Ξ .

Chapter III

Heat conduction beyond Fourier's law

In engineering praxis, heat conduction is usually described via the Fourier law. A principal limitation of this model is that Fourier's heat conduction leads to a parabolic differential equation for temperature, where the signal propagation speed is infinite. Moreover, several experiments justify deviation from the Fourier-like behaviour, *e.g.*, low-temperature measurements of heat conduction in superfluid helium [5, 6, 7] and in NaF crystals [10, 11, 12], and room-temperature measurements on heterogeneous samples like rocks and layered structures [21, 22, 23].

According to heat pulse experiments performed at the Department of Energy Engineering of the Budapest University of Technology and Economics, the deviation from Fourier's law measured at room temperature can be explained via the Guyer–Krumhansl equation. This equation is derived by Guyer and Krumhansl via linearizing the Boltzmann equation [8, 9], thus microscopic and statistical considerations are in the background. In parallel, the Guyer–Krumhansl equation can also be derived by IVM; what's more, a generalized and systematic structure of heat conduction equations can also be obtained by this latter methodology. In the IVM approach, the background phenomena is not known, and only some physical principles have to be fulfilled.

In this chapter, first, a possible and *known* background phenomenon is investigated, which can cause the measured deviations from the Fourier law. Namely, when thermal expansion is considered then mechanical phenomena couple to heat conduction, which modifies the usual and well-known Fourier heat conduction equation. Via investigating the characteristic parameters of the thermal expansion-modified heat conduction equation one can determine that, in room-temperature heat pulse experiments, the measured deviations from Fourier's law are not caused by thermal expansion.

In the second part of this chapter, a theoretical case study is presented. IVM applies internal variables and an assumed entropy current density – heat current density relationship, in which the so-called entropy current multipliers appear. These multipliers are unknown constitutive functions, and nothing else is known about them. Applying the IVM and GENERIC methodologies simultaneously, an interpretation of entropy current multipliers can be given. Namely, entropy current multipliers can be interpreted as relaxed state variables. Along these lines, a comparison of IVM and GENERIC is also performed. These results may pave the way for microscopic/multiscale understanding of beyond-Fourier heat conduction, and can also lead to new numerical solution methods for these phenomena.

This chapter is based on the publications [23, 114]. The contributions by the author of this dissertation are as follows:

- Investigating the effect of thermal expansion on heat conduction in heat-pulse experiments;
- Identification of the entropy conjugate vectorial internal variable with the heat current density;
- GENERIC representation of ballistic-diffusive heat conduction;
- Interpretation of entropy current multipliers as extra state variables that have already relaxed to a quasi-stationary state.

III.1 Thermal expansion coupled to heat conduction

In general, there is no direct physical interpretation of a phenomenon that leads to, at the phenomenological level, non-Fourier heat conduction. Here, a case is investigated where the background phenomenon is known, namely, the effect of thermal expansion on heat conduction is analyzed. Without thermal expansion, elasticity—a tensorial behavior—is not coupled to Fourier heat conduction—a vectorial one in isotropic materials. However, with nonzero thermal expansion, mechanical and thermal processes are coupled. Based on the balance equations, the kinematic equation, Fourier heat conduction and the Duhamel–Neumann law of thermal expansion, a beyond-Fourier type equation for temperature can be derived. Analyzing this equation for some materials investigated in heat pulse experiments, a possible physical explanation of non-Fourier like behavior can be given. Nevertheless, as one will see in this section, the reason of the measured non-Fourier like behavior at room temperature is not thermal expansion.

III.1.1 The effect of thermal expansion on heat conduction

» Let us consider homogeneous and isotropic solids in the small-strain approximation, hence,

$$\partial_t \boldsymbol{\varepsilon} = \left(\mathbf{v} \otimes \boldsymbol{\nabla} \right)^{\mathbf{S}} \tag{III.1}$$

[(II.25) is repeated here for convenience]. The derivation presented here is restricted to linear elastic solids with linear thermal expansion, which is usually described by the Duhamel–Neumann law, *i.e.*,

$$\boldsymbol{\sigma}(T,\boldsymbol{\varepsilon}^{\mathrm{d}},\boldsymbol{\varepsilon}^{\mathrm{s}}) = E^{\mathrm{d}}\boldsymbol{\varepsilon}^{\mathrm{d}} + E^{\mathrm{s}}[\boldsymbol{\varepsilon}^{\mathrm{s}} - \alpha(T - T_{0})\mathbf{1}], \qquad (\mathrm{III.2})$$

where E^{d} and E^{s} are the deviatoric and spherical elasticity coefficients¹, respectively, and α is the linear thermal expansion coefficient. For simplicity—and as it is sufficient for the examinations done in this work—it is assumed that specific heat capacity along a constant-strain process—the generalization of isochoric specific heat capacity for solids—is constant, *i.e.*,

$$c_{\varepsilon}(T, \varepsilon) = c_{\varepsilon} = \text{const.}$$
 (III.3)

The internal energy and entropy functions being compatible with the Duhamel–Neumann law and this constant specific heat capacity are

$$e(T,\boldsymbol{\varepsilon}) = e_0 + c_{\boldsymbol{\varepsilon}}(T - T_0) + \frac{E^{\mathrm{d}}}{2\varrho} \operatorname{tr}(\boldsymbol{\varepsilon}^{\mathrm{d}}\boldsymbol{\varepsilon}^{\mathrm{d}}) + \frac{E^{\mathrm{s}}}{2\varrho} \operatorname{tr}(\boldsymbol{\varepsilon}^{\mathrm{s}}\boldsymbol{\varepsilon}^{\mathrm{s}}) + \frac{E^{\mathrm{s}}\alpha T_0}{\varrho} \operatorname{tr}\boldsymbol{\varepsilon}, \qquad (\text{III.4})$$

$$s(T, \boldsymbol{\varepsilon}) = s_0 + c_{\boldsymbol{\varepsilon}} \ln \frac{T}{T_0} + \frac{E^s \alpha}{\varrho} \operatorname{tr} \boldsymbol{\varepsilon}, \qquad (\text{III.5})$$

with the arbitrary constants e_0 , s_0 and T_0 .

The balance of internal energy (II.23) with (III.1) can be given as

$$\varrho \partial_t e = -\nabla \cdot \mathbf{j}_E + \operatorname{tr}(\boldsymbol{\sigma} \partial_t \boldsymbol{\varepsilon}). \tag{III.6}$$

Substituting (III.2), (III.4) and the classic Fourier law

$$\mathbf{j}_E = -\lambda \nabla T \tag{III.7}$$

(with λ denoting thermal conductivity) into (III.6), one obtains

$$\varrho c_{\varepsilon} \partial_t T = \nabla \cdot (\lambda \nabla T) - E^{\mathsf{s}} \alpha T \operatorname{tr}(\partial_t \varepsilon).$$
(III.8)

¹Customarily, the notations $E^{d} = 2G$ and $E^{s} = 3K$ are applied, where G and K are called shear and bulk moduli, respectively.

In heat pulse experiments, the temperature change in the sample is relatively small, therefore, the nonlinear term, *i.e.*, the second one on the lhs of (III.8), can be linearized and thermal conductivity can be treated as a constant, through which (III.8) reduces to

$$\rho c_{\varepsilon} \partial_t T = \lambda \Delta T - E^{\mathsf{s}} \alpha T_0 \operatorname{tr}(\partial_t \varepsilon), \qquad (\text{III.9})$$

where Δ is the Laplace operator. In light of (III.1), this can be rewritten as

$$E^{s}\alpha T_{0}\nabla \cdot \mathbf{v} = \lambda \Delta T - \varrho c_{\varepsilon} \partial_{t} T, \qquad (\text{III.10})$$

which, together with the balance of linear momentum (II.21) (with neglected volumetric force density),

$$\varrho \partial_t \mathbf{v} = \boldsymbol{\sigma} \cdot \overleftarrow{\nabla}, \tag{III.11}$$

forms a closed system of equations.

To obtain an equation that only contains temperature as unknown function, let us investigate the expression $E^{s} \alpha T_{0} \nabla \cdot \partial_{t}^{2} \mathbf{v}$, *i.e.*,

$$E^{s} \alpha T_{0} \nabla \cdot \partial_{t}^{2} \mathbf{v} \stackrel{(III.11)}{=} \frac{E^{s} \alpha T_{0}}{\varrho} \Big(\partial_{t} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \Big) \cdot \boldsymbol{\nabla} \\ \stackrel{(III.2)}{=} \frac{E^{s} \alpha T_{0}}{\varrho} \Big\{ \Big[E^{d} \partial_{t} \boldsymbol{\varepsilon}^{d} + E^{s} (\partial_{t} \boldsymbol{\varepsilon}^{s} - \alpha \partial_{t} T \mathbf{1}) \Big] \cdot \boldsymbol{\nabla} \Big\} \cdot \boldsymbol{\nabla} \\ = \frac{E^{s} \alpha T_{0}}{\varrho} \Big\{ \Big[E^{d} \partial_{t} \boldsymbol{\varepsilon} + (E^{s} - E^{d}) \partial_{t} \boldsymbol{\varepsilon}^{s} - E^{s} \alpha \partial_{t} T \mathbf{1} \Big] \cdot \boldsymbol{\nabla} \Big\} \cdot \boldsymbol{\nabla} \\ \stackrel{(III.1)}{=} \frac{E^{s} \alpha T_{0}}{\varrho} \Big\{ \Big[\frac{E^{d}}{2} \Big(\mathbf{v} \otimes \boldsymbol{\nabla} + \boldsymbol{\nabla} \otimes \mathbf{v} \Big) + \frac{E^{s} - E^{d}}{3} (\boldsymbol{\nabla} \cdot \mathbf{v}) \mathbf{1} - E^{s} \alpha \partial_{t} T \mathbf{1} \Big] \cdot \boldsymbol{\nabla} \Big\} \cdot \boldsymbol{\nabla} \\ = \frac{E^{s} \alpha T_{0}}{\varrho} \Big\{ \Big[\frac{2E^{d} + E^{s}}{3} \Delta (\boldsymbol{\nabla} \cdot \mathbf{v}) - E^{s} \alpha \Delta \partial_{t} T \Big] \\ = \frac{2E^{d} + E^{s}}{3\varrho} \Delta (E^{s} \alpha T_{0} \boldsymbol{\nabla} \cdot \mathbf{v}) - \frac{(E^{s} \alpha)^{2} T_{0}}{\varrho} \Delta \partial_{t} T \\ \stackrel{(III.10)}{=} \frac{2E^{d} + E^{s}}{3\varrho} \Delta (\lambda \Delta T - \varrho c_{\varepsilon} \partial_{t} T) - \frac{(E^{s} \alpha)^{2} T_{0}}{\varrho} \Delta \partial_{t} T.$$
(III.12)

In parallel, the second time derivative of (III.10) yields

$$E^{s} \alpha T_{0} \nabla \cdot \partial_{t}^{2} \mathbf{v} = \lambda \Delta \partial_{t}^{2} T - \varrho c_{\varepsilon} \partial_{t}^{3} T.$$
(III.13)

In (III.12), the coefficient $\frac{2E^d + E^s}{3\varrho}$ is actually the square of the longitudinal elastic wave propagation velocity so, hereafter, it will be denoted by c_{\parallel}^2 . From the equality of (III.12) and (III.13), a non-Fourier like heat conduction equation on temperature is obtained, *i.e.*,

$$\frac{1}{c_{\parallel}^2}\partial_t^2(\varrho c_{\varepsilon}\partial_t T - \lambda\Delta T) = \Delta \left[\left(\varrho c_{\varepsilon} + \frac{(E^s\alpha)^2 T_0}{\varrho c_{\parallel}^2} \right) \partial_t T - \lambda\Delta T \right],$$
(III.14)

in which a wave equation of the heat conduction equation can be recognized.

When thermal expansion is neglected, heat conduction in solids is described via the well-known equation

$$\rho c_{\sigma} \partial_t T = \lambda \Delta T, \tag{III.15}$$

where c_{σ} is the specific heat capacity along a constant-stress process—the generalization of isobaric specific heat capacity for solids. Since this c_{σ} heat capacity is measurable, c_{ε} can be calculated. Namely, the difference between these two specific heat capacities can be determined as

$$c_{\sigma} - c_{\varepsilon} = T \left(\frac{\partial s}{\partial T} \Big|_{\sigma} - \frac{\partial s}{\partial T} \Big|_{\varepsilon} \right).$$
(III.16)

By considering specific entropy as $s(T, \varepsilon(T, \sigma))$, the first partial derivative in (III.16) can be given as

$$\frac{\partial s}{\partial T}\Big|_{\sigma} = \frac{\partial s}{\partial T}\Big|_{\varepsilon} + \operatorname{tr}\left(\frac{\partial s}{\partial \varepsilon}\Big|_{T}\frac{\partial \varepsilon}{\partial T}\Big|_{\sigma}\right)$$
(III.17)

so one finds

$$c_{\sigma} - c_{\varepsilon} = T \operatorname{tr} \left(\frac{\partial s}{\partial \varepsilon} \Big|_{T} \frac{\partial \varepsilon}{\partial T} \Big|_{\sigma} \right).$$
(III.18)

Since the specific entropy of the Duhamel–Neumann material depends only on the spherical part of strain and the deviatoric part of stress (thus also the inverse relation, *i.e.*, the deviatoric part of strain) does not depend on temperature (see equations (III.2) and (III.5)), the above expression can explicitly be given as

$$c_{\sigma} - c_{\varepsilon} = T \operatorname{tr} \left(\frac{\partial s}{\partial \varepsilon^{s}} \bigg|_{T} \frac{\partial \varepsilon^{s}}{\partial T} \bigg|_{\sigma^{s}} \right).$$
(III.19)

Replacing $\boldsymbol{\varepsilon}^{\mathrm{s}} = \frac{1}{E^{\mathrm{s}}} \boldsymbol{\sigma}^{\mathrm{s}} + \alpha (T - T_0) \mathbf{1}$ and (III.5), the result is

$$c_{\sigma} - c_{\varepsilon} = 3 \frac{E^{s} \alpha^{2}}{\varrho} T.$$
 (III.20)

It is now obvious from (III.20) that, when thermal expansion is neglected (*i.e.*, $\alpha = 0$), then $c_{\sigma} = c_{\varepsilon}$. The messages of the above derivation are as follows:

- 1. When thermal expansion is considered then c_{ε} appears in the heat conduction equation instead of c_{σ} . In parallel, instead of the (usual) 'constant-stress' thermal diffusivity $a_{\sigma} = \frac{\lambda}{\varrho c_{\sigma}}$ (denoted usually by *a*), the 'constant-strain' thermal diffusivity $a_{\varepsilon} = \frac{\lambda}{\varrho c_{\varepsilon}}$ appears on the lhs of (III.14).
- 2. Thermal expansion modifies the 'constant-strain' thermal diffusivity $a_{\varepsilon} = \frac{\lambda}{\rho c_{\varepsilon}}$ to an 'effective' one $a_{\text{eff}} = \frac{\lambda}{\rho c_{\text{eff}}} = \frac{c_{\varepsilon}}{c_{\text{eff}}} a_{\varepsilon}$ [see the rhs of (III.14)], where $c_{\text{eff}} = c_{\varepsilon} + \frac{(E^{s}\alpha)^{2}T_{0}}{\rho^{2}c_{\parallel}^{2}}$ is an 'effective' specific heat capacity.
- 3. For a length scale ℓ and the corresponding 'effective' Fourier time scale $\tau_{\rm F} = \frac{\ell^2}{a_{\rm eff}}$, the rhs of (III.14) is, to a rough estimate, $\frac{1}{\ell^2}$ times a heat conduction equation, while the lhs is (similarly roughly) $\frac{1}{\tau_{\rm F}^2} \cdot \frac{1}{c_{\parallel}^2}$ times the (nearly) same heat conduction equation (a one with a_{ε}). In other words, the lhs of (III.14) provides a contribution to the rhs via a dimensionless factor $\frac{\ell^2}{\tau_{\rm F}^2} \cdot \frac{1}{c_{\parallel}^2} = \frac{a_{\rm eff}}{\ell^2 c_{\parallel}^2}$.

III.1.2 Parameter testing

Now, a parameter testing is performed to investigate the effect of thermal expansion in heat-pulse experiments. A typical size (relevant length scale) of the samples during the experiment is $\ell = 3$ mm. A typical ambient temperature is 293 K during the experiments. Five materials, which can be considered isotropic, are investigated.

Material	$\varrho/\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$	$E^{\rm d}/{\rm GPa}$	$E^{\rm s}/{\rm GPa}$	$\alpha / \left(10^{-6} \frac{1}{\mathrm{K}} \right)$	$c_{\boldsymbol{\sigma}}/\left(\frac{\mathrm{J}}{\mathrm{kgK}}\right)$	$\lambda / \left(\frac{W}{mK}\right)$
Steel	7800	161.54	525	12	473	46
Aluminum	2700	51.65	207.53	23.6	896	222
Copper	8900	81.18	379.31	17.6	385	386
PA6	1150	0.86	4.57	0.8	1700	0.27
Granite	2750	41.71	95	11.1	790	3.2

Table III.1: Measurable material coefficients of some materials.

From the measurable material coefficients given in Table III.1 via the previously given formulas, the characteristic dimensionless coefficients are shown in Table III.2.

Material	$c_{\parallel}/\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$	$c_{\epsilon}/(\frac{\mathrm{J}}{\mathrm{kgK}})$	$c_{\rm eff} / \left(\frac{J}{\rm kgK}\right)$	$\frac{a_{\rm eff}}{a_{\varepsilon}} = \frac{c_{\varepsilon}}{c_{\rm eff}}$	$\frac{a_{\mathrm{eff}}}{\tau_{\mathrm{F}}c_{\parallel}^{2}}$
Steel	6020.18	464.48	469.75	0.9888	$4.83 \cdot 10^{-13}$
Aluminum	6194.67	858.37	883.494	0.9716	$2.51 \cdot 10^{-11}$
Copper	4504.15	373.4	381.522	0.9787	$7.08 \cdot 10^{-11}$
PA6	1350.79	1700	1700	1	$1.16 \cdot 10^{-15}$
Granite	4650.38	786.26	788.25	0.9975	$1.12 \cdot 10^{-14}$

Table III.2: Calculated material coefficients and the characteristic dimensionless coefficients of some materials.

The 'effective' thermal diffusivity gets shifted by a few percent, relatively to 'constant-strain' thermal diffusivity, at room temperature. The dimensionless factor $\frac{a_{\text{eff}}}{\tau_{\text{F}}c_{\parallel}^2}$ is about 10^{-15} to 10^{-11} , consequently, the effect of the lhs appears to be negligible w.r.t. the rhs of (III.14) from an engineering point of view.

As a conclusion, thermal expansion coupled elasticity may introduce a few-percent effect in determining thermal diffusivity from flash experiments or other transient processes while its other consequences may be negligible. Therefore, the deviation from Fourier heat conduction measured in roomtemperature heat-pulse experiments cannot be explained by thermal expansion.

«

III.2 An interpretation of entropy current multipliers via GENERIC

The theory of CIT has a limited region of validity only and, accordingly, such heat conduction phenomena that are out of scope of the Fourier law cannot be explained within this framework.

Several models of other type have been born to explain beyond-Fourier behavior. Based on kinetic theory, the Maxwell–Cattaneo–Vernotte (MCV) equation [78, 115, 116] and the Guyer–Krumhansl (GK) equation [8, 9] can be derived. Furthermore, at the phenomenological side, extended theories of thermo-dynamics have their own methodology to obtain these equations. The approach of EIT proposes to use current densities as additional state variables beside specific internal energy [90, 91, 92, 93, 117, 118]. When this additional current density is the heat current density then the result is the MCV equation. In parallel, it is also possible to extend the entropy current density as well, by a term proportional to the gradient of heat current density. Using this modified entropy current density (and without modifying the specific entropy), one obtains Ginzburg–Landau (GL) type [119] heat conduction. Combining the previous extensions, the Guyer–Krumhansl (GK) equation [8, 9] can also be derived.

These extensions of specific entropy and its current density can be kept at a more general and systematic level, using internal variables and Nyíri multipliers. Assuming a vectorial internal variable with the usual entropy current density – heat current density relationship, one obtains the so-called Jeffreys' type heat conduction. Usually, the vectorial internal variable is identified with the heat current density, and then Jeffreys' heat conduction reduces to the MCV equation. However, this kind of identification is theoretically not entirely correct since, as it will be shown, it is the conjugate of internal variable that should be identified with the heat current density. This statement holds actually more generally, namely, identification of a vectorial internal variable with the heat current density is applicable only in the special case when there is linear constitutive relationship between the internal variable and its conjugate [117].

Introducing a second-order tensorial internal variable together with heat current density as an extended state space, entropy current density is generalized accordingly, and the construction yields a ballistic–diffusive model (BD) [119]. Actually, this model covers the previously mentioned ones as special cases, as well as many more beyond them. The approach of IVM has recently been compared to the framework of RET [63]—juxtaposing these non-equilibrium frameworks helps to find compatibility conditions and relations that make these approaches equivalent, and are helpful in evaluating experimental data [120]. The approach of RET is based on principles inherited from kinetic theory, hence, it offers a method to calculate some of the coefficients [87, 88]. However, the solution to the Boltzmann equation is often too difficult to determine and thus a Grad-like momentum series expansion is applied, which results in an infinite number of partial differential equations. For ballistic–diffusive heat conduction, *i.e.*, thermal wave propagation with the speed of sound, one has to consider at least 30 momentum equations to satisfactorily reproduce the value of the propagation speed [25, 121]. Despite these facts, it has highlighted what kind of coupling should be included in the modeling. An instructive comparison between the frameworks RET and GENERIC is presented in [62].

GENERIC formulation of heat conduction is given for instance in [117] and [122], however, in these works, the full system of generalized heat conduction equations given in [119] is not reproduced. The GENERIC implementation of all the models appearing in [119] is provided in this section. A GENERIC interpretation of the generalized heat conduction equations may serve two purposes. First, for viewing a phenomenological heat-conduction model as the outcome of some—possibly even multi-level—reduction procedure from microscopic to macroscopic, GENERIC is a suitable framework. Second, regarding numerical solutions to heat conduction problems, structure-preserving numerical methods provide high-quality solutions so the structure of GENERIC comes practical².

The main result of this section is to give a physical explanation of Nyíri's entropy current multipliers. The generalization of entropy current density has long been an active field of research, including but not limited to Müller's K vector [84, 85], and the works by Verhás [96] and Nyíri [95]. Nyíri's entropy current multipliers lead to heat conduction equations beyond Fourier's law, but a physical interpretation of the multiplier constitutive tensors themselves has been missing so far. Here, the simultaneous application of IVM and GENERIC leads us to the recognition that, in the theory of heat conduction, Nyíri multipliers can be understood as extra state variables of a higher tensorial order in a relaxed state. It will be shown that several generalized heat conduction equations that are deduced in IVM via generalizing the entropy current density can be derived in the GENERIC framework, as a reduction of a more detailed model. It means that the same models can be derived both via generalization and via reduction³.

III.2.1 Systematic generalization of heat conduction beyond the Fourier theory

Now let us focus on heat conduction phenomena. Let us restrict ourselves to rigid, homogeneous and isotropic heat conductors at rest w.r.t. a given reference frame so mass density ρ is constant, the velocity field v is zero and the material time derivative can be identified with the partial time derivative: $D_v = \partial_t$. Due to homogeneity, there is no explicit space dependence in the material parameters and, based on Curie's principle, there are no couplings between quantities with different tensorial orders and characters in isotropic materials [70].

In order to avoid technical complications and to direct the attention to the essential aspects, hereafter this work is presented in a one space dimensional treatment. Accordingly, as a warning for this, we will use the notation of partial space derivative ∂_r instead of the nabla operator ∇ . Nevertheless, in notation, quantities that have different tensorial orders in a three dimensional full treatment are distinguished, denoting scalars by italic letters (*e.g.*, *T*), vectors by boldface lowercase ones (*e.g.*, \mathbf{j}_E), second-order tensors by boldface uppercase letters (*e.g.*, **C**), and third-order tensors by blackboard bold lowercase letters (*e.g.*, w). By the same reason, the \cdot notation is kept displayed, which is informative whenever one is interested in the possible three space dimensional counterpart of a formula. In further respects, the three space dimensional treatment can be given via similar tools as utilized in [123].

 $^{^{2}}$ In parallel, some advantages of the internal-variable approach have been that it keeps balances more directly in the foreground, may be fruitfully connected to, *e.g.*, the structure of equations on momentum-type quantities of kinetic theory, and may suggest natural boundary conditions. Here, the intention is to work on unifying these advantages with that of a GENERIC approach.

³Note that GENERIC \rightarrow GENERIC reductions and GENERIC \rightarrow non-GENERIC reductions should be distinguished, as done in [111]. Nevertheless, for our present conclusions, this distinction does not play any role so, in short, we refer to both of them as reductions hereafter.

Also to keep the treatment simpler, let us assume that there are no volumetric heat sources. Then the balance of internal energy (II.23) can be given, with these restrictions, in the form

$$\varrho \partial_t e = -\partial_r \mathbf{j}_E. \tag{III.21}$$

As it is already mentioned, the balance of internal energy will be used as a constraint to evaluate the entropy production rate density π_S from the balance of entropy [(II.24) is repeated here for convenience]

$$\varrho \partial_t s = -\partial_r \mathbf{j}_S + \pi_S. \tag{III.22}$$

In what follows, we only rely on the balances of internal energy and entropy. Assuming different (concrete) expressions on the extended entropy (II.29) and on the heat current density – entropy current density relationship (II.33), different generalized heat conduction models can be derived.

In parallel, the GENERIC realizations of the same heat conduction models are presented. Due to its structure, GENERIC is suitable for multilevel description of processes [103, 124, 125]. If one assumes in the heat conduction theory that the characteristic time of the state variable of the highest tensorial order is the smallest, then fast changes of this variable are quickly damped and the variable becomes a function of the remaining variables. This kind of reduction technique leads, as is proposed below, to a compatible derivation of heat conduction equations within the GENERIC framework. Furthermore, when GENERIC is viewed as a microscopically motivated framework, the physical interpretation of the state variables determines the time-reversal parities as even–odd–even–odd *etc*. with increasing tensorial orders, which can be connected to the velocity moments in the BBGKY⁴ or Grad hierarchies [126, 127].

This section is partitioned by the number of independent state variables assumed in the thermodynamic potentials internal energy and entropy. Based on the number of dimensions of the thermodynamic state space, we can speak about different levels of description, the more variables resulting the more detailed description. Both IVM and GENERIC generate the same number of time evolution equations as the dimensions of the state spaces are equal. Since IVM treats spatial differential equations naturally, non-local extensions can be generated easily at the same level of description, which, in some cases, is a challenge within GENERIC. In other words, some models that are difficult to be directly formulated within GENERIC can be seen as a reduction of more detailed GENERIC models.

III.2.1.1 One-dimensional state space

Let us first assume that the state space is spanned only by energy density, which can be written in the state vector form⁵ \mathbf{x}_1^S as the one-component state vector

$$\mathbf{x}_1^S := (e) \,. \tag{III.23}$$

Then the Gibbs relation is simply

$$\mathrm{d}s = \frac{1}{T}\mathrm{d}e.\tag{III.24}$$

III.2.1.1.1 Fourier heat conduction Time evolution of entropy is, consequently (the equations employed are displayed above the equality signs),

$$\varrho\partial_t s \stackrel{(III.24)}{=} \frac{\varrho}{T} \partial_t e \stackrel{(III.21)}{=} -\frac{1}{T} \partial_r \mathbf{j}_E = -\partial_r \left(\frac{1}{T} \mathbf{j}_E\right) + \mathbf{j}_E \cdot \partial_r \frac{1}{T}, \tag{III.25}$$

⁴A common abbreviation for the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy in statistical physics.

⁵The subscript displays the dimension of the state space, and the superscript shows the representation, here, entropic representation. The importance of distinguishing representations will be apparent later.

where a term in the form of divergence of a vector field is separated. Comparing (III.25) to (III.22), the usual entropy current density $\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E$ and the entropy production rate density

$$\pi_S = \mathbf{j}_E \cdot \partial_r \frac{1}{T} \ge 0, \tag{III.26}$$

can be recognised. Positive semi-definiteness of entropy production is ensured via the linear Onsagerian equation

$$\mathbf{j}_E = l\partial_r \frac{1}{T},\tag{III.27}$$

where, due to the isotropy, l is a non-negative scalar function depending on the only state variable e. Assuming that the function $\frac{1}{T}(e)$ —the constitutive function of temperature—is invertible, then l(e(T)) = l(T). In what follows, to focus on the main aim, all the appearing coefficients will be treated as constants. Then Fourier heat conduction leads to

$$\varrho \partial_t e = -l \partial_r^2 \frac{1}{T}.$$
 (III.28)

Here, we mention that, for measurements and calculations, thermal conductivity λ is defined as $\lambda(T) = \frac{l(T)}{T^2}$, and then (III.27) is

$$\mathbf{j}_E = l\partial_r \frac{1}{T} = -\frac{l}{T^2} \partial_r T = -\lambda \partial_r T, \qquad (III.29)$$

which is the classic form of Fourier's law.

Now let us switch to the GENERIC formulation of the Fourier heat conduction. In general, the reversible contribution of the evolution equations is simpler in the energetic representation, while the irreversible contribution is simpler in the entropic representation. Fourier heat conduction describes a purely dissipative process, therefore, in the GENERIC formulation (II.41), no Hamiltonian structure is expected to appear, and, indeed, an 1×1 matrix operator is antisymmetric if and only if its only element is zero. Since volumetric densities fit better to GENERIC than mass-specific quantities, we introduce the state vector $\boldsymbol{\xi}_1^S$ in the form

$$\boldsymbol{\xi}_1^S := \left(\varrho_E\right),\tag{III.30}$$

where $\rho_E = \rho e$ is the internal volumetric energy density.⁶ The dissipative part—in this case, the whole equation—can be generated from a convex dissipation potential. A convenient way is to formulate the dissipation potential in the entropy conjugated state variable

$$\boldsymbol{\xi}_1^{S^*} = \frac{\delta S}{\delta \boldsymbol{\xi}_1^S}.\tag{III.31}$$

Entropy can be written as

$$S = \int_{V} \varrho_{S} \left(\boldsymbol{\xi}_{1}^{S} \right) \mathrm{d}V \tag{III.32}$$

with entropy density ρ_S , and, assuming that no non-local terms appear in this functional, the entropy conjugated state variable is found to be

$$\boldsymbol{\xi}_{1}^{S^{*}} = \frac{\delta S}{\delta \boldsymbol{\xi}_{1}^{S}} = \left(\frac{1}{T}\right) \tag{III.33}$$

⁶In the present case with 'muted' mechanics and the corresponding constant ρ , the transformation from specific quantities to densities is trivial. In more general cases, it is more complicated.

[cf. (III.24)]. For the simple linear cases like ours, convexity can be guaranteed by a quadratic expression, which we choose to be the volume integral of half of the entropy production rate density. Namely, integrating (along the one space dimensional region L w.r.t. the spatial coordinate r) (III.26), with the substitution (III.27), the dissipation potential is

$$\Xi_{\rm F}\left(\boldsymbol{\xi}_{1}^{S^{*}}\right) = \int_{L} \frac{l}{2} \left(\partial_{r} \frac{1}{T}\right)^{2} \mathrm{d}r,\tag{III.34}$$

from which the time evolution of internal energy density is

$$\partial_t \varrho_E = \left. \frac{\delta \Xi_F}{\delta \boldsymbol{\xi}_1^{S^*}} \right|_{\boldsymbol{\xi}_1^{S^*} = \frac{\delta S}{\delta \boldsymbol{\xi}_1^S}} = -l \partial_r \partial_r \frac{1}{T} = -l \partial_r^2 \frac{1}{T}$$
(III.35)

[via applying (II.40) together with (III.33) and (III.34), as well as by performing the functional derivation]. Rewriting (III.35) as

$$\partial_t \varrho_E = -\partial_r \left(l \partial_r \frac{1}{T} \right) \tag{III.36}$$

and comparing with (III.21), the constitutive equation of heat current density, $\mathbf{j}_E = l\partial_r \frac{1}{T}$, can be read off. Note however, that the relation between heat current density and the gradient of temperature is a consequence of the choice of the dissipation potential made here.

Entropy density is a function of the energy density and thus its evolution reads

$$\partial_t \varrho_S = \frac{\mathrm{d}\varrho_S}{\mathrm{d}\varrho_E} \partial_t \varrho_E = -\frac{1}{T} l \partial_r^2 \frac{1}{T},\tag{III.37}$$

which is equivalent to

$$\partial_t \varrho_S = -\partial_r \left(\frac{l}{T} \partial_r \frac{1}{T}\right) + l \left(\partial_r \frac{1}{T}\right)^2 \ge 0, \tag{III.38}$$

where the former term on the right hand side is interpreted as the divergence of the entropy current density and the latter as entropy production. The relation between entropy current density and heat current density is the same as in the preceding approach, and it is again a consequence of the choice of the dissipation potential. Comparing the equations derived in the two formulations, one finds a complete match. Nevertheless, the directions of the two derivations are opposite.

III.2.1.1.2 Ginzburg–Landau type heat conduction Next, let us assume that, instead of the usual relationship for entropy current density, $\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E$, the generalized

$$\mathbf{j}_S = \left(\frac{1}{T}\mathbf{1} + \mathbf{C}\right) \cdot \mathbf{j}_E \tag{III.39}$$

relation is valid [a special case of (II.33)], where C is a second order constitutive tensor. Then, entropy production rate density is

$$\pi_S = \varrho \partial_t s + \partial_r \mathbf{j}_S = \partial_r \left(\frac{1}{T} \mathbf{1} + \mathbf{C} \right) \cdot \mathbf{j}_E + \mathbf{C} : \partial_r \mathbf{j}_E \ge 0.$$
(III.40)

In a whole three space dimensional treatment, the first term here would describe a vector–vector coupling and the second term a tensor–tensor one; consequently, using Curie's principle, positive semidefiniteness of the entropy production rate density could be ensured by the Onsagerian equations

$$\mathbf{j}_E = l_1 \partial_r \left(\frac{1}{T} + \mathbf{C} \right), \tag{III.41a}$$

$$\mathbf{C} = l_2 \partial_r \mathbf{j}_E \tag{III.41b}$$

with non-negative constants l_1 and l_2 . To reflect this, in the one space dimensional version, we also stick to this structure in (III.41a)–(III.41b).

Now let us insert (III.41b) into (III.41a). Then we obtain a generalized—non-Fourier type constitutive relationship for heat current density—the Ginzburg–Landau-type relationship—, which reads

$$\mathbf{j}_E = l_1 \partial_r \frac{1}{T} + l_1 l_2 \partial_r^2 \mathbf{j}_E.$$
(III.42)

Substituting equations (III.41a) and (III.41b) into (III.40), one obtains

$$\pi_S = l_1 \left[\partial_r \left(\frac{1}{T} + l_2 \partial_r \mathbf{j}_E \right) \right]^2 + l_2 \left(\partial_r \mathbf{j}_E \right)^2.$$
(III.43)

From this entropy production rate density, it seems rather nontrivial to construct a dissipation potential. In other words, assuming a one space dimensional state space, this model seems very difficult to be embedded in the GENERIC formulation. More closely, rewriting equation (III.42) in the form

$$\left(1 - l_1 l_2 \partial_r^2\right) \mathbf{j}_E = l_1 \partial_r \frac{1}{T} \tag{III.44}$$

and acting on (III.21) by the operator $(1 - l_1 l_2 \partial_r^2)$, one obtains

$$\varrho\partial_t e - \varrho l_1 l_2 \partial_t \partial_r^2 e = -l_1 \partial_r^2 \frac{1}{T},$$
(III.45)

which is difficult to formulate within GENERIC because dissipative coefficients appear on both sides of the equation. On the other hand, it will be shown that, via model reduction, the Ginzburg–Landau type heat conduction can also be incorporated in the GENERIC framework.

III.2.1.2 Two-dimensional state space

Stepping forward, now let us assume that, besides the usual state variable e, a further specific extensive vectorial state variable—denoted by y—is required to span the state space, *i.e.*,

$$\mathbf{x}_2^S := \begin{pmatrix} e \\ \mathbf{y} \end{pmatrix},\tag{III.46}$$

for which the energetic and entropic representations of the Gibbs relation are

$$de = Tds + \mathbf{z} \cdot d\mathbf{y}, \tag{III.47a}$$

$$\mathrm{d}s = \frac{1}{T}\mathrm{d}e - \frac{\mathbf{z}}{T} \cdot \mathrm{d}\mathbf{y},\tag{III.47b}$$

where the energy conjugated intensive function z and the entropy conjugated intensive function $-\frac{z}{T}$ are defined by the partial derivatives $\frac{\partial e}{\partial y}\Big|_{s}$ and $\frac{\partial s}{\partial y}\Big|_{e}$, respectively. One can think of y as an internal variable in the IVM sense, with the difference that, usually, IVM does not introduce and utilize the corresponding conjugate variable but works solely in terms of the internal variable, shifting entropy by a concave—in the simplest cases a quadratic—function of the internal variable. For instance, formula (8) of [128] presents the relationship

$$s(e, \mathbf{y}) = s_0(e) - \frac{\hat{m}}{2}\mathbf{y} \cdot \mathbf{y}$$
(III.48)

with $\frac{\partial s}{\partial e}\Big|_{\mathbf{y}} = \frac{\mathrm{d}s_0}{\mathrm{d}e} = \frac{1}{T}$ and a non-negative \hat{m} —a constant for simplicity. By deducing the differential of (III.48) and comparing it with (III.47b), one can read off the constitutive relationship between \mathbf{y} and \mathbf{z} in this simplest case:

$$\frac{\mathbf{z}}{T} = \hat{m}\mathbf{y}.$$
 (III.49)

Later, we will show that, without such a constitutive relationship, one cannot eliminate the internal variable(s) from the resulting system of equations.

III.2.1.2.1 Jeffreys-type heat conduction Assuming the two-component state vector (III.46) and the usual entropy current density $\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E$, one obtains for entropy production rate density

$$\pi_{S} = \varrho \partial_{t} s + \partial_{r} \mathbf{j}_{S} \stackrel{(III.47b)}{=} \frac{1}{T} \varrho \partial_{t} e - \frac{\mathbf{z}}{T} \varrho \partial_{t} \mathbf{y} + \frac{1}{T} \partial_{r} \mathbf{j}_{E} + \mathbf{j}_{E} \partial_{r} \frac{1}{T} \stackrel{(III.21)}{=} - \frac{\mathbf{z}}{T} \varrho \partial_{t} \mathbf{y} + \mathbf{j}_{E} \partial_{r} \frac{1}{T} \ge 0,$$
(III.50)

the positive semi-definiteness of which is ensured by the linear Onsagerian equations

$$\mathbf{j}_E = l_{11}\partial_r \frac{1}{T} + l_{12} \left(-\frac{\mathbf{z}}{T}\right), \qquad (\text{III.51a})$$

$$\varrho \partial_t \mathbf{y} = l_{21} \partial_r \frac{1}{T} + l_{22} \left(-\frac{\mathbf{z}}{T} \right), \qquad \text{(III.51b)}$$

with the requirements

$$l_{11} \ge 0, \qquad l_{22} \ge 0, \qquad l_{11}l_{22} - l_{12}l_{21} \ge 0$$
 (III.52)

on the coefficients l_{ij} . Equations (III.51a) and (III.51b) can be rewritten in the forms

$$\mathbf{j}_E = l_{12}^{\mathrm{A}} \left(-\frac{\mathbf{z}}{T} \right) + l_{11} \partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \left(-\frac{\mathbf{z}}{T} \right), \qquad (\text{III.53})$$

$$\varrho \partial_t \mathbf{y} = -l_{12}^{\mathrm{A}} \partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \partial_r \frac{1}{T} + l_{22} \left(-\frac{\mathbf{z}}{T} \right), \qquad (\text{III.54})$$

respectively, where the terms with the coefficients $l_{12}^{A} := (l_{12} - l_{21})/2$ do not increase the entropy and only the terms with the coefficients l_{11} , l_{22} and $l_{12}^{S} := (l_{12} + l_{21})/2$ do so. This can be seen from the conveniently rewritten entropy production rate density:

$$\pi_S = l_{11} \left(\partial_r \frac{1}{T} \right)^2 + 2l_{12}^{\rm S} \left(\partial_r \frac{1}{T} \right) \left(-\frac{\mathbf{z}}{T} \right) + l_{22} \left(-\frac{\mathbf{z}}{T} \right)^2. \tag{III.55}$$

In order to eliminate the internal variable y and its conjugate z, we have to assume a constitutive relationship among these quantities. Let this relation be (III.49). Substituting it into (III.51a) and (III.51b), one obtains

$$\mathbf{j}_E = l_{11}\partial_r \frac{1}{T} + l_{12} \left(-\hat{m}\mathbf{y}\right), \qquad \text{(III.56a)}$$

$$\varrho \partial_t \mathbf{y} = l_{21} \partial_r \frac{1}{T} + l_{22} \left(-\hat{m} \mathbf{y} \right), \qquad \text{(III.56b)}$$

the latter being rewritable as

$$\left(\varrho\partial_t + l_{22}\hat{m}\right)\mathbf{y} = l_{21}\partial_r \frac{1}{T}.$$
(III.57)

Letting the operator $(\varrho \partial_t + l_{22} \hat{m})$ [observed on the lhs of (III.57)] act on (III.56a), one finds a thermodynamic version of the Jeffreys-type equation (originally proposed by Sir Harold Jeffreys in [129] regarding viscoelastic fluids—for heat conduction, the model has been introduced by Joseph and Preziosi [130, 131]),

$$\tau \partial_t \mathbf{j}_E + \mathbf{j}_E = \lambda_1 \partial_r \frac{1}{T} + \lambda_2 \partial_t \partial_r \frac{1}{T}$$
(III.58)

with the coefficients $\tau := \frac{\varrho}{l_{22}\hat{m}}$, $\lambda_1 := \frac{\det l_{ij}}{l_{22}}$ and $\lambda_2 := \frac{\varrho l_{11}}{l_{22}\hat{m}} = l_{11}\tau$. Let us now give the GENERIC representation of this model. To obtain the reversible contribution of

Let us now give the GENERIC representation of this model. To obtain the reversible contribution of the time evolution, we use the energetic representation with the variables

$$\boldsymbol{\xi}_{2}^{E} = \begin{pmatrix} \varrho_{S} \\ \boldsymbol{\varrho}_{y} \end{pmatrix}, \qquad (\text{III.59})$$

where ρ_y is the density of the internal variable y, *i.e.*, $\rho_y = \rho y$. Since all mechanical interactions are neglected, total energy is equal to internal energy, *i.e.*,

$$E = \int_{V} \varrho_E \left(\boldsymbol{\xi}_2^E \right) \, \mathrm{d}V. \tag{III.60}$$

Supposing that there are no non-local terms in the energy, its functional derivative w.r.t. to the state vector $\boldsymbol{\xi}_2^E$ is

$$\frac{\delta E}{\delta \boldsymbol{\xi}_2^E} = \begin{pmatrix} T \\ \mathbf{z} \end{pmatrix} \tag{III.61}$$

[cf. the energetic representation of the Gibbs-relation (III.47a)]. Assuming a Hamiltonian structure, the time evolution of the state variables under the reversible dynamics can be expressed as

$$\begin{pmatrix} \partial_t \varrho_S |_{\text{rev}} \\ \partial_t \boldsymbol{\varrho}_{\mathbf{y}} |_{\text{rev}} \end{pmatrix} = \begin{pmatrix} 0 & -\partial_r \\ -\partial_r & 0 \end{pmatrix} \begin{pmatrix} T \\ \mathbf{z} \end{pmatrix}, \quad (\text{III.62})$$

where the reversible operator matrix (or Poisson bivector) $\begin{pmatrix} 0 & -\partial_r \\ -\partial_r & 0 \end{pmatrix}$ is an antisymmetric operator (one can for instance construct the Poisson bracket to verify that) and it is state independent so it automatically satisfies the Jacobi identity as well. The reversible evolution of the internal energy density is, accordingly,

$$\partial_t \varrho_E|_{\rm rev} = \left. \frac{\partial \varrho_E}{\partial \varrho_S} \right|_{\boldsymbol{\varrho}_{\mathbf{y}}} \partial_t \varrho_S|_{\rm rev} + \left. \frac{\partial \varrho_E}{\partial \boldsymbol{\varrho}_{\mathbf{y}}} \right|_{\varrho_S} \partial_t \boldsymbol{\varrho}_{\mathbf{y}}|_{\rm rev} = -T \partial_r \mathbf{z} - \mathbf{z} \partial_r T = -\partial_r \left(T \mathbf{z} \right), \tag{III.63}$$

hence, total energy (space integral of this total divergence) is conserved.

Such a Hamiltonian structure can be obtained by reduction of the Hamilton canonical equations for the cotangent bundle for fields [132]. Therefore, since entropy is even (not changing sign) with respect to the time-reversal transformation (TRT), the other field z is odd. The Onsager–Casimir reciprocal relations then tell that the coupling between those variables occurs via an operator antisymmetric with respect to the simultaneous adjoint and time-reversal, see e.g. [103]. Since that operator is constant (consisting only of gradients) here, it has to be antisymmetric, which is in agreement with the structure of the operator employed here. Hamiltonian mechanics is compatible with the Onsager–Casimir reciprocal relations, and z is an odd quantity with respect to TRT.

To formulate the irreversible contribution to the time evolution, we switch to the entropic representation with the state vector

$$\boldsymbol{\xi}_{2}^{S} = \begin{pmatrix} \varrho_{E} \\ \boldsymbol{\varrho}_{\mathbf{y}} \end{pmatrix}. \tag{III.64}$$

Then entropy is

$$S = \int_{V} \varrho_{S} \left(\boldsymbol{\xi}_{2}^{S} \right) \mathrm{d}V \tag{III.65}$$

and the entropy conjugate state variables are

$$\boldsymbol{\xi}_{2}^{S^{*}} = \frac{\delta S}{\delta \boldsymbol{\xi}_{2}^{S}} = \begin{pmatrix} \frac{1}{T} \\ -\frac{\mathbf{z}}{T} \end{pmatrix}.$$
 (III.66)

Entropy production rate density (III.55) is given in just these variables, thus the dissipation potential

$$\Xi_{\rm J}\left(\boldsymbol{\xi}_{2}^{S^*}\right) = \int_{L} \left\{ \frac{l_{11}}{2} \left(\partial_{r} \frac{1}{T} \right)^{2} + \frac{l_{12}^{\rm S}}{2} \left[\left(\partial_{r} \frac{1}{T} \right) \left(-\frac{\mathbf{z}}{T} \right) - \frac{1}{T} \partial_{r} \left(-\frac{\mathbf{z}}{T} \right) \right] + \frac{l_{22}}{2} \left(-\frac{\mathbf{z}}{T} \right)^{2} \right\} \mathrm{d}r \quad (\text{III.67})$$

can be introduced. Correspondingly, the evolution of $\boldsymbol{\xi}_2^{S^*}$ restricted to the irreversible dynamics is

$$\partial_t \boldsymbol{\xi}_2^{S^*} \Big|_{\mathrm{irr}} = \begin{pmatrix} \partial_t \varrho_E \big|_{\mathrm{irr}} \\ \partial_t \boldsymbol{\varrho}_{\mathbf{y}} \big|_{\mathrm{irr}} \end{pmatrix} = \frac{\delta \Xi_{\mathrm{J}}}{\delta \boldsymbol{\xi}_2^{S^*}} \Big|_{\boldsymbol{\xi}_2^{S^*} = \frac{\delta S}{\delta \boldsymbol{\xi}_2^{S}}} = \begin{pmatrix} -l_{11} \partial_r^2 \frac{1}{T} - l_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{z}}{T}\right) \\ l_{12}^{\mathrm{S}} \partial_r \frac{1}{T} + l_{22} \left(-\frac{\mathbf{z}}{T}\right) \end{pmatrix}.$$
(III.68)

Here, one can see coupling between $\frac{1}{T}$, which is even with respect to TRT, and -z/T, which is odd. The Onsager–Casimir reciprocal relations then tell that the coupling is provided by an operator antisymmetric w.r.t. the simultaneous transposition (adjoint) and TRT. Therefore, the coefficients $l_{12}^{\rm S}$ must be odd with respect to TRT. In particular, they cannot be constant but must depend on an odd quantity, here, ρ_y or z. In other words, the dissipation potential has to be even w.r.t. TRT, which requires that the coefficients $l_{12}^{\rm S}$ be odd.

Calculating the irreversible contribution to time evolution of entropy density yields

$$\partial_{t}\varrho_{S}|_{irr} = \frac{\partial\varrho_{S}}{\partial\varrho_{E}}\Big|_{\boldsymbol{\varrho}_{\mathbf{y}}} \partial_{t}\varrho_{E}|_{irr} + \frac{\partial\varrho_{S}}{\partial\boldsymbol{\varrho}_{\mathbf{y}}}\Big|_{\boldsymbol{\varrho}_{E}} \partial_{t}\boldsymbol{\varrho}_{\mathbf{y}}|_{irr} = -\partial_{r}\left\{\frac{1}{T}\left[l_{11}\partial_{r}\frac{1}{T} + l_{12}^{S}\left(-\frac{\mathbf{z}}{T}\right)\right]\right\} + l_{11}\left(\partial_{r}\frac{1}{T}\right)^{2} + 2l_{12}^{S}\left(\partial_{r}\frac{1}{T}\right)\left(-\frac{\mathbf{z}}{T}\right) + l_{22}\left(-\frac{\mathbf{z}}{T}\right)^{2}.$$
 (III.69)

The final time evolution equations are the sum of the reversible and irreversible contributions,

$$\partial_t \varrho_E = -\partial_r \left[T \mathbf{z} + l_{11} \partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \left(-\frac{\mathbf{z}}{T} \right) \right], \qquad (\text{III.70a})$$

$$\partial_t \varrho_S = -\partial_r \left\{ \mathbf{z} + \frac{1}{T} \left[l_{11} \partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \left(-\frac{\mathbf{z}}{T} \right) \right] \right\} + l_{11} \left(\partial_r \frac{1}{T} \right)^2 + 2l_{12}^{\mathrm{S}} \left(\partial_r \frac{1}{T} \right) \left(-\frac{\mathbf{z}}{T} \right) + l_{22} \left(-\frac{\mathbf{z}}{T} \right)^2,$$
(III.70b)

$$\partial_t \boldsymbol{\varrho}_{\mathbf{y}} = -\partial_r T + l_{12}^{\mathrm{S}} \partial_r \frac{1}{T} + l_{22} \left(-\frac{\mathbf{z}}{T} \right). \tag{III.70c}$$

Note, however, that only two of them are independent while the equation for entropy or energy can be seen as an implication of the remaining two equations. One can also see that the part of the right hand side of these equations that transforms under TRT as the left hand side comes from the Hamiltonian (reversible) dynamics while the part that flips sign under TRT w.r.t. the left hand side stems from the dissipation potentials.

Comparing (III.70a) with (III.21) and (III.70b) with (III.22), the heat and entropy current densities

$$\mathbf{j}_E = T\mathbf{z} + l_{11}\partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \left(-\frac{\mathbf{z}}{T}\right), \qquad \mathbf{j}_S = \mathbf{z} + \frac{1}{T} \left[l_{11}\partial_r \frac{1}{T} + l_{12}^{\mathrm{S}} \left(-\frac{\mathbf{z}}{T}\right) \right] \qquad (\text{III.71})$$

can be recognized, and the relationship

$$\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E \tag{III.72}$$

is valid between them. The first expression of (III.71) is equal to (III.53) in the approximation $\frac{l_{12}^{A}}{T^{2}} \approx -1$, then (III.70c), and then (III.56a) are also equivalent, thus a full match is found between the equations generated by the two methodologies.

III.2.1.2.2 Maxwell–Cattaneo–Vernotte heat conduction The Maxwell–Cattaneo–Vernotte equation is usually derived in the way that, in addition to specific internal energy, heat current density is also assumed as a state variable, and specific entropy is usually assumed in the form

$$\tilde{s}(e, \mathbf{j}_E) = s(e) - \frac{m}{2\varrho} \mathbf{j}_E \cdot \mathbf{j}_E$$
(III.73)

with $\frac{\partial \tilde{s}}{\partial e}\Big|_{\mathbf{j}_E} = \frac{1}{T}$ and the positive constant m. (Here, the presence of ρ is to show that we respect that \mathbf{j}_E is a specific extensive quantity.) Constructing the differential of this expression, one obtains

$$\mathrm{d}\tilde{s} = \frac{1}{T}\mathrm{d}e - \frac{m}{\varrho}\mathbf{j}_E \cdot \mathrm{d}\mathbf{j}_E, \qquad (\mathrm{III.74a})$$

and its rearranged form

$$de = Td\tilde{s} + \frac{m}{\varrho}T\mathbf{j}_E \cdot d\mathbf{j}_E, \qquad (\text{III.74b})$$

which tells us that specific internal energy depends on (extended) entropy and heat current density both. When thinking of e and \mathbf{j}_E as the temporal and spatial parts of a single internal energy spacetime quantity, it appears highly inconsistent that the temporal part of a spacetime quantity depends on the spatial part of the same spacetime quantity.

Consequently, instead of this assumption, let us get back to equations (III.53) and let us identify heat current density with the entropy conjugated internal variable as

$$\mathbf{j}_E = l_{12}^{\mathrm{A}} \left(-\frac{\mathbf{z}}{T} \right), \tag{III.75}$$

which means that $l_{11} = 0$ and $l_{12}^{S} = 0$. Then (III.54) reduces to

$$\varrho \partial_t \mathbf{y} = -l_{12}^{\mathbf{A}} \partial_r \frac{1}{T} + \frac{l_{22}}{l_{12}^{\mathbf{A}}} \mathbf{j}_E, \qquad (\text{III.76})$$

and, substituting the constitutive equation (III.49), one obtains

$$-\frac{\varrho}{\hat{m}l_{12}^{\mathrm{A}}}\partial_t \mathbf{j}_E = -l_{12}^{\mathrm{A}}\partial_r \frac{1}{T} + \frac{l_{22}}{l_{12}^{\mathrm{A}}} \mathbf{j}_E.$$
 (III.77)

Introducing the coefficients $l := l_{22} = l_{12}^A$ and $\tau := \frac{\varrho}{\hat{m}l}$, one can recognize the well-known Maxwell–Cattaneo–Vernotte equation

$$\tau \partial_t \mathbf{j}_E + \mathbf{j}_E = l \partial_r \frac{1}{T}.$$
 (III.78)

Let us make here two remarks. Firstly, to obtain the MCV equation, the usual entropy current density relationship $\mathbf{j}_S = \frac{1}{T}\mathbf{j}_E$ has been assumed. Secondly, the heat current density has been identified with the entropy conjugate internal variable (apart from a constant multiplier), but not with the internal variable itself. When a simple linear relationship (III.49) is assumed between the internal variable and its conjugate then the identification between the heat current density and the internal variable also holds. More generally, however, the situation is more complicated. When deriving heat conduction models in GENERIC, the step of identification is a key ingredient, see *e.g.*, in [117] and [122].

For the GENERIC treatment of MCV model, let us refer on [122]. Due to microscopic considerations, the vectorial variable is connected to the momentum of phonons and, correspondingly, the density of the internal variable ρ_y is identified with the conjugate of entropy current density⁷ w. The reversible time evolution of the variables

$$\tilde{\boldsymbol{\xi}}_{2}^{E} = \begin{pmatrix} \varrho_{S} \\ \mathbf{w} \end{pmatrix}$$
(III.79)

⁷As far as the reversible part is concerned, **w** is typically conjugate to the entropy current density. However, if the dissipation potential contains some non-local terms, entropy current density picks up additional terms—we will show this, for example, in Sec. (III.2.1.2.4). Therefore, calling **w** the conjugate entropy current density is completely correct when we speak about the reversible evolution but, more precisely, conjugate **w** is a part of the entropy current density. Furthermore, **w** can be identified with the momentum density of phonons divided by the entropy density so it could also be called specific phonon momentum [103].

is given as

$$\begin{pmatrix} \partial_t \varrho_S|_{\rm rev} \\ \partial_t \mathbf{w}|_{\rm rev} \end{pmatrix} = \begin{pmatrix} 0 & -\partial_r \\ -\partial_r & 0 \end{pmatrix} \begin{pmatrix} T \\ \mathbf{j} \end{pmatrix}.$$
 (III.80)

The irreversible contribution to time evolution is derived in the variables of the entropic representation

$$\tilde{\boldsymbol{\xi}}_{2}^{S} = \begin{pmatrix} \varrho_{E} \\ \mathbf{w} \end{pmatrix}. \tag{III.81}$$

Dissipation potential is assumed in the entropy conjugated variables

$$\tilde{\boldsymbol{\xi}}_{2}^{S^{*}} = \frac{\delta S}{\delta \boldsymbol{\xi}_{2}^{S}} = \begin{pmatrix} \frac{1}{T} \\ -\frac{\mathbf{j}}{T} \end{pmatrix}$$
(III.82)

with the form

$$\Xi_{\rm MCV}\left(\tilde{\boldsymbol{\xi}}_{2}^{S^*}\right) = \int_{L} \frac{k}{2} \left(-\frac{\mathbf{j}}{T}\right)^2 \mathrm{d}r,\tag{III.83}$$

where k is a non-negative constant. The generated gradient dynamics of $ilde{m{\xi}}_2^{S^*}$ is then

$$\partial_t \tilde{\boldsymbol{\xi}}_2^S \Big|_{\rm irr} = \begin{pmatrix} \partial_t \varrho_E |_{\rm irr} \\ \partial_t \mathbf{w} |_{\rm irr} \end{pmatrix} = \frac{\delta \Xi_{\rm MCV}}{\delta \tilde{\boldsymbol{\xi}}_2^{S*}} \Big|_{\tilde{\boldsymbol{\xi}}_2^{S*} = \frac{\delta S}{\delta \tilde{\boldsymbol{\xi}}_2^S}} = \begin{pmatrix} 0 \\ k \left(-\frac{\mathbf{j}}{T} \right) \end{pmatrix}, \quad (III.84)$$

from which the irreversible contribution to the time evolution of entropy density is

$$\partial_t \varrho_S|_{\rm irr} = k \left(-\frac{\mathbf{j}}{T}\right)^2.$$
 (III.85)

Finally, the system of time evolution equations is

$$\partial_t \varrho_S = -\partial_r \mathbf{j} + k \left(-\frac{\mathbf{j}}{T}\right)^2,$$
 (III.86a)

$$\partial_t \mathbf{w} = -\partial_r T + k \left(-\frac{\mathbf{j}}{T} \right);$$
 (III.86b)

comparing (III.86a) with (III.22) the entropy current density $\mathbf{j}_S = \mathbf{j}$ can be identified. Time evolution of internal energy density is then

$$\partial_t \varrho_E = \partial_t \varrho_E|_{\text{rev}} + \partial_t \varrho_E|_{\text{irr}} = -\partial_r \left(T\mathbf{j}\right) + 0 = -\partial_r \left(T\mathbf{j}\right), \qquad \text{(III.87)}$$

and, comparing this with (III.21), the heat current density – entropy current density relationship

$$\mathbf{j}_E = T\mathbf{j}_S \qquad \Longleftrightarrow \qquad \mathbf{j}_S = \frac{1}{T}\mathbf{j}_E$$
 (III.88)

can be read off. Assuming a linear relationship between j and w, in the linear approximation the equivalence of (III.86b) can (III.78) be recognized.

III.2.1.2.3 Model reduction: Fourier heat conduction Now let us suppose that the equilibration time of w is much shorter than that of s. In this approximation, (III.86b) reduces to

$$0 = -\partial_r T + k \left(-\frac{\mathbf{j}}{T}\right),\tag{III.89}$$

which can be treated as a constitutive equation among \mathbf{j} and T, moreover, it is (also in the linear approximation) equal to Fourier's law.

III.2.1.2.4 Guyer–Krumhansl heat conduction In the framework of IVM, the GK equation is derived with the assumptions of an extended specific entropy in the form of (III.73) and of a generalized entropy current density as defined in (III.39). With these, the entropy production rate density is

$$\pi_S = \mathbf{j}_E \cdot \left(-m\partial_t \mathbf{j}_E + \partial_r \frac{1}{T} + \partial_r \mathbf{C} \right) + \mathbf{C} \cdot \partial_r \mathbf{j}_E.$$
(III.90)

The linear equations

$$\mathbf{j}_E = l_1 \left(-m\partial_t \mathbf{j}_E + \partial_r \frac{1}{T} + \partial_r \mathbf{C} \right), \qquad (\text{III.91})$$

$$\mathbf{C} = l_2 \partial_r \mathbf{j}_E \tag{III.92}$$

with non-negative constants l_1 and l_2 ensure the positive semi-definiteness of the entropy production rate density (III.90). Inserting (III.92) into (III.91), one obtains the Guyer–Krumhansl equation

$$\tau \partial_t \mathbf{j}_E + \mathbf{j}_E = l_1 \partial_r \frac{1}{T} + \kappa^2 \partial_r^2 \mathbf{j}_E$$
(III.93)

with the coefficients $\tau := l_1 m$ and $\kappa^2 := l_1 l_2$.

As for GENERIC, since the GK equation can be considered as a nonlocal extension of the MCV model, the reversible dynamics needs no modification, but it is only the dissipation potential defined in (III.83) that has to be extended by a non-local term, *viz.*,

$$\Xi_{\rm GK}\left(\tilde{\boldsymbol{\xi}}_{2}^{S^*}\right) = \Xi_{\rm MCV}\left(\tilde{\boldsymbol{\xi}}_{2}^{S^*}\right) + \int_{L} \frac{k_2}{2} \left[\partial_r \left(-\frac{\mathbf{j}}{T}\right)\right]^2 \mathrm{d}r = \int_{L} \left\{\frac{k_1}{2} \left(-\frac{\mathbf{j}}{T}\right)^2 + \frac{k_2}{2} \left[\partial_r \left(-\frac{\mathbf{j}}{T}\right)\right]^2\right\} \mathrm{d}r,\tag{III.94}$$

where k_1 and k_2 are non-negative constants. Consequently, the GENERIC representation of GK heat conduction is

$$\partial_t \varrho_E = -\partial_r \left(T \mathbf{j} \right), \tag{III.95}$$

$$\partial_t \varrho_S = -\partial_r \left[\mathbf{j} + k_2 \left(-\frac{\mathbf{j}}{T} \right) \partial_r \left(-\frac{\mathbf{j}}{T} \right) \right] + k_1 \left(-\frac{\mathbf{j}}{T} \right)^2 + k_2 \left[\partial_r \left(-\frac{\mathbf{j}}{T} \right) \right]^2, \quad (\text{III.96})$$

$$\partial_t \mathbf{w} = -\partial_r T + k_1 \left(-\frac{\mathbf{j}}{T} \right) - k_2 \partial_r^2 \left(-\frac{\mathbf{j}}{T} \right).$$
(III.97)

Now one can recognize the heat and entropy current densities as

$$\mathbf{j}_E = T\mathbf{j}$$
 and $\mathbf{j}_S = \mathbf{j} + k_2 \left(-\frac{\mathbf{j}}{T}\right) \partial_r \left(-\frac{\mathbf{j}}{T}\right)$. (III.98)

In an appropriate approximation, and utilizing what we had in and below (III.88) for w, j, and j_E , (III.97) proves equivalent to (III.93) (see more on it in [122]) and, in this approximation, the entropy current density – heat current density relationship

$$\mathbf{j}_{S} = \frac{1}{T}\mathbf{j}_{E} + k_{2}\left(-\frac{\mathbf{j}_{E}}{T^{2}}\right)\partial_{r}\left(-\frac{\mathbf{j}_{E}}{T^{2}}\right) \approx \left(\frac{1}{T} + \tilde{k}_{2}\partial_{r}\mathbf{j}_{E}\right) \cdot \mathbf{j}_{E}$$
(III.99)

can be read off, which proves equivalent to (III.39) via substituting (III.92).

III.2.1.2.5 Model reduction: the Ginzburg–Landau equation When fast evolution of w is relaxed, equation (III.97) reduces to

$$0 = -\partial_r T + k_1 \left(-\frac{\mathbf{j}}{T}\right) - k_2 \partial_r^2 \left(-\frac{\mathbf{j}}{T}\right), \qquad (\text{III.100})$$

in which the structure of the Ginzburg-Landau type equation (III.42) can be recognized.

III.2.1.2.6 Summary As a conclusion, one finds the equivalence of Jeffreys, MCV and GK time evolution equations and the corresponding entropy current density – heat current density relationships. It is shown that GL-type heat conduction (which seems to be incompatible with GENERIC) can be obtained in the framework by reducing GK time evolution. It is obvious that non-local terms in the dissipation potential give additional contributions to the entropy current density. In what follows, the state space will be extended with an additional tensorial state variable and, accordingly, the BD heat conduction equation will be derived within IVM and GENERIC, and we show that higher order tensorial terms in the entropy current density – heat current density relationship or in the dissipation potential lead to such equations that can be seen as a reduced model of the dynamics in a higher dimensional state space.

III.2.1.3 Three-dimensional state space

For describing heat conduction phenomena beyond the MCV and GK models, a further state variable is also required (which is a second-order tensor when treated in three space dimensions). In this case, the thermodynamical state space is spanned by the variables

$$\mathbf{x}_3^S := \begin{pmatrix} e \\ \mathbf{j}_E \\ \mathbf{Q} \end{pmatrix}, \tag{III.101}$$

where \mathbf{Q} is the additional internal variable and, furthermore, let us refer to Section III.2.1.2.2, where heat current density is understood as a state variable after the identification (III.75), and a linear relationship among the internal variable and its conjugate holds.

III.2.1.3.1 Ballistic–diffusive heat conduction Let us assume that specific entropy (III.73) is shifted by a concave expression of the new internal variable Q as well:

$$\tilde{\tilde{s}}(e, \mathbf{j}_E, \mathbf{Q}) = s(e) - \frac{m_1}{2\varrho} \mathbf{j}_E \cdot \mathbf{j}_E - \frac{m_2}{2\varrho} \mathbf{Q} \cdot \mathbf{Q}, \qquad \text{(III.102)}$$

where m_1 and m_2 are non-negative constants (for simplicity—in general, these can again be functions depending on the state variables) and that a generalized entropy current density relationship (III.39) holds. Then entropy production rate density is

$$\pi_{S} = \mathbf{j}_{E} \cdot \left(-m_{1}\partial_{t}\mathbf{j}_{E} + \partial_{r}\frac{1}{T} + \partial_{r}\mathbf{C} \right) - m_{2}\mathbf{Q} \cdot \partial_{t}\mathbf{Q} + \mathbf{C} \cdot \partial_{r}\mathbf{j}_{E}.$$
(III.103)

Here, the first term a vector-vector coupling while the second and third terms are tensor-tensor couplings (in a three space dimensional sense). Therefore, in the spirit of Curie's principle, the linear Onsagerian equations

$$-m_1\partial_t \mathbf{j}_E + \partial_r \frac{1}{T} + \partial_r \mathbf{C} = l \mathbf{j}_E, \qquad (\text{III.104a})$$

$$-m_2\partial_t \mathbf{Q} = l_{11}\mathbf{Q} + l_{12}\partial_r \mathbf{j}_E, \qquad \text{(III.104b)}$$

$$\mathbf{C} = l_{21}\mathbf{Q} + l_{22}\partial_r \mathbf{j}_E \tag{III.104c}$$

are taken to ensure positive-semidefiniteness of (III.103) with the coefficients fulfilling the requirements

$$l \ge 0,$$
 $l_{11} \ge 0,$ $l_{22} \ge 0,$ $l_{11}l_{22} - l_{12}l_{21} \ge 0.$ (III.105)

Similarly to (III.53) and (III.54), equations (III.104b) and (III.104c) can be rewritten into entropy-preserving and entropy-increasing contributions, *viz.*,

$$-m_2\partial_t \mathbf{Q} = \left(-l_{12}^{\mathrm{A}}\partial_r \mathbf{j}_E\right) + \left(l_{11}\mathbf{Q} + l_{12}^{\mathrm{S}}\partial_r \mathbf{j}_E\right), \qquad (\text{III.106})$$

$$\mathbf{C} = \left(l_{12}^{\mathbf{A}}\mathbf{Q}\right) + \left(l_{12}^{\mathbf{S}}\mathbf{Q} + l_{22}\partial_{r}\mathbf{j}_{E}\right).$$
(III.107)

After eliminating the entropy current density multiplier C from (III.104a), the time evolution equations

$$\begin{pmatrix} -m_1\partial_t \mathbf{j}_E\\ -m_2\partial_t \mathbf{Q} \end{pmatrix} = \begin{pmatrix} -\partial_r \frac{1}{T} - l_{12}^{\mathrm{A}}\partial_r \mathbf{Q}\\ -l_{12}^{\mathrm{A}}\partial_r \mathbf{j}_E \end{pmatrix} + \begin{pmatrix} l\mathbf{j}_E - l_{12}^{\mathrm{S}}\partial_r \mathbf{Q} - l_{22}\partial_r^2 \mathbf{j}_E\\ l_{11}\mathbf{Q} + l_{12}^{\mathrm{S}}\partial_r \mathbf{j}_E \end{pmatrix}$$
(III.108)

follow. At this point, one has to recognize that, although the antisymmetric part has no contribution in the entropy production rate density, it influences the evolution equations. At first sight, this separation may look unusual and artificial but will be clarified later when presenting the derivation in the framework of GENERIC. The first term on the right hand side of (III.108) represents the reversible contribution, while the second term is the irreversible contribution of time evolution. Now writing the second equation of (III.108) in time-derivative operator form, namely,

$$(m_2\partial_t + l_{11})\mathbf{Q} = \left(l_{12}^{\mathrm{A}} - l_{12}^{\mathrm{S}}\right)\partial_r \mathbf{j}_E,$$
(III.109)

and letting the operator $(m_2\partial_t + l_{11})$ act on the first equation of (III.108), the outcome is the extended constitutive equation of heat current density, *i.e.*,

$$m_1 m_2 \partial_t^2 \mathbf{j}_E + (m_1 l_{11} + m_2 l) \partial_t \mathbf{j}_E - m_2 l_{22} \partial_t \partial_r^2 \mathbf{j}_E - (l_{11} l_{22} - l_{12} l_{21}) \partial_r^2 \mathbf{j}_E + l l_{11} \mathbf{j}_E = m_2 \partial_t \partial_r \frac{1}{T} + l_{11} \partial_r \frac{1}{T}$$
(III.110)

One can observe that this equation is a non-local extension of the ballistic–diffusive heat conduction equation. If $l_{22} = 0$ is assumed then one obtains for (III.104c)

$$\mathbf{C} = l_{21}\mathbf{Q},\tag{III.111}$$

which means that the entropy current multiplier is identified with the internal variable, thus

$$\mathbf{j}_S = \left(\frac{1}{T}\mathbf{1} + l_{21}\mathbf{Q}\right)\mathbf{j}_E.$$
 (III.112)

Then the first equation of (III.108) is

$$-m_1\partial_t \mathbf{j}_E = \left(-\partial_r \frac{1}{T} - l_{12}^{\mathrm{A}} \partial_r \mathbf{Q}\right) + \left(l \mathbf{j}_E - l_{12}^{\mathrm{S}} \partial_r \mathbf{Q}\right)$$
(III.113)

and, finally, the constitutive equation of ballistic-diffusive heat conduction is

$$m_1 m_2 \partial_t^2 \mathbf{j}_E + (m_1 l_{11} + m_2 l) \,\partial_t \mathbf{j}_E - (l_{11} l_{22} - l_{12} l_{21}) \,\partial_r^2 \mathbf{j}_E + l l_{11} \mathbf{j}_E = m_2 \partial_t \partial_r \frac{1}{T} + l_{11} \partial_r \frac{1}{T}.$$
 (III.114)

In the GENERIC framework, we look for the time evolution of the variables

$$\boldsymbol{\xi}_{3}^{E} = \begin{pmatrix} \varrho_{S} \\ \mathbf{w} \\ \mathbf{W} \end{pmatrix}$$
(III.115)

(where W is a second-order tensorial variable—not required to be symmetric and/or traceless—if treated in three space dimensions). The partial derivatives of internal energy density $\rho_E(\boldsymbol{\xi}_3^E)$ defines the energy conjugate variables

$$T = \frac{\partial \varrho_E}{\partial \varrho_S} \Big|_{\mathbf{w}, \mathbf{W}}, \qquad \mathbf{j} = \frac{\partial \varrho_E}{\partial \mathbf{w}} \Big|_{\varrho_S, \mathbf{W}}, \qquad \mathbf{P} = \frac{\partial \varrho_E}{\partial \mathbf{W}} \Big|_{\varrho_S, \mathbf{w}}. \tag{III.116}$$

Time evolution of $\boldsymbol{\xi}_3^E$ restricted to reversible dynamics is

$$\begin{pmatrix} \partial_t \varrho_S|_{\rm rev} \\ \partial_t \mathbf{w}|_{\rm rev} \\ \partial_t \mathbf{W}|_{\rm rev} \end{pmatrix} = \begin{pmatrix} 0 & -\partial_r & 0 \\ -\partial_r & 0 & -\partial_r \\ 0 & -\partial_r & 0 \end{pmatrix} \begin{pmatrix} T \\ \mathbf{j} \\ \mathbf{P} \end{pmatrix}.$$
 (III.117)

Why is the Poisson bivector chosen this way here? In general, there are several routes towards the bivectors (or Poisson brackets): (i) analogy with quantum mechanical commutators, (ii) the theory of Lie groups and algebras, and (iii) reduction from a more detailed Poisson bracket. None of these routes has been taken here, so the chosen Poisson bivector can only be seen as a suitable choice advantageous for the comparison with IVM. We believe, however, that it can be interpreted as an approximation of a more detailed and microscopically motivated Poisson bivector, as for instance the top left 2×2 block can be obtained from the Poisson bivector of fluid mechanics when neglecting the momentum density.

From the Onsager–Casimir reciprocal relations it again follows that the parity of W is even so that the coupling can be antisymmetric.

To formulate the irreversible contribution of time evolution, we switch to the variables of entropic representation: the dissipation potential is taken in the entropy conjugated variables

$$\boldsymbol{\xi}_{3}^{S} = \begin{pmatrix} \varrho_{E} \\ \mathbf{w} \\ \mathbf{W} \end{pmatrix}, \qquad \Longrightarrow \qquad \boldsymbol{\xi}_{3}^{S^{*}} = \frac{\delta S}{\delta \boldsymbol{\xi}_{3}^{S}} = \begin{pmatrix} \frac{1}{T} \\ -\frac{\mathbf{j}}{T} \\ -\frac{\mathbf{P}}{T} \end{pmatrix}$$
(III.118)

as the quadratic expression

$$\Xi_{\rm BD}\left(\boldsymbol{\xi}_{3}^{S^{*}}\right) = \int_{L} \left\{ \frac{k}{2} \left(-\frac{\mathbf{j}}{T} \right)^{2} + \frac{k_{11}}{2} \left(-\frac{\mathbf{P}}{T} \right)^{2} + \frac{k_{12}^{S}}{2} \left[\left(-\frac{\mathbf{P}}{T} \right) \partial_{r} \left(-\frac{\mathbf{j}}{T} \right) - \left(-\frac{\mathbf{j}}{T} \right) \partial_{r} \left(-\frac{\mathbf{P}}{T} \right) \right] + \frac{k_{22}}{2} \left[\partial_{r} \left(-\frac{\mathbf{j}}{T} \right) \right]^{2} \right\} dr$$
(III.119)

with the convexity-ensuring requirements

$$k \ge 0,$$
 $k_{11} \ge 0,$ $k_{22} \ge 0,$ $k_{11}k_{22} - (k_{12}^{\rm S})^2 \ge 0.$ (III.120)

The Onsager–Casimir reciprocal relations then require that k, k_{11} , and k_{22} be even w.r.t. TRT while k_{12}^{S} be odd, *e.g.*, a linear function of w or j. This dissipation potential generates the irreversible contribution to the time evolution of $\boldsymbol{\xi}_{3}^{S}$ as

$$\partial_t \boldsymbol{\xi}_3^{S^*} \Big|_{\text{irr}} = \begin{pmatrix} \partial_t \varrho_E |_{\text{irr}} \\ \partial_t \mathbf{w} |_{\text{irr}} \\ \partial_t \mathbf{W} |_{\text{irr}} \end{pmatrix} = \frac{\delta \Xi_{\text{BD}}}{\delta \boldsymbol{\xi}_3^{S^*}} \Big|_{\boldsymbol{\xi}_3^{S^*} = \frac{\delta S}{\delta \boldsymbol{\xi}_3^S}} = \begin{pmatrix} 0 \\ k \left(-\frac{\mathbf{j}}{T} \right) - k_{12}^S \partial_r \left(-\frac{\mathbf{P}}{T} \right) - k_{22} \partial_r^2 \left(-\frac{\mathbf{j}}{T} \right) \\ k_{11} \left(-\frac{\mathbf{P}}{T} \right) + k_{12}^S \partial_r \left(-\frac{\mathbf{j}}{T} \right) \end{pmatrix}. \quad \text{(III.121)}$$

The irreversible contribution to the time evolution of entropy density is

$$\partial_{t}\varrho_{S}|_{irr} = -\partial_{r}\left\{\left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right)\right\} + k\left(-\frac{\mathbf{j}}{T}\right)^{2} + k_{11}\left(-\frac{\mathbf{P}}{T}\right)^{2} + 2k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right)\partial_{r}\left(-\frac{\mathbf{j}}{T}\right) + k_{22}\left[\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]^{2}, \quad (III.122)$$

and, the time evolution of $\boldsymbol{\xi}_3^E$ is

$$\partial_{t}\varrho_{S} = -\partial_{r}\left\{\mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right)\right\} + k\left(-\frac{\mathbf{j}}{T}\right)^{2} + k_{11}\left(-\frac{\mathbf{P}}{T}\right)^{2} + 2k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right)\partial_{r}\left(-\frac{\mathbf{j}}{T}\right) + k_{22}\left[\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]^{2}, \quad (\text{III.123a})$$

$$\partial_t \mathbf{w} = -\partial_r T - \partial_r \mathbf{P} + k \left(-\frac{\mathbf{J}}{T} \right) - k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{F}}{T} \right) - k_{22} \partial_r^2 \left(-\frac{\mathbf{J}}{T} \right), \qquad (\text{III.123b})$$

$$\partial_t \mathbf{W} = -\partial_r \mathbf{j} + k_{11} \left(-\frac{\mathbf{P}}{T} \right) + k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{j}}{T} \right).$$
(III.123c)

Comparing (III.123b) and (III.123c) with (III.108), the same structures can be recognized. Naturally, if $k_{22} = 0$, we simply omit the last term from the dissipation potential (III.119) and obtain the ballistic–diffusive heat conduction. Time evolution of internal energy density is then

$$\partial_t \varrho_E = -T \partial_r \mathbf{j} - \mathbf{j} \left(\partial_r T + \partial_r \mathbf{P} \right) - \mathbf{P} \partial_r \mathbf{j} = -\partial_r \left[\left(T \mathbf{1} + \mathbf{P} \right) \mathbf{j} \right].$$
(III.124)

Heat current and entropy current densities

$$\mathbf{j}_{E} = (T\mathbf{1} + \mathbf{P})\mathbf{j}, \qquad \mathbf{j}_{S} = \mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right) \qquad (III.125)$$

can be read off. Expressing j with j_E and replacing it with j_S , in an appropriate approximation, the entropy current density – heat current density relationship obtained in (III.125) is found to be equivalent with (III.39) by substituting (III.104c). This means that (apart from non-linear terms) one finds a whole agreement between the equations derived in two ways. We remark that in the full 3D treatment the second order tensor T1 + P has to be inverted. Since T > 0, T1 and T1 + P are non-singular and, based on [133], the inverse of T1 + P can be expressed as

$$(T\mathbf{1} + \mathbf{P})^{-1} = \frac{1}{T}\mathbf{1} + \mathbf{R}$$
(III.126)

with

$$\mathbf{R} = -\frac{1}{T^2} \left(\mathbf{1} + \frac{1}{T} \mathbf{P} \right)^{-1} \mathbf{P}.$$
 (III.127)

III.2.1.3.2 Model reduction: Guyer–Krumhansl and Ginzburg–Landau equations Supposing $k_{12}^{S} = 0$ and $k_{22} = 0$, (III.119) is an algebraic dissipation potential, and the time evolution equations are

$$\partial_t \varrho_S = -\partial_r \mathbf{j} + k \left(-\frac{\mathbf{j}}{T} \right)^2 + k_{11} \left(-\frac{\mathbf{P}}{T} \right)^2, \qquad \text{(III.128a)}$$

$$\partial_t \mathbf{w} = -\partial_r T - \partial_r \mathbf{P} + k \left(-\frac{\mathbf{j}}{T}\right),$$
 (III.128b)

$$\partial_t \mathbf{W} = -\partial_r \mathbf{j} + k_{11} \left(-\frac{\mathbf{P}}{T} \right).$$
 (III.128c)

First of all, one can recognize that $j_S = j$, and, from the balance of internal energy,

$$\mathbf{j}_E = (T\mathbf{1} + \mathbf{P})\,\mathbf{j} = (T\mathbf{1} + \mathbf{P})\,\mathbf{j}_S,\tag{III.129}$$

Assuming that fast time evolution of W is over,

$$0 = -\partial_r \mathbf{j} + k_{11} \left(-\frac{\mathbf{P}}{T}\right), \qquad \text{(III.130)}$$

which can be treated as a constitutive relation between **j** and $\frac{P}{T}$ [122]. Inserting (III.130) into (III.128b), one can recognize a GK-like relationship

$$\partial_t \mathbf{w} = -\partial_r T + \partial_r \left(\frac{T}{k_{11}}\partial_r \mathbf{j}\right) + k\left(-\frac{\mathbf{j}}{T}\right).$$
 (III.131)

We remark that we obtained the entropy current density – heat current density relationship (III.129), which is equivalent to (III.99) or (III.39) and that entropy current density \mathbf{j}_S is purely the conjugate to w.

If fast evolution of w is also already relaxed then the Ginzburg–Landau type heat conduction can be recognized, *viz.*,

$$0 = -\partial_r T + \partial_r \left(\frac{T}{k_{11}}\partial_r \mathbf{j}\right) + k\left(-\frac{\mathbf{j}}{T}\right).$$
(III.132)

In these approximations, **P** inherits the time dependence from T and **j** while **P** and **j** inherit the time dependence from T, respectively. Thus the heat current density – entropy current density relationship $\mathbf{j}_E = (T\mathbf{1} + \mathbf{P})\mathbf{j}$ is revealed. This means that, via reducing a more detailed description, a complete agreement can be found among the theories.

III.2.1.3.3 Generalized ballistic–diffusive heat conduction A non-local generalization of ballistic– diffusive heat conduction equation via using a third-order entropy current multiplier was derived in [119]. Namely, a generalized entropy (III.102) and an extended entropy current density

$$\mathbf{j}_{S} = \left(\frac{1}{T}\mathbf{1} + \mathbf{C}\right) \cdot \mathbf{j}_{E} + \varepsilon \cdot \mathbf{Q}, \qquad (\text{III.133})$$

with the third-order Nyíri multiplier c, yield the entropy production density rate

$$\pi_{S} = \mathbf{j}_{E} \cdot \left(-m_{1}\partial_{t}\mathbf{j}_{E} + \partial_{r}\frac{1}{T} + \partial_{r}\mathbf{C} \right) + \mathbf{Q} \cdot \left(-m_{2}\partial_{t}\mathbf{Q} + \partial_{r}\mathbf{c} \right) + \mathbf{C} \cdot \partial_{r}\mathbf{j}_{E} + \mathbf{c} \cdot \partial_{r}\mathbf{Q}, \quad (\text{III.134})$$

where the first term is a vector–vector coupling, the last one is a third-order–third-order one, and the rest terms prescribe second-order tensorial couplings. (Again, all these are three space dimensional terminologies.) Positive semi-definiteness of (III.134) is ensured by the equations

$$-m_1\partial_t \mathbf{j}_E + \partial_r \frac{1}{T} + \partial_r \mathbf{C} = l \mathbf{j}_E, \qquad (\text{III.135a})$$

$$-m_2\partial_t \mathbf{Q} + \partial_r \mathbf{c} = l_{11} \mathbf{Q} + l_{12}\partial_r \mathbf{j}_E, \qquad \text{(III.135b)}$$

$$\mathbf{C} = l_{21}\mathbf{Q} + l_{22}\partial_r \mathbf{j}_E, \qquad (\text{III.135c})$$

$$\mathbf{c} = L\partial_r \mathbf{Q} \tag{III.135d}$$

with $L \ge 0$ and (III.105). After eliminating entropy current multipliers C and c, we have

$$\begin{pmatrix} -m_1\partial_t \mathbf{j}_E \\ -m_2\partial_t \mathbf{Q} \end{pmatrix} = \begin{pmatrix} -\partial_r \frac{1}{T} - l_{12}^{\mathrm{A}}\partial_r \mathbf{Q} \\ -l_{12}^{\mathrm{A}}\partial_r \mathbf{j}_E \end{pmatrix} + \begin{pmatrix} l\mathbf{j}_E - l_{12}^{\mathrm{S}}\partial_r \mathbf{Q} - l_{22}\partial_r^2 \mathbf{j}_E \\ l_{11}\mathbf{Q} + l_{12}^{\mathrm{S}}\partial_r \mathbf{j}_E - L\partial_r^2 \mathbf{Q} \end{pmatrix}.$$
 (III.136)

Similarly to (III.108), the first and second terms of rhs of (III.136) represent the reversible and irreversible contributions to time evolution, respectively. Let the operator $(m_2\partial_t + l_{11} - L\partial_r^2)$ act on the first equation of (III.136): then one obtains the constitutive equation on heat current density, *i.e.*,

$$m_{1}m_{2}\partial_{t}^{2}\mathbf{j}_{E} + (m_{1}l_{11} + m_{2}l)\,\partial_{t}\mathbf{j}_{E} - (m_{1}L + m_{2}l_{22})\,\partial_{t}\partial_{r}^{2}\mathbf{j}_{E} - (l_{11}l_{22} - l_{12}l_{21})\,\partial_{r}^{2}\mathbf{j}_{E} - l_{22}L\partial_{r}^{4}\mathbf{j}_{E} + ll_{11}\mathbf{j}_{E}$$
$$= m_{2}\partial_{t}\partial_{r}\frac{1}{T} + l_{11}\partial_{r}\frac{1}{T} - L\partial_{r}^{3}\frac{1}{T}.$$
(III.137)

We look for a non-local extension of the ballistic–diffusive heat conduction equation, consequently, total energy and the Hamiltonian structure of the reversible contribution presented in Sec. III.2.1.3.1 are not modified. On the other side, the dissipation potential is extended via a further non-local term, *viz.*,

$$\Xi_{\rm eBD}\left(\tilde{\boldsymbol{\xi}}_{3}^{S^*}\right) = \Xi_{\rm BD}\left(\tilde{\boldsymbol{\xi}}_{3}^{S^*}\right) + \int_{L} \frac{K}{2} \left[\partial_r \left(-\frac{\mathbf{P}}{T}\right)\right]^2 \mathrm{d}r \qquad (\text{III.138})$$

with non-negative constant K. This dissipation potential leads to the time evolution equations

$$\partial_{t}\varrho_{E} = -\partial_{r}\left[\left(T\mathbf{1} + \mathbf{P}\right)\mathbf{j}\right], \qquad \text{(III.139a)}$$
$$\partial_{t}\varrho_{S} = -\partial_{r}\left\{\mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right) + K\partial_{r}\left(-\frac{\mathbf{P}}{T}\right)\left(-\frac{\mathbf{P}}{T}\right)\right\} \qquad \text{(III.139b)}$$

$$+k\left(-\frac{\mathbf{j}}{2}\right)^{2}+k_{11}\left(-\frac{\mathbf{P}}{2}\right)^{2}+2k_{12}^{S}\left(-\frac{\mathbf{P}}{2}\right)\partial_{z}\left(-\frac{\mathbf{j}}{2}\right)+k_{22}\left[\partial_{z}\left(-\frac{\mathbf{j}}{2}\right)\right]^{2}+K\left[\partial_{z}\left(-\frac{\mathbf{P}}{2}\right)\right]^{2}$$

$$h_{t} \mathbf{w} = -\partial_{r} T - \partial_{r} \mathbf{P} + k \left(-\frac{\mathbf{j}}{T}\right) - k_{12}^{\mathrm{S}} \partial_{r} \left(-\frac{\mathbf{P}}{T}\right) - k_{22} \partial_{r}^{2} \left(-\frac{\mathbf{j}}{T}\right), \qquad (\text{III.139c})$$

$$\partial_t \mathbf{W} = -\partial_r \mathbf{j} + k_{11} \left(-\frac{\mathbf{P}}{T} \right) + k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{j}}{T} \right) - K \partial_r^2 \left(-\frac{\mathbf{P}}{T} \right).$$
(III.139d)

Heat and entropy current densities

$$\mathbf{j}_{E} = (T\mathbf{1} + \mathbf{P})\mathbf{j}, \qquad \mathbf{j}_{S} = \mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right) + K\partial_{r}\left(-\frac{\mathbf{P}}{T}\right)\left(-\frac{\mathbf{P}}{T}\right) \tag{III.140}$$

can be recognized. The third-order tensorial coupling in the dissipation potential gives additional contribution to entropy current density and, based on the conclusions of Sec. III.2.1.3.1, the equivalence with (III.133) can be obtained. Furthermore, the equivalence of time evolution equations also holds.

III.2.1.4 Generalized ballistic-conductive heat conduction reduced from a four-dimensional state space

Instead of further generalizations, we show that a four-dimensional state space, spanned by variables

$$\tilde{\boldsymbol{\xi}}_{4}^{E} = \begin{pmatrix} \varrho_{S} \\ \mathbf{w} \\ \mathbf{W} \\ \mathbf{W} \\ \mathbf{w} \end{pmatrix}, \qquad (III.141)$$

results in a time evolution system whose variable with highest tensorial order is reduced to obtain the non-local extension of the ballistic–diffusive heat conduction equation presented in Sec. III.2.1.3.3, and that the heat current density – entropy current density relationship obtained from IVM and GENERIC is also the same. Here, w denotes a third-order tensorial state variable (when in three space dimensions), the physical interpretation of which is not known. Now let us formulate this model within the GENERIC framework.

Supposing that total energy $E = \int_V \varrho_E \left(\boldsymbol{\xi}_4^E \right) dV$ does not contain non-local terms, the partial derivatives are

$$T = \frac{\partial \varrho_E}{\partial \varrho_S} \Big|_{\mathbf{w}, \mathbf{W}, \mathbf{w}}, \quad \mathbf{j} = \frac{\partial \varrho_E}{\partial \mathbf{w}} \Big|_{\varrho_S, \mathbf{W}, \mathbf{w}}, \quad \mathbf{P} = \frac{\partial \varrho_E}{\partial \mathbf{W}} \Big|_{\varrho_S, \mathbf{w}, \mathbf{w}}, \quad \mathbf{p} = \frac{\partial \varrho_E}{\partial \mathbf{w}} \Big|_{\varrho_S, \mathbf{w}, \mathbf{W}}.$$
(III.142)

Assuming a canonical structure, one obtains the time evolution of $\boldsymbol{\xi}_4^E$ restricted to reversible dynamics, *viz.*,

$$\begin{pmatrix} \partial_t \varrho_S|_{\text{rev}} \\ \partial_t \mathbf{w}|_{\text{rev}} \\ \partial_t \mathbf{w}|_{\text{rev}} \\ \partial_t \mathbf{w}|_{\text{rev}} \end{pmatrix} = \begin{pmatrix} 0 & -\partial_r & 0 & 0 \\ -\partial_r & 0 & -\partial_r & 0 \\ 0 & -\partial_r & 0 & -\partial_r \\ 0 & 0 & -\partial_r & 0 \end{pmatrix} \begin{pmatrix} T \\ \mathbf{j} \\ \mathbf{P} \\ \mathbf{p} \end{pmatrix}.$$
(III.143)

This means, due to the Onsager-Casimir reciprocal relation, that w is a quantity that is odd w.r.t. TRT.

Variables in entropic representation and entropy conjugated variables are

$$\boldsymbol{\xi}_{4}^{S} = \begin{pmatrix} \varrho_{E} \\ \mathbf{w} \\ \mathbf{W} \\ \mathbf{W} \\ \mathbf{w} \end{pmatrix}, \qquad \Longrightarrow \qquad \boldsymbol{\xi}_{4}^{S^{*}} = \frac{\delta S}{\delta \boldsymbol{\xi}_{3}^{S}} = \begin{pmatrix} \frac{1}{T} \\ -\frac{\mathbf{j}}{T} \\ -\frac{\mathbf{p}}{T} \\ -\frac{\mathbf{p}}{T} \end{pmatrix}, \qquad (\text{III.144})$$

respectively. The chosen dissipation potential

$$\Xi_{4\mathrm{D}}\left(\boldsymbol{\xi}_{4}^{S^{*}}\right) = \Xi_{\mathrm{BD}}\left(\boldsymbol{\xi}_{3}^{S^{*}}\right) + \int_{L} \frac{K}{2} \left(-\frac{\mathbb{P}}{T}\right)^{2} \mathrm{d}r \qquad (\mathrm{III.145})$$

and the above-presented Hamiltonian structure provide the time evolution of $\tilde{\boldsymbol{\xi}}_4^E$, *i.e.*,

$$\partial_{t}\varrho_{S} = -\partial_{r}\left\{\mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right)\right\} + k\left(-\frac{\mathbf{j}}{T}\right)^{2} + k_{11}\left(-\frac{\mathbf{P}}{T}\right)^{2} + 2k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right)\partial_{r}\left(-\frac{\mathbf{j}}{T}\right) + k_{22}\left[\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]^{2} + K\left(-\frac{\mathbb{P}}{T}\right)^{2},$$
(III.146)

$$\partial_t \mathbf{w} = -\partial_r T - \partial_r \mathbf{P} + k \left(-\frac{\mathbf{j}}{T} \right) - k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{P}}{T} \right) - k_{22} \partial_r^2 \left(-\frac{\mathbf{j}}{T} \right), \qquad (\text{III.147})$$

$$\partial_t \mathbf{W} = -\partial_r \mathbf{j} - \partial_r \mathbf{p} + k_{11} \left(-\frac{\mathbf{P}}{T} \right) + k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{j}}{T} \right), \qquad (\text{III.148})$$

$$\partial_t w = -\partial_r \mathbf{P} + K \left(-\frac{\mathbf{p}}{T} \right). \tag{III.149}$$

Time evolution of internal energy density is

$$\partial_t \varrho_E = -\partial_r \left[(T\mathbf{1} + \mathbf{P}) \,\mathbf{j} + \mathbf{p} \mathbf{P} \right], \qquad (\text{III.150})$$

thus heat and entropy current densities are

$$\mathbf{j}_{E} = (T\mathbf{1} + \mathbf{P})\mathbf{j} + \mathbf{p}\mathbf{P}, \qquad \mathbf{j}_{S} = \mathbf{j} + \left[k_{12}^{S}\left(-\frac{\mathbf{P}}{T}\right) + k_{22}\partial_{r}\left(-\frac{\mathbf{j}}{T}\right)\right]\left(-\frac{\mathbf{j}}{T}\right). \qquad (III.151)$$

As we have expected, no additional terms appear in the entropy current density with respect to the ballistic–diffusive one, but a third-order tensorial contribution appears in the heat current density.

If fast evolution of w is relaxed then

$$0 = -\partial_r \mathbf{P} + K\left(-\frac{\mathbf{p}}{T}\right),\tag{III.152}$$

which is the analogue of (III.135d) and can be treated as a constitutive relation among **P** and $\frac{\mathbb{P}}{T}$. Accordingly, substituting $\mathbb{P} = -\frac{T}{K}\partial_r \mathbf{P}$ into (III.148), one obtains

$$\partial_t \mathbf{W} = -\partial_r \mathbf{j} + k_{11} \left(-\frac{\mathbf{P}}{T} \right) + k_{12}^{\mathrm{S}} \partial_r \left(-\frac{\mathbf{j}}{T} \right) + \partial_r \left(\frac{T}{K} \partial_r \mathbf{P} \right), \qquad (\text{III.153})$$

which has the same structure as the second equation of (III.136) and, with the above approximations, the heat current density – entropy current density relationships obtained in both frameworks proved to be equivalent.

GENERIC allows for constructing of a hierarchy of models of heat conduction varying in the level of detail involved, and the more detailed models (with more state variables) can be reduced to the less detailed ones. This is a demonstration of the multiscale nature of GENERIC.

III.2.2 A short comparison of IVM and GENERIC

Similarly to CIT, IVM determines the entropy production density rate from a concave expression of entropy and an assumed entropy current density - heat current density relationship constraint, utilizing the classical balances on mass, linear and angular momenta, and internal energy, e.g., in case of the Navier-Stokes-Fourier system and its extensions, like in [63]. Since entropy is expressed as a concave function of the state variables, the chosen representation is usually the entropic representation. Positive semi-definiteness of the derived entropy production rate density is ensured by Onsagerian equations. When internal variables, for which no balance equation is known, are also variables of entropy, then the Onsagerian equations contain time derivative terms, too. As we have shown, when no assumption is made regarding reciprocal relations on the coefficients of the Onsagerian equations, then the framework of IVM generates both entropy preserving and entropy increasing terms in the time evolution equations (see, in this respect, [134]). Very often, internal variables have no known physical interpretation, hence, measuring them and performing calculations with them (without the knowledge of the related coefficients) is not feasible. Assuming a linear relation among the internal variable and its conjugate-which is almost always built in the concave expression of entropy-, internal variables and entropy current multipliers can be eliminated, thus extended constitutive laws can be obtained for the usual, known, and measurable physical quantities.

In contrast to IVM, GENERIC yields all evolution equations from the two generators, total energy and entropy (and the related operator matrices), from a Poisson bracket (or bivector) and a dissipation potential. GENERIC gives the non-dissipative, entropy-preserving, part and the irreversible, entropy-increasing, part of time evolution separately; the first one is convenient in the variables of the energetic representation while the second one in the entropic representation. The Hamiltonian structure of the reversible contribution is expressed by Poisson brackets, which can often be deduced from microscopic theories or by means of differential geometry on Lie groups. The irreversible contribution to time evolution can be deduced from a usually convex dissipation potential, which may also be determined from statistical theories [135]. In case of a quadratic dissipation potential, the generated system of time evolution is linear in the conjugate variables.

	NET-IV	GENERIC	
Representation	Entropy representation	Both energy and entropic representation	
Input	Internal energy entropy relationships	Internal energy entropy relationships	
	Extended relationship on \mathbf{j}_S	Poisson bracket	
	Classical balance equations	Dissipation potential	
Output	Entropy production rate density	Time evolution equations	
	Time evolution equations	Relationship of \mathbf{j}_S and \mathbf{j}_E	

The differences between the two approaches are summarized in Table III.3.

Table III.3: Differences between the NET-IV and GENERIC approaches. j_S : entropy current density, j_E : heat current density.

III.2.3 Conclusions

In this section, first, known derivations of beyond-Fourier heat conduction in the frameworks of IVM and of GENERIC have been revisited. Since known GENERIC realizations of beyond-Fourier heat conduction treat models up to the GK equation [117, 122], we formulated also the *ballistic–diffusive heat conduction model in GENERIC*.

The two derivations have led to the same structure of evolution equations and to the same relationship between entropy current density and heat current density. GENERIC recognizes both heat and entropy current densities from the evolution equations of internal energy and entropy densities, and connects them to the conjugate of the vectorial variable w. After algebraic reformulations, the entropy current density – heat current density relationship can be obtained. This derivation has lead us to our main recognition.

When the dissipation potential contains non-local terms, which has higher tensorial orders than the state variable with highest tensorial order, then non-local extensions will appear in the generated evolution equations, as well as in the relationship between entropy current density and heat current density also higher order multipliers can be obtained, see, *e.g.*, the MCV and GK equations for two-dimensional state space and BC and its generalization for three-dimensional state space. To get the same relations with algebraic dissipation potentials, one has to extend the state space with a variable of tensorial order larger than the highest tensorial order of the variables of the starting state space. Subsequently, deriving an evolution equation for this variable, and reducing it, the resulting entropy current density – heat current density relationships are also found equivalent, see *e.g.*, the GK equation reduced from BC heat conduction.

After the fast attenuation of the variable with the highest tensorial order, its time dependence becomes enslaved by the variables with lower tensorial orders, thus the explicit time dependence of this variable disappears. However, the implicit time dependence of that variable contributes to the entropy current density – heat current density relationship. In this limit, a spatial partial differential equation is obtained, which can be treated as a constitutive equation among the quantities which are included in this equation. Assuming a generalized entropy current density within IVM, only the spatial contributions of its variables appear in the entropy production rate density. Based on these, *entropy current multipliers can be interpreted as relaxed state variables*.

Heat current density is frequently identified with a vectorial internal variable, however, we have shown that, from a general theoretical point of view, *identification of heat current density with the conjugate of the vectorial internal variable is more advantageous*.

The derivation presented in this section strengthens the GENERIC background for beyond-Fourier heat conduction models, with a possible (and hoped) consequence that microscopic/multiscale (see, *e.g.*, [107, 122, 103, 125]) understanding of these phenomena becomes available. In parallel, the GENERIC formulation of heat conduction opens a way towards new and efficient numerical methods (for example, along the lines of [52, 136]) for heat-conduction problems (like in [137]).

Chapter IV

Kluitenberg–Verhás rheology of solids in the GENERIC framework

Starting from this chapter, rheology of solids is investigated.

Solids may be less "solid" than expected. Beyond elastic behaviour, they may exhibit damped and delayed response. This rheological/viscoelastic reaction may not simply be explained by a viscosity-related additional stress (the Kelvin–Voigt model of rheology) but the time derivative of stress may also be needed in the description, the simplest such model being the so-called standard or Poynting–Thomson–Zener (PTZ) one [see its details in Chapter V]. Namely, the PTZ model is the simplest model that enables to describe both creep (declining increase of strain during constant stress) and relaxation (declining decrease of stress during constant strain). The internal variable approach of irreversible thermodynamics, with a symmetric tensorial internal variable, provides a more general model family—the Kluitenberg–Verhás model family [43] (covering Hooke's elasticity, the previously mentioned Kelvin–Voigt and Poynting–Thomson–Zener models, and also the Maxwell and Jeffreys models as special cases)—for the rheology of solids. This family is significant not only from a theoretical perspective but also for experimental and engineering applications [1, 42, 40, 41].

Usually, models derived within the framework of internal variable methodology contain higher-order time and space derivatives [see *e.g.*, equations (IV.23) and (IV.24)], however, the treatment of initial and boundary conditions faces no problem. In contrast, the appearing higher-order derivatives complicate the solvability, thus accurate and reliable (numerical) methods are required. In parallel, the GENERIC formulation motivates new and efficient numerical methods (for example, along the lines of [108, 56, 52, 136]), however, the treatment of boundary conditions can be complicated. Nevertheless, it is advantageous and recommended to check how a model derived by the internal variable methodology suits the frame of GENERIC. This chapter analyzes how the internal variable formulation leading to the Kluitenberg–Verhás model family can be represented in GENERIC. This investigation is remarkable not only from a pure theoretical point of view, but it also motivates a direct numerical application, which is presented in Chapter V.

This chapter is based on the publications [138, 139]. The author's contributions are as follows:

- Generalization of Kluitenberg–Verhás model family by thermal expansion;
- Implementation of Kluitenberg–Verhás model family into the frame of GENERIC:
 - Isotropic decomposition of second-order tensors as independent state variables,
 - specific entropy-based formulation (a choice natural from principal aspects),
 - temperature-based formulation (a choice natural from engineering applications);
- Representation of antisymmetric irreversible coupling terms in the symplectic (thus reversible and entropy preserving) part of the equations, which increases the numerical opportunities.

IV.1 The internal variable formulation of rheology of solids

First, a summary and generalization of the internal variable approach to the Kluitenberg–Verhás rheological model family of solids is presented [43]. The discussion is generalized in that the derivation in [43] neglected thermal expansion and started from Hookean elasticity, while the version here is free of those restrictions, only isotropy of the material being assumed.

The small-strain regime is considered, thus mass density ρ is constant, and one can relate time derivative (partial coinciding with substantial, abbreviated in this Chapter by overdot) of strain with the symmetrized gradient of the velocity field v,

$$\dot{\boldsymbol{\varepsilon}} = \left(\mathbf{v} \otimes \boldsymbol{\nabla} \right)^{\mathbf{S}} \tag{IV.1}$$

[(II.25) is repeated here for convenience]. Due to the isotropy of the material, the deviatoric–spherical decomposition of symmetric tensors plays here an important role (as a reminder, the spherical part of, *e.g.*, strain is proportional to the identity tensor, $\varepsilon^{s} = \frac{1}{3} (\operatorname{tr} \varepsilon) \mathbf{1}$, while $\varepsilon^{d} = \varepsilon - \varepsilon^{s}$ is its deviatoric part). With s_{0} denoting specific entropy, the variables will be

$$\mathbf{x}_0 = \left(\mathbf{v}, \boldsymbol{\varepsilon}^{\mathsf{d}}, \boldsymbol{\varepsilon}^{\mathsf{s}}, s_0\right). \tag{IV.2}$$

The balance of linear momentum (II.21) with neglected field strength is

$$\rho \dot{\mathbf{v}} = \boldsymbol{\sigma}_0 \cdot \overleftarrow{\nabla} \tag{IV.3}$$

with the divergence of stress σ_0 on the rhs, where σ_0 is related to a specific internal energy $e_{\text{int},0}(\varepsilon^d, \varepsilon^s, s_0)$ as shown by the partial derivatives¹

$$\frac{\partial e_{\text{int},0}}{\partial \boldsymbol{\varepsilon}^{d}} = \frac{1}{\varrho} \boldsymbol{\sigma}_{0}^{d}, \qquad \frac{\partial e_{\text{int},0}}{\partial \boldsymbol{\varepsilon}^{s}} = \frac{1}{\varrho} \boldsymbol{\sigma}_{0}^{s}, \qquad \frac{\partial e_{\text{int},0}}{\partial s_{0}} = T,$$
(IV.4)

naturally, T standing for temperature [cf. (II.28)].

Rheology is a behavior most manifest in the mechanical aspect so, for an internal variable description of it, in conform with that strain and stress are second-order symmetric tensors, a symmetric tensorial internal variable $\boldsymbol{\xi}$ is introduced as an additional state variable. Mechanical effects of rheology are to be embodied by a $\boldsymbol{\xi}$ dependent extension of stress:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_0 + \hat{\boldsymbol{\sigma}},\tag{IV.5}$$

$$\varrho \dot{\mathbf{v}} = \boldsymbol{\sigma} \cdot \nabla. \tag{IV.6}$$

Rheology is irreversibility-related, thus specific entropy is also assumed to be influenced; concavity concerns combined with Morse's lemma for smooth enough $\boldsymbol{\xi}$ dependence and nonzero second derivative in $\boldsymbol{\xi}$ conclude in the variable transformation $s_0 \rightarrow s$ [94]

$$s = s_0 - \frac{1}{2} \operatorname{tr} \left(\boldsymbol{\xi}^{\mathsf{d}} \boldsymbol{\xi}^{\mathsf{d}} \right) - \frac{1}{2} \operatorname{tr} \left(\boldsymbol{\xi}^{\mathsf{s}} \boldsymbol{\xi}^{\mathsf{s}} \right).$$
(IV.7)

Correspondingly, specific internal energy expressed in terms of the extended collection of variables,

$$\mathbf{x} = \left(\mathbf{v}, \boldsymbol{\varepsilon}^{\mathsf{d}}, \boldsymbol{\varepsilon}^{\mathsf{s}}, s, \boldsymbol{\xi}^{\mathsf{d}}, \boldsymbol{\xi}^{\mathsf{s}}\right), \tag{IV.8}$$

is of the form

$$e_{\text{int}}(\mathbf{x}) = e_{\text{int},0} \Big(\boldsymbol{\varepsilon}^{d}, \boldsymbol{\varepsilon}^{s}, s_{0} \big(s, \boldsymbol{\xi}^{d}, \boldsymbol{\xi}^{s} \big) \Big).$$
(IV.9)

 ${}^{1}\frac{\partial e_{\mathrm{int},0}}{\partial \varepsilon^{\mathrm{d}}} \text{ is purely deviatoric since, for any two tensors } \mathbf{A}, \mathbf{B}, \ A^{\mathrm{s}}{}_{ij}B^{\mathrm{d}}{}_{ij} = 0 \text{ so } \frac{\partial e_{\mathrm{int},0}}{\partial \varepsilon^{\mathrm{d}}_{ij}} \mathrm{d}\varepsilon^{\mathrm{d}}_{ij} = \left(\frac{\partial e_{\mathrm{int},0}}{\partial \varepsilon^{\mathrm{d}}_{ij}}\right)^{\mathrm{d}} \mathrm{d}\varepsilon^{\mathrm{d}}_{ij}.$
The balance of internal energy [(II.23) is repeated here for convenience] is

$$\rho \dot{e}_{int} = -\mathbf{j}_E \cdot \overleftarrow{\nabla} + \operatorname{tr} \left(\boldsymbol{\sigma} \dot{\boldsymbol{\varepsilon}} \right), \qquad (IV.10)$$

where the only source term considered is related to mechanical power. Substituting (IV.4), (IV.5) and (IV.7) into (IV.10), on the one hand, we obtain

$$\varrho \dot{e}_{int} = \varrho \left\{ tr \left(\frac{\partial e_{int,0}}{\partial \boldsymbol{\varepsilon}^{d}} \dot{\boldsymbol{\varepsilon}}^{d} \right) + tr \left(\frac{\partial e_{int,0}}{\partial \boldsymbol{\varepsilon}^{s}} \dot{\boldsymbol{\varepsilon}}^{s} \right) + \frac{\partial e_{int,0}}{\partial s_{0}} \left[\frac{\partial s_{0}}{\partial s} \dot{\boldsymbol{s}} + tr \left(\frac{\partial s_{0}}{\partial \boldsymbol{\xi}^{d}} \dot{\boldsymbol{\xi}}^{d} \right) + tr \left(\frac{\partial s_{0}}{\partial \boldsymbol{\xi}^{s}} \dot{\boldsymbol{\xi}}^{s} \right) \right] \right\} = tr \left(\boldsymbol{\sigma}_{0}^{d} \dot{\boldsymbol{\varepsilon}}^{d} \right) + tr \left(\boldsymbol{\sigma}_{0}^{s} \dot{\boldsymbol{\varepsilon}}^{s} \right) + \varrho T \dot{\boldsymbol{s}} + \varrho T tr \left(\boldsymbol{\xi}^{d} \dot{\boldsymbol{\xi}}^{d} \right) + \varrho T tr \left(\boldsymbol{\xi}^{s} \dot{\boldsymbol{\xi}}^{s} \right), \tag{IV.11}$$

and, on the other hand,

$$\varrho \dot{e}_{\text{int}} = -\mathbf{j}_E \cdot \overleftarrow{\nabla} + \text{tr} \left(\boldsymbol{\sigma}_0^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} \right) + \text{tr} \left(\boldsymbol{\sigma}_0^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} \right) + \text{tr} \left(\hat{\boldsymbol{\sigma}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} \right) + \text{tr} \left(\hat{\boldsymbol{\sigma}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} \right).$$
(IV.12)

The rhs of (IV.11) is to be equal to the rhs of (IV.12), which leads to

$$\rho \dot{s} = -\frac{1}{T} \mathbf{j}_E \cdot \overleftarrow{\nabla} + \frac{1}{T} \operatorname{tr} \left(\hat{\boldsymbol{\sigma}}^{\mathsf{d}} \dot{\boldsymbol{\varepsilon}}^{\mathsf{d}} \right) + \frac{1}{T} \operatorname{tr} \left(\hat{\boldsymbol{\sigma}}^{\mathsf{s}} \dot{\boldsymbol{\varepsilon}}^{\mathsf{s}} \right) - \rho \operatorname{tr} \left(\boldsymbol{\xi}^{\mathsf{d}} \dot{\boldsymbol{\xi}}^{\mathsf{d}} \right) - \rho \operatorname{tr} \left(\boldsymbol{\xi}^{\mathsf{s}} \dot{\boldsymbol{\xi}}^{\mathsf{s}} \right).$$
(IV.13)

Since the balance of the extended entropy [based on (II.24)] is to be of the form

$$\rho \dot{s} = -\mathbf{j}_S \cdot \nabla + \pi_s \tag{IV.14}$$

with entropy current density \mathbf{j}_S chosen to be the usual $\mathbf{j}_S = \frac{1}{T} \mathbf{j}_E$, and entropy production π_s , in the light of (IV.13), one can write

$$\pi_{s} = \varrho \dot{s} + \mathbf{j}_{S} \cdot \overleftarrow{\nabla} = \mathbf{j}_{E} \cdot \left(\frac{1}{T} \otimes \overleftarrow{\nabla}\right) + \frac{1}{T} \operatorname{tr}\left(\hat{\boldsymbol{\sigma}}^{\mathsf{d}} \dot{\boldsymbol{\varepsilon}}^{\mathsf{d}}\right) + \frac{1}{T} \operatorname{tr}\left(\hat{\boldsymbol{\sigma}}^{\mathsf{s}} \dot{\boldsymbol{\varepsilon}}^{\mathsf{s}}\right) - \varrho \operatorname{tr}\left(\boldsymbol{\xi}^{\mathsf{d}} \dot{\boldsymbol{\xi}}^{\mathsf{d}}\right) - \varrho \operatorname{tr}\left(\boldsymbol{\xi}^{\mathsf{s}} \dot{\boldsymbol{\xi}}^{\mathsf{s}}\right).$$
(IV.15)

Positive semidefiniteness of entropy production can be ensured for the first term via $\mathbf{j}_E = \lambda \left(\frac{1}{T} \otimes \nabla\right)$, $\lambda \ge 0$ (Fourier heat conduction, a vectorial part that cannot isotropically couple to the remaining, tensorial, terms; hence, for simplicity, heat conduction is neglected in what follows), and via Onsagerian equations concerning the further terms, with independent deviatoric and spherical parts because of isotropy:

$$\hat{\boldsymbol{\sigma}}^{\mathrm{d}} = l_{11}^{\mathrm{d}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{d}} + l_{12}^{\mathrm{d}} \left(-\varrho T \boldsymbol{\xi}^{\mathrm{d}} \right), \qquad \hat{\boldsymbol{\sigma}}^{\mathrm{s}} = l_{11}^{\mathrm{s}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{s}} + l_{12}^{\mathrm{s}} \left(-\varrho T \boldsymbol{\xi}^{\mathrm{s}} \right), \qquad (\mathrm{IV.16})$$

$$\dot{\boldsymbol{\xi}}^{\mathrm{d}} = l_{21}^{\mathrm{d}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{d}} + l_{22}^{\mathrm{d}} \left(-\varrho T \boldsymbol{\xi}^{\mathrm{d}}\right), \qquad \dot{\boldsymbol{\xi}}^{\mathrm{s}} = l_{21}^{\mathrm{s}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{s}} + l_{22}^{\mathrm{s}} \left(-\varrho T \boldsymbol{\xi}^{\mathrm{s}}\right), \qquad (\mathrm{IV.17})$$

with appropriate conditions on the deviatoric coefficients l_{ij}^{d} and the spherical ones l_{ij}^{s} , each of which are going to be assumed constant for simplicity². These conditions can be read off from the quadratic form obtained by substituting (IV.16)–(IV.17) into (IV.15), which yields³

$$T\pi_{s} = \left(\dot{\boldsymbol{\varepsilon}}^{d} - \varrho T\boldsymbol{\xi}^{d} \dot{\boldsymbol{\varepsilon}}^{s} - \varrho T\boldsymbol{\xi}^{s}\right) \begin{pmatrix} l_{11}^{d} & l_{S}^{d} & 0 & 0\\ l_{S}^{d} & l_{22}^{d} & 0 & 0\\ 0 & 0 & l_{11}^{s} & l_{S}^{s}\\ 0 & 0 & l_{S}^{s} & l_{22}^{s} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{\varepsilon}}^{d} \\ -\varrho T\boldsymbol{\xi}^{d} \\ \dot{\boldsymbol{\varepsilon}}^{s} \\ -\varrho T\boldsymbol{\xi}^{s} \end{pmatrix}$$
(IV.18)

²No principal difficulties are expected when these coefficients are \mathbf{x} dependent, and here we intend to keep formulae relatively short.

³The upper right and lower left two-by-two submatrices contain only zero elements due to the isotropic decoupling of deviatoric and spherical parts.

with $l_{\rm S}^{\rm d} = \frac{1}{2} \left(l_{12}^{\rm d} + l_{21}^{\rm d} \right)$ and $l_{\rm S}^{\rm s} = \frac{1}{2} \left(l_{12}^{\rm s} + l_{21}^{\rm s} \right)$. Hence, the four-by-four coefficient matrix in the middle is required to be positive semidefinite, which necessitates for the coefficients, using Sylvester's criteria,

$$l_{11}^{\rm d} \ge 0, \qquad l_{22}^{\rm d} \ge 0, \qquad \det l_{\rm S}^{\rm d} \ge 0,$$
 (IV.19)

$$l_{11}^{s} \ge 0, \qquad l_{22}^{s} \ge 0, \qquad \det l_{S}^{s} \ge 0.$$
 (IV.20)

We remark that, both in (IV.19) and (IV.20), the three conditions are not independent: the third one and either of the first two ones imply the remaining one. It is important to notice that the antisymmetric part of the coefficient matrix does not contribute to entropy production. We can emphasize this by dividing the Onsagerian equations (IV.16)–(IV.17) into two parts:

$$\hat{\boldsymbol{\sigma}}^{d} = \left[l_{A}^{d} \left(-\varrho T \boldsymbol{\xi}^{d} \right) \right] + \left[l_{11}^{d} \dot{\boldsymbol{\varepsilon}}^{d} + l_{S}^{d} \left(-\varrho T \boldsymbol{\xi}^{d} \right) \right], \quad \hat{\boldsymbol{\sigma}}^{s} = \left[l_{A}^{s} \left(-\varrho T \boldsymbol{\xi}^{s} \right) \right] + \left[l_{11}^{s} \dot{\boldsymbol{\varepsilon}}^{s} + l_{S}^{s} \left(-\varrho T \boldsymbol{\xi}^{s} \right) \right],$$
(IV.21)

$$\dot{\boldsymbol{\xi}}^{d} = \left[-l_{A}^{d} \dot{\boldsymbol{\varepsilon}}^{d} \right] + \left[l_{S}^{d} \dot{\boldsymbol{\varepsilon}}^{d} + l_{22}^{d} \left(-\varrho T \boldsymbol{\xi}^{d} \right) \right], \qquad \dot{\boldsymbol{\xi}}^{s} = \left[-l_{A}^{s} \dot{\boldsymbol{\varepsilon}}^{s} \right] + \left[l_{S}^{s} \dot{\boldsymbol{\varepsilon}}^{s} + l_{22}^{s} \left(-\varrho T \boldsymbol{\xi}^{s} \right) \right] \quad (IV.22)$$

with $l_{\rm A}^{\rm d} = \frac{1}{2} (l_{12}^{\rm d} - l_{21}^{\rm d})$ and $l_{\rm A}^{\rm s} = \frac{1}{2} (l_{12}^{\rm s} - l_{21}^{\rm s})$.

It is to be noted that, in general, the coefficient matrices l^d , l^s need not be symmetric nor antisymmetric, corresponding to that the concrete physical interpretation of $\boldsymbol{\xi}$ may not be available and the behavior of $\boldsymbol{\xi}$ under time reflection might not be purely sign preserving/flipping⁴.

To see that this model family covers classic rheological models like Kelvin–Voigt and Poynting– Thomson, one can start with the special case of Hooke elasticity, and eliminating the internal variable leads, in the isothermal approximation (constant $l_{11}^{d,s}$, $l_A^{d,s}$, $\rho T l_S^{d,s}$, $\rho T l_{22}^{d,s}$), to the Kluitenberg–Verhás model family [43],

$$\boldsymbol{\sigma}^{\mathrm{d}} + \tau^{\mathrm{d}} \dot{\boldsymbol{\sigma}}^{\mathrm{d}} = E_0^{\mathrm{d}} \boldsymbol{\varepsilon}^{\mathrm{d}} + E_1^{\mathrm{d}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{d}} + E_2^{\mathrm{d}} \ddot{\boldsymbol{\varepsilon}}^{\mathrm{d}}, \qquad (\mathrm{IV.23})$$

$$\boldsymbol{\sigma}^{\mathrm{s}} + \tau^{\mathrm{s}} \dot{\boldsymbol{\sigma}}^{\mathrm{s}} = E_0^{\mathrm{s}} \boldsymbol{\varepsilon}^{\mathrm{s}} + E_1^{\mathrm{s}} \dot{\boldsymbol{\varepsilon}}^{\mathrm{s}} + E_2^{\mathrm{s}} \ddot{\boldsymbol{\varepsilon}}^{\mathrm{s}}, \qquad (\mathrm{IV.24})$$

with necessary and sufficient thermodynamical inequality conditions on the coefficients $\tau^{d,s}$, $E_0^{d,s}$, $E_1^{d,s}$, $E_2^{d,s}$ stemming from (IV.19)–(IV.20) (for further details on the elimination and the inequalities, see [43], Section 2.3).

IV.2 Internal variable rheology of solids realized in the GENERIC formulation

Section IV.1 has actually been given in a form to provide preparations for the present one, where the GENERIC form for the ξ -described rheology of solids is established. The set of variables x is (IV.8), the energy functional consists of the internal energy contribution (IV.9) supplemented by the kinetic energy related one, and the entropy functional is straightforward:

$$E = \int_{V} \varrho e_{\text{total}} dV = \int_{V} \varrho \left[\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + e_{\text{int},0} \left(\boldsymbol{\varepsilon}^{\text{d}}, \boldsymbol{\varepsilon}^{\text{s}}, s_{0} \left(s, \boldsymbol{\xi}^{\text{d}}, \boldsymbol{\xi}^{\text{s}} \right) \right) \right] dV, \qquad (\text{IV.25})$$

$$S = \int_{V} \rho s \mathrm{d}V. \tag{IV.26}$$

The corresponding functional derivatives are

$$\frac{\delta E}{\delta \mathbf{x}} = \begin{pmatrix} \varrho \mathbf{v} \\ \boldsymbol{\sigma}_0^{\mathrm{d}} \\ \boldsymbol{\sigma}_0^{\mathrm{s}} \\ \varrho T \\ \varrho T \boldsymbol{\xi}^{\mathrm{d}} \\ \varrho T \boldsymbol{\xi}^{\mathrm{s}} \end{pmatrix}, \qquad \qquad \frac{\delta S}{\delta \mathbf{x}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \varrho \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \tag{IV.27}$$

⁴Rocks and biomaterials are examples for complex enough materials that may require such a description.

The nontrivial task is to identify the operator matrices L and M. Concerning the time evolution of the state variables, we know (IV.6), (IV.1), (IV.13) and (IV.16)-(IV.17) so we conjecture the decomposition to reversible and irreversible parts as ⁵

$$\begin{pmatrix} \dot{\mathbf{v}} \\ \dot{\boldsymbol{\varepsilon}}^{d} \\ \dot{\boldsymbol{\varepsilon}}^{s} \\ \dot{\boldsymbol{\varepsilon}}^{s} \\ \dot{\boldsymbol{\xi}}^{s} \\ \dot{\boldsymbol{\xi}}^{s} \\ \dot{\boldsymbol{\xi}}^{s} \\ \boldsymbol{\xi}^{s} \\ \boldsymbol{\delta} \\ \boldsymbol{\delta} \\ \boldsymbol{\xi}^{s} \\ \boldsymbol{\delta} \\ \boldsymbol{\delta}$$

The governing principle for this decision for decomposition is that, since dissipation and irreversibility are related to entropy production and to the internal variable, the reversible vector field should not contain them but only pure fluid mechanics.

Then L can directly read off from the first term on the rhs of (IV.28):

$$\mathbf{L} = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \mathbf{0} & \mathbf{0} \cdot & \mathbf{0} \cdot \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{d}} & 0 & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} & 0 & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} \cdot & \mathbf{0} : & \mathbf{0} : & \mathbf{0} \cdot & \mathbf{0} : \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix},$$
(IV.29)

with • denoting the 'slot' where the operator acts. This L apparently fulfils the degeneracy condition $L\frac{\delta S}{\delta x} = 0$. To prove antisymmetry of L, let us take the corresponding bracket (II.38):

$$\{A,B\} = \int_{V} \frac{1}{\varrho} \left[A_{v} \cdot \left(B_{\varepsilon^{\mathsf{d}}} \cdot \overleftarrow{\nabla} + B_{\varepsilon^{\mathsf{s}}} \cdot \overleftarrow{\nabla} \right) + \operatorname{tr} \left\{ A_{\varepsilon^{\mathsf{d}}} \left[\left(B_{v} \otimes \overleftarrow{\nabla} \right)^{\mathsf{S}} \right]^{\mathsf{d}} \right\} + \operatorname{tr} \left\{ A_{\varepsilon^{\mathsf{s}}} \left[\left(B_{v} \otimes \overleftarrow{\nabla} \right)^{\mathsf{S}} \right]^{\mathsf{s}} \right\} \right] \mathrm{d}V,$$
(IV.30)

where A and B are arbitrary functionals of the state variables, and abbreviations of the kind

$$A_{v} := \frac{\delta A}{\delta \mathbf{v}}, \quad A_{\varepsilon^{\mathsf{d}}} := \frac{\delta A}{\delta \varepsilon^{\mathsf{d}}}, \quad A_{\varepsilon^{\mathsf{s}}} := \frac{\delta A}{\delta \varepsilon^{\mathsf{s}}}, \quad A_{s} := \frac{\delta A}{\delta s}, \quad A_{\xi^{\mathsf{d}}} := \frac{\delta A}{\delta \xi^{\mathsf{d}}}, \quad A_{\xi^{\mathsf{s}}} := \frac{\delta A}{\delta \xi^{\mathsf{s}}}$$
(IV.31)

have been introduced. Using indices (with Einstein convention and the Kronecker symbol δ_{ij}), we have

$$\left[\left(B_v \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} = \frac{1}{3} \operatorname{tr} \left[\left(B_v \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right] \mathbf{1} = \frac{1}{3} \partial_k (B_v)_k \delta_{ij}, \tag{IV.32}$$

$$\left[\left(B_v\otimes\overleftarrow{\nabla}\right)^{\mathbf{S}}\right]^{\mathbf{d}} = \left(B_v\otimes\overleftarrow{\nabla}\right)^{\mathbf{S}} - \left[\left(B_v\otimes\overleftarrow{\nabla}\right)^{\mathbf{S}}\right]^{\mathbf{s}} = \frac{1}{2}\left[\partial_j(B_v)_i + \partial_i(B_v)_j\right] - \frac{1}{3}\partial_k(B_v)_k\delta_{ij}, \quad (IV.33)$$

⁵Beware that, if we prefer to write x and \dot{x} as column vectors then (IV.27) should contain row vectors, as being covectors with respect to the vector space of \mathbf{x} . However, then \mathbf{L} and \mathbf{M} could not be displayed as customary square matrices. The misleading double meaning of column vectors could be resolved by writing x-covectors like in (IV.27) as column vectors but within [] instead of (). Then, correspondingly, L, M were to be written within (]. Here, we decided not to use this convention but at least to draw attention to that distinction between vectors and covectors is not only principally important but also avoids considerable confusion during calculations.

leading to

$$\{A, B\} = \int_{V} \frac{1}{\varrho} \left[(A_{v})_{i} \left[\partial_{j} (B_{\varepsilon^{d}})_{ij} + \partial_{j} (B_{\varepsilon^{s}})_{ij} \right] + (A_{\varepsilon^{d}})_{ij} \left\{ \frac{1}{2} \left[\partial_{j} (B_{v})_{i} + \partial_{i} (B_{v})_{j} \right] - \frac{1}{3} \partial_{k} (B_{v})_{k} \delta_{ij} \right\} + (A_{\varepsilon^{s}})_{ij} \frac{1}{3} \partial_{k} (B_{v})_{k} \delta_{ij} \right] dV.$$
(IV.34)

Via integration by parts and omitting surface terms,

$$\{A, B\} = -\int_{V} \frac{1}{\varrho} \left[\partial_{j} (A_{v})_{i} (B_{\varepsilon^{d}})_{ij} + \partial_{j} (A_{v})_{i} (B_{\varepsilon^{s}})_{ij} + \frac{1}{2} \left[\partial_{j} (A_{\varepsilon^{d}})_{ij} (B_{v})_{i} + \partial_{i} (A_{\varepsilon^{d}})_{ij} (B_{v})_{j} \right] - \frac{1}{3} \partial_{k} (A_{\varepsilon^{d}})_{ij} (B_{v})_{k} \delta_{ij} + \frac{1}{3} \partial_{k} (A_{\varepsilon^{s}})_{ij} (B_{v})_{k} \delta_{ij} \right] dV.$$
(IV.35)

Now, taking into consideration that the functional derivative of a scalar functional with respect to a symmetric tensor is symmetric, with respect to a deviatoric tensor is deviatoric, and with respect to a spherical tensor is spherical, the first term in the integrand can be reformulated as

$$\operatorname{tr}\left\{B_{\varepsilon^{\mathrm{d}}}\left[\left(A_{v}\otimes\stackrel{\leftarrow}{\nabla}\right)^{\mathrm{S}}\right]^{\mathrm{d}}\right\},\tag{IV.36}$$

and the second term can be treated analogously. Next, it is easy to show that the third term is $B_v \cdot (A_{\varepsilon^d} \cdot \nabla)$. Further, in the terms that contain δ_{ij} , the *j* index can be changed to *i*, hence, in these terms we find the gradient of the trace of a tensor. Therefore, the fourth term contains trace of a deviatoric tensor—which is traceless—so this term gives zero contribution. Finally, the fifth term contains a spherical tensor and thus can be rewritten as $\frac{1}{3}\partial_k(A_{\varepsilon^s})_{ii}(B_v)_k = \partial_k(A_{\varepsilon^s})_{ik}(B_v)_i$. To sum up, we find

$$\{A, B\} = -\int_{V} \frac{1}{\varrho} \left[B_{v} \cdot \left(A_{\varepsilon^{d}} \cdot \overleftarrow{\nabla} + A_{\varepsilon^{s}} \cdot \overleftarrow{\nabla} \right) + \operatorname{tr} \left\{ B_{\varepsilon^{d}} \left[\left(A_{v} \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{d}} \right\} + \operatorname{tr} \left\{ B_{\varepsilon^{s}} \left[\left(A_{v} \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} \right\} \right] dV = -\{B, A\},$$
(IV.37)

that is, antisymmetry is revealed.

Since L is independent of the state variables and is antisymmetric, the generalized Poisson bracket also satisfies the Jacobi identity [107].

Now let us turn towards the irreversible side: the operator matrix M can be constructed from the second term of the time evolution equation (IV.28) and the degeneracy condition (II.44); we find

$$\mathbf{M} = \begin{pmatrix} M_{11} & \mathbf{0} \cdot & \mathbf{0} \cdot & M_{14} & M_{15} & M_{16} \\ \mathbf{0} \otimes & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} \otimes & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ M_{41} & \mathbf{0} : & \mathbf{0} : & M_{44} & M_{45} & M_{46} \\ M_{51} & \mathbf{0} & \mathbf{0} & M_{54} & M_{55} & \mathbf{0} \\ M_{61} & \mathbf{0} & \mathbf{0} & M_{64} & \mathbf{0} & M_{66} \end{pmatrix}$$
(IV.38)

with⁶

One can notice that this M is not symmetric—see the elements that contain l_{12}^d vs. l_{21}^d , as well as the ones with l_{12}^s vs. l_{21}^s . As mentioned in Section IV.1, when we have no additional microscopic or experimental information about $\boldsymbol{\xi}$ and about the corresponding coefficients l^d , l^s then we cannot exclude that antisymmetric parts l_A^d , l_A^s appear in the dynamics.

On the other side, positive semidefiniteness can be shown by reformulating the integrand of the irreversible bracket [A, A] to a quadratic expression. More closely, we can form a matrix that contains non-negative elements and the Onsagerian coefficients, and (IV.19)–(IV.20) just prove to be the conditions that ensure positive semidefiniteness. The calculation is straightforward but lengthy.

Actually, the whole realization of $\boldsymbol{\xi}$ -based rheology provided above is straightforward (if lengthy), and is expected to work for non-constant coefficient matrices l^{d} , l^{s} as well. However, specifically for constant coefficients, an alternative version is also possible: implementing the antisymmetric part of the coefficient matrices, that is, the constants l_{A}^{d} , l_{A}^{s} , in the reversible part of the time evolution.

For this case, let us use the prepared (IV.21)–(IV.22) form of the Onsagerian equations. Rearranging the time evolution equation is straightforward, and one finds for the alternative reversible operator matrix

⁶An outline and order of obtaining the components is as follows: $M_{24} = 0$ and $M_{34} = 0$ from (IV.28), $M_{42} = 0$ and $M_{43} = 0$ from (II.42), $M_{56} = 0$ and $M_{65} = 0$ from (IV.28), M_{44} from (IV.28), M_{54} and M_{64} from (IV.28), M_{45} and M_{46} from (II.42), M_{41} from (II.44), M_{14} from (II.42), M_{51} and M_{55} from (IV.28), M_{61} and M_{66} from (IV.28), M_{15} and M_{16} from (II.42), M_{11} from (II.44), the unconstrained remaining components can be set to zero.

$$\mathbf{L}' = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & 0 & -\frac{l_{A}^{d}}{\varrho} \bullet \cdot \overleftarrow{\nabla} & -\frac{l_{A}^{s}}{\varrho} \bullet \cdot \overleftarrow{\nabla} \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{d}} & 0 & 0 & 0 & 0 \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} & 0 & 0 & 0 & 0 \\ \mathbf{0} \cdot & \mathbf{0} : & \mathbf{0} : & 0 & \mathbf{0} : & \mathbf{0} : \\ -\frac{l_{A}^{d}}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{d}} & 0 & 0 & \mathbf{0} & 0 \\ -\frac{l_{A}^{s}}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} & 0 & 0 & \mathbf{0} & 0 \\ 0 \cdot & \mathbf{0} : & \mathbf{0} : & \mathbf{0} : & \mathbf{0} : \\ \mathbf{0} \cdot & \mathbf{0} : & \mathbf{0} : & \mathbf{0} : & \mathbf{0} : \\ -\frac{l_{A}^{s}}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} & 0 & 0 & \mathbf{0} & \mathbf{0} & 0 \\ 0 \cdot & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\frac{l_{A}^{s}}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^{\mathbf{s}} & 0 & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \end{array} \right],$$
(IV.40)

while the elements of the alternative irreversible operator matrix \mathbf{M}' are very similar to (IV.39): we just have to change all l_{12}^d and l_{21}^d to l_{S}^d and, similarly, l_{12}^s and l_{21}^s to l_{S}^s . The degeneracy criteria, antisymmetry of \mathbf{L}' , the Jacobi identity for the generalized Poisson brackets,

The degeneracy criteria, antisymmetry of L', the Jacobi identity for the generalized Poisson brackets, and positive semidefiniteness for M' prove to be satisfied. Moreover, in this case the symmetric property of M' also holds.

We repeat that this alternative realization is valid only for constant Onsagerian coefficients as otherwise the Jacobi identity can be violated.

This latter variant appears rather counter-intuitive from principal point of view but may be beneficial for numerical solutions, *e.g.*, , to have as much symplectic part in the numerical scheme as possible—see [108, 56] about the importance of this.

IV.2.1 Temperature as state variable

For mechanical engineering applications and evaluations of experiments (see, *e.g.*, [1]), it can be beneficial to use temperature, instead of entropy, as state variable. Then the collection of state variables is

$$\tilde{\mathbf{x}} = \left(\mathbf{v}, \boldsymbol{\varepsilon}^{\mathrm{d}}, \boldsymbol{\varepsilon}^{\mathrm{s}}, T, \boldsymbol{\xi}^{\mathrm{d}}, \boldsymbol{\xi}^{\mathrm{s}}\right).$$
(IV.41)

To keep the discussion as concrete and basic as possible, let us choose the simplest constitutive equation for the internal energy, linear in temperature with constant specific heat *c*, containing elastic energy related to Hooke's law,

$$\boldsymbol{\sigma}_0 = E^{\mathrm{d}} \boldsymbol{\varepsilon}^{\mathrm{d}} + E^{\mathrm{s}} \boldsymbol{\varepsilon}^{\mathrm{s}}, \qquad E^{\mathrm{d}} = 2G, \quad E^{\mathrm{s}} = 3K, \tag{IV.42}$$

and neglecting thermal expansion—which is manifested in the separation of strain dependence and temperature dependence—:

$$\tilde{e}_{\text{int},0}(\tilde{\mathbf{x}}) = \tilde{e}_{\text{thermal}}(T) + \tilde{e}_{\text{elastic}}(\boldsymbol{\varepsilon}^{d}, \boldsymbol{\varepsilon}^{s}) = cT + \frac{E^{d}}{2\varrho} \operatorname{tr}\left(\boldsymbol{\varepsilon}^{d}\boldsymbol{\varepsilon}^{d}\right) + \frac{E^{s}}{2\varrho} \operatorname{tr}\left(\boldsymbol{\varepsilon}^{s}\boldsymbol{\varepsilon}^{s}\right).$$
(IV.43)

Temperature has the same relationship to specific entropy as seen in Section IV.2, now utilized in the opposite direction (*i.e.*, what is a variable and what is a function): The thermodynamical consistency condition $\frac{d\tilde{s}_0}{dT} = \frac{1}{T} \frac{d\tilde{e}_{\text{thermal}}}{dT}$ that follows from the Gibbs relation [and which is the manifestation of the third equation of (IV.4)] leads to

$$\tilde{s}_0\left(\tilde{\mathbf{x}}\right) = \tilde{s}_{\text{aux}} + c \ln \frac{T}{T_{\text{aux}}},\tag{IV.44}$$

with auxiliary constants \tilde{s}_{aux} , T_{aux} , and the extension (IV.7) induces

$$\tilde{s}\left(\tilde{\mathbf{x}}\right) = \tilde{s}_{0}\left(\tilde{\mathbf{x}}\right) - \frac{1}{2}\operatorname{tr}\left(\boldsymbol{\xi}^{\mathsf{d}}\boldsymbol{\xi}^{\mathsf{d}}\right) - \frac{1}{2}\operatorname{tr}\left(\boldsymbol{\xi}^{\mathsf{s}}\boldsymbol{\xi}^{\mathsf{s}}\right),\tag{IV.45}$$

or, expressing temperature,

$$T\left(\tilde{s}_0\left(\tilde{s}, \boldsymbol{\xi}^{\mathrm{d}}, \boldsymbol{\xi}^{\mathrm{s}}\right)\right) = T_{\mathrm{aux}} \exp\left(\frac{\tilde{s}_0\left(\tilde{s}, \boldsymbol{\xi}^{\mathrm{d}}, \boldsymbol{\xi}^{\mathrm{s}}\right) - \tilde{s}_{\mathrm{aux}}}{c}\right).$$
(IV.46)

Now the energy and entropy functionals are

$$\tilde{E} = \int_{V} \varrho \tilde{e}_{\text{total}} dV = \int_{V} \varrho \left[\frac{1}{2} \mathbf{v} \cdot \mathbf{v} + cT + \frac{E^{d}}{2\varrho} \operatorname{tr} \left(\boldsymbol{\varepsilon}^{d} \boldsymbol{\varepsilon}^{d} \right) + \frac{E^{s}}{2\varrho} \operatorname{tr} \left(\boldsymbol{\varepsilon}^{s} \boldsymbol{\varepsilon}^{s} \right) \right] dV, \quad (IV.47)$$

$$\tilde{S} = \int_{V} \rho \tilde{s} dV = \int_{V} \rho \left[\tilde{s}_{aux} + c \ln \frac{T}{T_{aux}} - \frac{1}{2} \operatorname{tr} \left(\boldsymbol{\xi}^{d} \boldsymbol{\xi}^{d} \right) - \frac{1}{2} \operatorname{tr} \left(\boldsymbol{\xi}^{s} \boldsymbol{\xi}^{s} \right) \right] dV, \qquad (IV.48)$$

with corresponding functional derivatives

$$\frac{\delta \tilde{E}}{\delta \tilde{\mathbf{x}}} = \begin{pmatrix} \varrho \mathbf{v} \\ E^{d} \boldsymbol{\varepsilon}^{d} \\ E^{s} \boldsymbol{\varepsilon}^{s} \\ \varrho c \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \qquad \qquad \frac{\delta \tilde{S}}{\delta \tilde{\mathbf{x}}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \frac{\varrho c}{T} \\ -\varrho \boldsymbol{\xi}^{d} \\ -\varrho \boldsymbol{\xi}^{s} \end{pmatrix}.$$
(IV.49)

A transformation of variables $\mathbf{x} \to \tilde{\mathbf{x}}$ is performed, to which the transformation (operator) matrix $\mathbf{Q} = \frac{\delta \tilde{\mathbf{x}}}{\delta \mathbf{x}}$ is accompanied. This \mathbf{Q} can be used to establish the relationship between the original and transformed reversible and irreversible operator matrices [107]:

$$\tilde{\mathbf{L}} = \mathbf{Q}\mathbf{L}\mathbf{Q}^{\mathrm{T}}, \qquad \tilde{\mathbf{M}} = \mathbf{Q}\mathbf{M}\mathbf{Q}^{\mathrm{T}}.$$
 (IV.50)

In the present current special case, we change only the fourth state variable (from s to T), so only the fourth row of **Q** contains nontrivial elements. Furthermore, since (IV.46) does not contain non-local (gradient) terms, we can realize the transformation directly in the form

$$\mathbf{Q} = \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}} = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbb{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbb{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \frac{1}{c}T & \frac{1}{c}T\boldsymbol{\xi}^{\mathsf{d}} & \frac{1}{c}T\boldsymbol{\xi}^{\mathsf{s}} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbb{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbb{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbb{I} \end{pmatrix},$$
(IV.51)

where \mathbb{I} denotes the fourth-order identity tensor [the identity that maps tensors to tensors, *i.e.*, to themselves]. Then, using (IV.50) yields⁷

$$\tilde{\mathbf{L}} = \mathbf{L}$$
 (IV.52)

so all the requirements of GENERIC—antisymmetry, Jacobi identity, degeneracy—prove to hold for L,

⁷Results (IV.52), (IV.53) can also be derived directly from the time evolution formula and the degeneracy conditions.

and we find that the structure of \tilde{M} is the same as of M [see (IV.38)], with the elements

$$\begin{split} \tilde{M}_{11} &= -\frac{l_{11}^{1}}{\varrho^{2}} \left\{ T \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{d} \right\} \cdot \tilde{\nabla} - \frac{l_{11}^{s}}{\varrho^{2}} \left\{ T \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{s} \right\} \cdot \tilde{\nabla}, \\ \tilde{M}_{14} &= \frac{1}{\varrho^{2}c} \left\{ l_{11}^{d} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{d} T \bullet + l_{11}^{s} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{s} T \bullet \right\} \cdot \tilde{\nabla}, \\ \tilde{M}_{15} &= \frac{l_{12}^{d}}{\varrho} (T \bullet) \cdot \tilde{\nabla}, \\ \tilde{M}_{15} &= \frac{l_{12}^{d}}{\varrho} (T \bullet) \cdot \tilde{\nabla}, \\ \tilde{M}_{41} &= -\frac{T}{\varrho^{2}c} \operatorname{tr} \left\{ l_{11}^{d} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{d} \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{d} + l_{11}^{s} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{s} \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{s} \right\}, \\ \tilde{M}_{44} &= \frac{T}{\varrho^{2}c^{2}} \operatorname{tr} \left\{ l_{11}^{d} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{d} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{d} \bullet + l_{11}^{s} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{s} \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{s} \bullet \right\}, \\ \tilde{M}_{45} &= \frac{l_{12}^{d}}{\varrho c} T \operatorname{tr} \left\{ \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{d} \bullet \right\}, \\ \tilde{M}_{51} &= -\frac{l_{21}^{d}}{\varrho} T \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{d}, \\ \tilde{M}_{51} &= -\frac{l_{21}^{d}}{\varrho} T \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{d}, \\ \tilde{M}_{61} &= -\frac{l_{21}^{s}}{\varrho} T \left[\left(\bullet \otimes \tilde{\nabla} \right)^{S} \right]^{s}, \\ \tilde{M}_{64} &= \frac{l_{21}^{s}}{\varrho c} T \left[\left(\mathbf{v} \otimes \tilde{\nabla} \right)^{S} \right]^{s}, \\ \tilde{M}_{66} &= l_{22}^{s} T. \end{split}$$

The variable transformation is expected to preserve the structure of GENERIC ([107], page 26 in Section 1.2.4). Indeed, by substituting (IV.43) into (IV.10) and rewriting it in terms of temperature, the evolution equation for T is obtained, and turns out to coincide with the fourth row of $\tilde{M}\frac{\delta \tilde{S}}{\delta \tilde{x}}$ so the whole evolution equation has been preserved under the transformation. Meanwhile, as in the variable *s* case M has proved nonsymmetric for nonzero l_{d}^{4} or l_{s}^{5} . \tilde{M} behaves the same way.

has proved nonsymmetric for nonzero l_A^d or l_A^s , \tilde{M} behaves the same way. Now let us repeat moving the l_A^d and l_A^s related part of the dynamics to the reversible part. We find the antisymmetric

$$\tilde{\mathbf{L}}' = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \tilde{L}'_{14} & -\frac{l_A^d}{\varrho} \bullet \cdot \overleftarrow{\nabla} & -\frac{l_A^s}{\varrho} \bullet \cdot \overleftarrow{\nabla} \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^d & 0 & 0 & \mathbf{0} & 0 \\ \frac{1}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^s & 0 & 0 & \mathbf{0} & 0 & 0 \\ \tilde{L}'_{41} & \mathbf{0} : & \mathbf{0} : & \mathbf{0} & \mathbf{0} : & \mathbf{0} : \\ -\frac{l_A^d}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^d & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 \\ -\frac{l_A^s}{\varrho} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \right]^s & 0 & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 \end{pmatrix} \end{pmatrix}$$
(IV.54)

with

$$\widetilde{L}_{14}' = -\frac{1}{\varrho c} \left(l_{A}^{d} T \boldsymbol{\xi}^{d} \bullet + l_{A}^{s} T \boldsymbol{\xi}^{s} \bullet \right) \cdot \overleftarrow{\nabla},
\widetilde{L}_{41}' = -\frac{T}{\varrho c} \operatorname{tr} \left\{ l_{A}^{d} \boldsymbol{\xi}^{d} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{S} \right]^{d} + l_{A}^{s} \boldsymbol{\xi}^{s} \left[\left(\bullet \otimes \overleftarrow{\nabla} \right)^{S} \right]^{s} \right\},$$
(IV.55)

and that $\tilde{\mathbf{M}}'$ can be obtained from $\tilde{\mathbf{M}}$ like \mathbf{M}' from \mathbf{M} , *i.e.*, changing all l_{12}^{d} and l_{21}^{d} to l_{s}^{d} and l_{12}^{s} and l_{21}^{s} to l_{s}^{s} . Symmetricity and positive semidefiniteness of $\tilde{\mathbf{M}}$, the degeneracy criteria, as well as the Jacobi identity related to $\tilde{\mathbf{L}}'$ are all satisfied.

It is to be noted here that, while the Jacobi property of $\tilde{\mathbf{L}}'$ is foreseen on general grounds – any variable transformation is expected to preserve the Jacobi identity ([107], page 26 in Section 1.2.4) –, checking it directly is nonstraightforward. The difficulty is related to the task of identifying total divergences of multiple products among the numerous terms. When we used the application jacobi.m [140] – with appropriately increased memory limit and run-time limit –, it could not confirm the Jacobi identity (while it found its validity for \mathbf{L} , \mathbf{L}' and $\tilde{\mathbf{L}}$ seamlessly). Instead, we have verified the Jacobi property of $\tilde{\mathbf{L}}'$ both by hand and via an own symbolic code. A key element was an advantageous convention for classifying and grouping terms, which has reduced the number of terms from thousands to hundreds, enabling to observe the remaining cancellations.

IV.3 Conclusions

The results can be summarized according to Table IV.1.

	variable s		variable T	
	$l_{\mathrm{A}}^{\mathrm{d}}, l_{\mathrm{A}}^{\mathrm{s}}$ in \mathbf{M}	$l_{\mathrm{A}}^{\mathrm{d}}, l_{\mathrm{A}}^{\mathrm{s}}$ in \mathbf{L}	$l_{\rm A}^{ m d}, l_{ m A}^{ m s}$ in ${f M}$	$l_{\mathrm{A}}^{\mathrm{d}}, l_{\mathrm{A}}^{\mathrm{s}}$ in \mathbf{L}
L fulfils Jacobi	\checkmark	\checkmark	\checkmark	\checkmark
M is symmetric	$ imes$ if $l_{ m A}^{ m d}, l_{ m A}^{ m s} eq 0$	\checkmark	$ imes$ if $l_{ m A}^{ m d}, l_{ m A}^{ m s} eq 0$	\checkmark

Table IV.1: How the four versions behave with respect to generic GENERIC expectations.

This means that the Kluitenberg–Verhás model family—which has been derived originally via the internal variable methodology—is compatible with the GENERIC framework. Nowadays, the demand to unify the several branches of irreversible thermodynamics is increasingly pronounced, thus this work contributes to this direction. In parallel, as it was already mentioned at the beginning of this chapter, this GENERIC realization is also significant for numerical applications. The next chapter presents a numerical solution method for calculating wave propagation in a Poynting–Thomson–Zener medium, which method is strongly based on the reversible–irreversible decomposition of the time evolution equations.

A challenge for GENERIC with its explicit time evolution formulation is the treatment of problems in the force-equilibrial approximation [zero lhs in (IV.6), an approximation valuable for various engineering situations]. In Chapter VI], analytical solutions for various situations are presented in this approximation, however, for more general situations, an effective and reliable numerical treatment would be welcome. Hopefully, the GENERIC-based reversible–irreversible decomposition can contribute such methods in the future.

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Chapter V

Thermodynamical extension of a symplectic numerical scheme

Numerical solution methods for dissipative problems are important and are a nontrivial topic. Already for reversible systems, the difference between a symplectic and nonsymplectic finite difference method is striking: the former can offer reliable prediction that stays near the exact solution even at extremely large time scales, while the latter may provide a solution that drifts away from the exact solution steadily. For dissipative systems, the situation is harder. Methods that were born with reversibility in mind may apparently fail for a nonreversible problem. For example, a finite element software is able to provide, at the expense of a large run time, a quantitatively and even qualitatively wrong outcome, while a simple finite difference scheme solves the same problem fast and precisely [27].

Partly inspired by, and partly based on, the intensive development on symplectic schemes for reversible problems, remarkable research has been done in recent years to develop geometric methods for dissipative systems, more on ones with finite degrees of freedom (including [52, 53, 54, 55, 56, 57] and less for continua (see, e.g., [50, 51, 101, 141]).

Thermodynamics also modifies the way of thinking concerning numerical modeling. Even if quantities known from mechanics form a closed system of equations to solve numerically, monitoring temperature (or other thermodynamical quantities) for a nonreversible system can give insight on the processes and phenomena, for example, pointing out the presence of viscoelasticity/rheology, and displaying when plastic changes start [1]. In addition, temperature can also react in the form of thermal expansion and heat conduction, even in situations where one is not prepared for this "surprise" [23].

Furthermore, in a sense, thermodynamics is a stability theory. Therefore, how thermodynamics ensures asymptotic stability for systems may give new ideas on how the stability and suppression of errors can be achieved for numerical methods. A conceptually closer relationship is desirable between these two areas.

Along these lines, this chapter presents a study where a new numerical scheme is suggested and applied for a continuum thermodynamical model. The scheme proves to be an extension of a symplectic method. In parallel, this finite difference scheme introduces a staggered arrangement of quantities by half space and time steps with respect to each other, according to the spacetime nature of the involved quantities and the nature of equations governing them. The shifts can be introduced by inspecting the equations. It turns out that balances, kinematic equations, and Onsagerian equations all have their own distinguished discretized realization. The shifts also render the scheme with one order of accuracy higher than the original symplectic scheme.

In many of the practical applications, numerical calculations must be performed many times with different material coefficients, for example, as part of a fitting procedure where experimental data are to be fitted. Hence, the numerical scheme should be fast, resource-friendly yet reliable and precise enough.

In addition, numerical calculations face at three frequent challenges:

1. instability (exponential blow-up of the solution),

- 2. dissipation error (artificial decrease of amplitudes and energies), and
- 3. dispersion error (artificial oscillations near fast changes).

A good scheme keeps these artefacts under control.

Now, if a numerical scheme exhibits dissipation error for conservative systems, then it is expected to behave similarly for nonconservative ones so one cannot separate the real dissipation of mechanical energy from the dissipation artefact of the scheme. And, similarly, a real wavy behaviour cannot be distinguished from the dispersion/wavy artefact.

In parallel, thermodynamics is important not only from the aspect of balances. Namely, traditional and well-known numerical methods and commercial finite element softwares focus only on the set of equations to solve, that is, on the minimally necessary equations to follow the minimally necessary quantities. However, knowing from the spacetime perspective that momentum and energy form a four-quantity (also in continuum theory on Galilean spacetime) [74], in addition to the customarily taken balance of momentum, the balance of energy is also present. This enables one to follow, in addition to the mechanically considered quantities, internal energy—or, if practice favours so, temperature—as well. The point in doing so (even in situations where thermomechanical coupling and heat conduction are neglected) is that, if, say, temperature is followed via a separate discretized evolution equation, then conservation of total energy—at the discretized level—is not built-in but is a property that will hold only approximately. Then, checking how well this conservation holds along the numerical solution can provide a diagnostic tool. Thus one may check the degree of dissipation error (*i.e.*, the degree of violation of total energy that should be a constant).

Driven by (primarily rock mechanical) applications in scope, the simulation of wave phenomena in the Poynting–Thomson–Zener (PTZ) rheological model for solids via commercial finite element softwares have been performed. The results—already for the Hookean case (but also for non-Fourier heat conduction [27])—were disappointing: the solutions ran very slowly, with large memory and CPU demand, and were burdened by considerable numerical artefacts of the mentioned kinds.

To see the problem more closely, let us consider numerical solutions obtained via a commercial finite element software, namely, COMSOL v5.3a. Wave propagation is studied in a finite-size one spatial dimensional Hookean sample, the wave is induced by a pulse at the left endpoint of the rod and, except for the duration of the pulse, the two endpoint boundaries are treated stress-free. In this problem, the only free (nondimensional) parameter is related to the temporal length of the pulse (for details, see Section V.2.2). Figures V.1, V.2 and V.3 present the rear-side velocity history of the sample in time with different methods and settings.



Figure V.1: Dimensionless rear-side velocity history in dimensionless time for dimensionless pulse length 0.2 calculated by Backward Differentiation Formula. *Left:* Maximum BDF order: 2. *Right:* Maximum BDF order: 5. The presented solutions prove that artificial damping of the lower-order version is stronger, while, with the higher-order scheme, the damping is less significant; therefore, the artificial oscillations are less suppressed.



Figure V.2: Dimensionless rear-side velocity history in dimensionless time calculated by the Runge–Kutta based fifth order Dormand—Prince scheme. *Left:* Dimensionless pulse length: 0.2. *Right:* Dimensionless pulse length: 0.04. For smaller pulse length the numerical originated dispersive and dissipative errors also are well visible.



Figure V.3: Dimensionless rear-side velocity history in dimensionless time calculated by the Runge–Kutta based method RK34, which is recommended by the COMSOL manual to solve oscillatory problems [142]. *Left:* Dimensionless pulse length: 0.2. *Right:* Dimensionless pulse length: 0.04. Again, for smaller pulse length the dispersive and dissipative errors are more visible.

The results demonstrate that the different solvers are sensitive to the different settings, thus choosing a reliable one is a difficult task. The above figures present that both dissipation and of dispersion errors occur in the results.

The dependence of the numerical solutions on the applied time integration algorithms is more visible in higher spatial dimensions (see Figure I.15). Taking into account that the full problem that will be analyzed in what follows has 16 coupled degrees of freedom in three spatial dimensions and with further time derivatives (in the PTZ model), it does not seem reasonable to try to represent it via any commercial finite element software as long as such a much simpler problem cannot be treated confidently.

These all motivated the development such a numerical scheme that performs better. Similarly to that the PTZ model can be obtained in a thermodynamical approach as an internal variable extension of Hooke elasticity [43], the starting point is a symplectic scheme for Hooke elasticity. Symplectic numerical schemes (see, *e.g.*, [143]) provide much better large-time approximations, thanks to the fact that a symplectic numerical integrator of a conservative system is actually the exact integrator of a 'nearby' (coinciding in the zeroth order of the time step) conservative system.

In recent years, numerous works have been born to develop extensions of symplectic schemes to nonconservative systems [52, 53, 54, 55, 56, 57, 50, 51, 101, 141]). Here, the same path is chosen, and such an extension is devised, on the example of the PTZ model, presented first in one spatial dimension and then in three spatial dimensions, with the novelties that some discretized field values reside with half space and time steps with respect to some other field values. This made the symplectic Euler method—an originally order-one accurate scheme—accurate to second order, and spatial accuracy was also second order.

The developed scheme performs well indeed: it produces, in a much faster and resource-friendlier way, much more artefact-free solutions.

This chapter is based on the publications [44, 48]. The author's contributions are as follows:

- Investigating the stability, dissipation and dispersive errors of the one spatial dimensional scheme;
- Numerical proof of the total energy preserving property of the scheme for a three spatial dimensional Cartesian grid.

V.1 Properties of the continuum Poynting–Thomson–Zener model and the thermodynamics behind

The continuum system that is the subject of the investigation is important on its own—it is the PTZ rheological model for solids. This model exhibits both dissipation and wave propagation (actually, dispersive wave propagation), and this is thus ideal for testing various aspects and difficulties. Meanwhile, its predictions are relevant for many solids, typically ones with complicated micro- or mesoscopic structure, such as rocks [42, 40, 41], plastics [1], and asphalt. This non-Newtonian rheological model can explain why slow and fast measurements and processes yield different results.

A homogeneous and isotropic solid, in the small-strain approximation (with respect to an inertial reference system) is considered, correspondingly, substantial time derivative coincides with partial time derivative, mass density ρ can be treated as constant, and the relationship between the symmetric strain tensor ε to the velocity field v is

$$\partial_t \boldsymbol{\varepsilon} = \left(\mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbf{S}} \tag{V.1}$$

[(II.25) is repeated here for convenience].

The symmetric stress tensor σ governs the time evolution of v according to balance of linear momentum

$$\varrho \partial_t \mathbf{v} = \boldsymbol{\sigma} \cdot \overleftarrow{\nabla}; \tag{V.2}$$

now, volumetric force density ρg is neglected [(II.21) is repeated here for convenience].

Hooke elasticity can be expressed as

$$\boldsymbol{\sigma}^{\mathrm{d}} = E^{\mathrm{d}} \boldsymbol{\varepsilon}^{\mathrm{d}}, \qquad \qquad \boldsymbol{\sigma}^{\mathrm{s}} = E^{\mathrm{s}} \boldsymbol{\varepsilon}^{\mathrm{s}}, \qquad \qquad (\mathrm{V.3})$$

and its PTZ generalization is

$$\boldsymbol{\sigma}^{d} + \tau^{d}\partial_{t}\boldsymbol{\sigma}^{d} = E^{d}\boldsymbol{\varepsilon}^{d} + \hat{E}^{d}\partial_{t}\boldsymbol{\varepsilon}^{d}, \qquad \boldsymbol{\sigma}^{s} + \tau^{s}\partial_{t}\boldsymbol{\sigma}^{s} = E^{s}\boldsymbol{\varepsilon}^{s} + \hat{E}^{s}\partial_{t}\boldsymbol{\varepsilon}^{s}; \qquad (V.4)$$

the material coefficients will be treated as constants hereafter (as a reminder, ^d and ^s denote the deviatoric and spherical parts of second order tensors, respectively). To make the subsequent formulae more intelligible, we introduce the irreversible stress contributions

$$\hat{\boldsymbol{\sigma}}^{d} = \boldsymbol{\sigma}^{d} - E^{d} \boldsymbol{\varepsilon}^{d}, \qquad \qquad \hat{\boldsymbol{\sigma}}^{s} = \boldsymbol{\sigma}^{s} - E^{s} \boldsymbol{\varepsilon}^{s} \qquad (V.5)$$

and the coefficient combinations

$$\hat{I}^{d} = \hat{E}^{d} - \tau^{d} E^{d}, \qquad \qquad \hat{I}^{s} = \hat{E}^{s} - \tau^{s} E^{s}, \qquad (V.6)$$

with the aid of which (V.4) gets simplified to

$$\hat{\boldsymbol{\sigma}}^{d} + \tau^{d} \partial_{t} \hat{\boldsymbol{\sigma}}^{d} = \hat{I}^{d} \partial_{t} \boldsymbol{\varepsilon}^{d}, \qquad \qquad \hat{\boldsymbol{\sigma}}^{s} + \tau^{s} \partial_{t} \hat{\boldsymbol{\sigma}}^{s} = \hat{I}^{s} \partial_{t} \boldsymbol{\varepsilon}^{s}. \qquad (V.7)$$

Taking (also for simplicity) a constant 'isobaric' specific heat capacity c_{σ} as well as neglected thermal expansion and heat conduction, the internal variable approach puts the following thermodynamical background behind the PTZ model: after eliminating the internal variable, it is specific total energy

$$e_{\text{total}} = e_{\text{kinetic}} + e_{\text{thermal}} + e_{\text{elastic}} + e_{\text{rheological}}, \qquad (V.8)$$

$$e_{\text{kinetic}} = \frac{1}{2} \mathbf{v}^{2}, \qquad e_{\text{elastic}} = \frac{E^{d}}{2\varrho} \operatorname{tr}(\boldsymbol{\varepsilon}^{d} \boldsymbol{\varepsilon}^{d}) + \frac{E^{s}}{2\varrho} \operatorname{tr}(\boldsymbol{\varepsilon}^{s} \boldsymbol{\varepsilon}^{s}),$$

$$e_{\text{thermal}} = c_{\sigma} T, \qquad e_{\text{rheological}} = \frac{\tau^{d}}{2\varrho \hat{I}^{d}} \operatorname{tr}(\hat{\boldsymbol{\sigma}}^{d} \hat{\boldsymbol{\sigma}}^{d}) + \frac{\tau^{s}}{2\varrho \hat{I}^{s}} \operatorname{tr}(\hat{\boldsymbol{\sigma}}^{s} \hat{\boldsymbol{\sigma}}^{s})$$

with absolute temperature T, and accompanied with specific entropy s and entropy production rate density π_s

$$s = c_{\sigma} \ln \frac{T}{T_{\text{aux}}},\tag{V.9}$$

$$\pi_s = \frac{1}{T} \left\{ \frac{1}{\hat{I}^{\mathsf{d}}} \operatorname{tr} \left(\hat{\boldsymbol{\sigma}}^{\mathsf{d}} \hat{\boldsymbol{\sigma}}^{\mathsf{d}} \right) + \frac{1}{\hat{I}^{\mathsf{s}}} \operatorname{tr} \left(\hat{\boldsymbol{\sigma}}^{\mathsf{s}} \hat{\boldsymbol{\sigma}}^{\mathsf{s}} \right) \right\},\tag{V.10}$$

for which the specific internal energy part $e_{\text{total}} - e_{\text{kinetic}}$ fulfils the balance with neglected heat conduction

$$\varrho \partial_t (e_{\text{total}} - e_{\text{kinetic}}) = \text{tr}(\boldsymbol{\sigma} \partial_t \boldsymbol{\varepsilon}) \tag{V.11}$$

and specific entropy the balance

$$\varrho \partial_t s = \pi_s, \tag{V.12}$$

as can be found along the lines of [43] (including its Appendix B), and is straightforward to check. Due to the second law of thermodynamics,

$$\hat{I}^{d} > 0, \qquad \hat{I}^{s} > 0$$
 (V.13)

and

$$\pi_s \ge 0 \tag{V.14}$$

follow for the PTZ model [43], where (V.14) is already apparent from the form (V.10). Recall that heat conduction is neglected so there are no heat and entropy current density terms in the balances. In parallel, there is no term in e_{total} that couples T and ϵ , and—correspondingly—there is no ϵ dependent term in s, due to neglected thermal expansion.

From either balance (V.11) or (V.12), the time derivative of temperature can also be expressed:

$$\frac{\partial T}{\partial t} = \frac{T}{\varrho c_{\sigma}} \pi_s. \tag{V.15}$$

As a simple analysis of the PTZ model, for 'slow' processes, which is to be understood with respect to the time scales

$$\tau^{\mathrm{d}}, \qquad \hat{\tau}^{\mathrm{d}} = \hat{E}^{\mathrm{d}}/E^{\mathrm{d}}, \qquad \tau^{\mathrm{s}}, \qquad \hat{\tau}^{\mathrm{s}} = \hat{E}^{\mathrm{s}}/E^{\mathrm{s}}, \tag{V.16}$$

a rule-of-thumb approximation is to neglect the time derivative terms (to keep only the lowest time derivative term for each quantity) in (V.4). The result is nothing but the Hooke model (V.3), for which the longitudinal and transversal wave propagation speeds are

$$c_{\text{longitudinal}} = \sqrt{\frac{2E^{\text{d}} + E^{\text{s}}}{3\varrho}}, \qquad c_{\text{transversal}} = \sqrt{\frac{E^{\text{d}}}{2\varrho}}.$$
 (V.17)

Now, as opposed to this 'static' limit, let us consider the limit of 'fast' processes: then it is the time derivative terms (the highest time derivative term for each quantity) that we keep. The result is the time derivative of an effective/'dynamic' Hooke model:

$$\boldsymbol{\sigma}^{d} = E_{\infty}^{d} \boldsymbol{\varepsilon}^{d}, \quad \boldsymbol{\sigma}^{s} = E_{\infty}^{s} \boldsymbol{\varepsilon}^{s}, \qquad E_{\infty}^{d} = \hat{E}^{d} / \tau^{d} > E^{d}, \quad E_{\infty}^{s} = \hat{E}^{s} / \tau^{s} > E^{s}, \qquad (V.18)$$

where the inequalities follow from (V.13). Accordingly, the wave propagation speeds

$$\hat{c}_{\text{longitudinal}} = \sqrt{\frac{2\hat{E}_{\infty}^{\text{d}} + \hat{E}_{\infty}^{\text{s}}}{3\varrho}} > c_{\text{longitudinal}}, \qquad \hat{c}_{\text{transversal}} = \sqrt{\frac{\hat{E}_{\infty}^{\text{d}}}{2\varrho}} > c_{\text{transversal}}$$
(V.19)

follow. This, on one side, illustrates how the PTZ model can interpret that dynamic elasticity coefficients of rocks are larger than their static counterpart [144, 46]. On the other side, the nontrivial—frequency dependent, therefore, dispersive—wave propagation indicates that numerical solution of PTZ wave propagation problems should contain the minimal possible amount of dispersion error, to give account of the dispersive property of the continuum model itself. In parallel, the dissipative nature of the PTZ model requires the minimal possible amount of dispersive the decrease of wave amplitudes.

V.2 The numerical scheme in one spatial dimension

When investigating the longitudinal wave propagation in a one spatial dimensional rod, equations (V.2) and (V.1) reduce to

$$\varrho \partial_t v = \frac{\partial \sigma}{\partial x} \tag{V.20}$$

$$\partial_t \varepsilon = \frac{\partial v}{\partial x} \tag{V.21}$$

and the one spatial dimensional versions of the constitutive laws (V.3) and (V.4) are

$$\sigma = E\varepsilon \tag{V.22}$$

$$\sigma + \tau \partial_t \sigma = E\varepsilon + \hat{E}\partial_t \varepsilon, \tag{V.23}$$

where E is Young's modulus and \hat{E}, τ are positive (rheological) coefficients. Accordingly, (V.8) and (V.9) are

$$e_{\text{total}} = e_{\text{kinetic}} + e_{\text{thermal}} + e_{\text{elastic}} + e_{\text{rheological}} \equiv \frac{1}{2}v^2 + c_{\sigma}T + \frac{E}{2\varrho}\varepsilon^2 + \frac{\tau}{2\varrho\hat{I}}\left(\sigma - E\varepsilon\right)^2$$
(V.24)

$$s = c_{\sigma} \ln \frac{T}{T_{\text{aux}}},\tag{V.25}$$

and (V.6) simplifies to

$$\hat{I} = \hat{E} - \tau E > 0, \tag{V.26}$$

and, instead of (V.15), equation

$$\rho c_{\sigma} \partial_t T = \frac{(\sigma - E\varepsilon)^2}{\hat{I}}.$$
(V.27)

is treated.

Remarkably, also thanks to our simplifications, the closed system of Equations (V.20)–(V.23) to be solved is linear. Having the solution for v, ε , and σ , the further quantities (T, s, and the various energy terms) can be obtained.

Our system admits two distinguished time scales, τ and

$$\hat{\tau} = \frac{\hat{E}}{E} > \tau, \tag{V.28}$$

the inequality following from (V.26). The wave propagation speed in the slow limit is

$$c = \sqrt{\frac{E}{\varrho}},\tag{V.29}$$

and in the fast limit is

$$\hat{c} = \sqrt{\frac{E_{\infty}}{\varrho}} = \sqrt{\frac{\hat{E}}{\tau \varrho}}, \qquad \hat{c} > c$$
 (V.30)

with the so-called "dynamic" Young's modulus

$$E_{\infty} = \frac{\dot{E}}{\tau}, \qquad E_{\infty} > E. \tag{V.31}$$

The classic attitude to finite difference schemes is that all quantities are registered at the same discrete positions and at the same discrete instants. An argument against this practice is that, when dividing a sample into finite pieces, some physical quantities have a meaning related to the bulk, the center of a piece, while others have a physical role related to the boundaries of a unit. For example, in Fourier heat conduction, heat current density is proportional to the gradient of temperature. A natural discretization of this, in one space dimension, is that temperature values sit at the centers and heat current density values at the boundaries—in other words, at a half space step distance from the centers [27]. In addition, in heat conduction, the change rate of specific internal energy is determined by the divergence of the heat current density. The natural one space dimensional discretization is then that, since heat current density values sit at the boundaries, specific internal energy values e_{thermal} are placed at the centers (at the same places where temperature values T are put, which is in tune with the fact that the two are related to one another via $e_{\text{thermal}} = c_{\sigma}T$) [27]. More generally, in continuum theories, specific extensive and density quantities would naturally live at a center, while currents/fluxes are boundary-related by their physical nature/role.

Here, this approach is generalized. Namely, when one has a full—at the general level, 4D—spacetime perspective (which unfolds that traditional physical quantities are time- and spacelike components of four-vectors, four-covectors, four-cotensors *etc.* governed by 4D equations with four-divergences, fourgradients *etc.*), then it turns out that quantities may "wish" to be staggered with respect to each other by a half in time as well. Taking again the example of the balance of internal energy in heat conduction, the finite-difference discretization of the change rate of specific internal energy e_{thermal} contains the change $\Delta e_{\text{thermal}}$ corresponding to a finite time difference Δt . This change is caused by the flux of heat leaving the spatial unit during this time interval Δt , which is the time average of the flux naturally realized at half-time $\Delta t/2$. Accordingly, heat current density values would be realized as half-shifted in time with respect to specific internal energy.

More generally, if an equation relates the change rate of a quantity to another quantity, then these two quantities would be realized as half-shifted in time with respect to one another.

To sum up, the space and time derivatives suggest how we can arrange the quantities with space and time half-shifts, respectively.

This approach is realized for the present system. Discrete space and time values are chosen as

$$x_n = n\Delta x, \quad n = 0, 1, \dots, N, \qquad t^j = j\Delta t, \quad j = 0, 1, \dots, J,$$
 (V.32)

and discrete values of stress are prescribed to these spatial and temporal coordinates:

$$\sigma_n^j$$
 at t^j , x_n . (V.33)

Next, investigating (V.20), velocity values are put half-shifted with respect to stress values both in space and time:

$$v_{n+1/2}^{j-1/2}$$
 at $t^j - \frac{\Delta t}{2}, \quad x_n + \frac{\Delta x}{2},$ (V.34)

and we discretize (V.20) as

$$\rho \frac{v_{n+1/2}^{j+1/2} - v_{n+1/2}^{j-1/2}}{\Delta t} = \frac{\sigma_{n+1}^j - \sigma_n^j}{\Delta x}.$$
(V.35)

Next, studying (V.21) suggests analogously that strain values should have half-shifted with respect to velocity values both in time and space. Therefore, strain is to reside at the same spacetime location as stress:

$$\varepsilon_n^j$$
 at t^j , x_n , (V.36)

and (V.21) is discretized as

$$\frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} = \frac{v_{n+1/2}^{j+1/2} - v_{n-1/2}^{j+1/2}}{\Delta x}.$$
(V.37)

Finally, for the Hooke model, (V.22) is discretized plainly as

$$\sigma_n^j = E\varepsilon_n^j,\tag{V.38}$$

as stress and strain are assigned to the same locations. In the Hooke case, bookkeeping both stress and strain is redundant.



Figure V.4: Visualization of the finite difference numerical scheme. Velocity values stay at triangles, strain and stress values at rhombuses, and filled symbols denote values calculated via the scheme, while empty ones represent initial and boundary conditions. First, new velocities are determined from (V.35), new strains are obtained according to (V.37), and new stress values are obtained from (V.38) or (V.40). Grey indicates initial condition values (which are typically known for a whole time interval in practice). If the "grey dashed triangles" are not available, then an explicit Euler step can be used to produce the "white dashed triangles" for starting the scheme.

Rewriting the scheme for the Hooke case as

$$v_{n+1/2}^{j+1/2} = v_{n+1/2}^{j-1/2} + \frac{E}{\varrho} \frac{\Delta t}{\Delta x} \left(\varepsilon_{n+1}^j - \varepsilon_n^j \right), \qquad \varepsilon_n^{j+1} = \varepsilon_n^j + \frac{\Delta t}{\Delta x} \left(v_{n+1/2}^{j+1/2} - v_{n-1/2}^{j+1/2} \right), \tag{V.39}$$

one can recognize the steps of the symplectic Euler method [143] (with the Hamiltonian corresponding to $e_{\text{kinetic}} + e_{\text{elastic}}$). Now, a symplectic method is highly favorable because of its extremely good large-time behavior, including the preservation of energy conservation. While (V.39) coincides with the symplectic Euler method computationally, the present interpretation of the quantities is different, because of the space and time staggering. One advantageous consequence is that, due to the reflection symmetries (see Figure V.4), our scheme makes second-order accurate predictions (understood in powers of Δt and Δx), while the symplectic Euler method makes only first-order accurate ones [143] (see the proof in [44]).

In case of the PTZ model, one has to discretize (V.23). Here, both σ and its derivative, and both ε and its derivative, appear. Hence, staggering does not directly help. This is what one can expect for dissipative, irreversible, relaxation-type equations in general. However, an interpolation-like solution is possible:

$$\alpha \sigma_n^j + (1-\alpha)\sigma_n^{j+1} + \tau \frac{\sigma_n^{j+1} - \sigma_n^j}{\Delta t} = E\left[\alpha \varepsilon_n^j + (1-\alpha)\varepsilon_n^{j+1}\right] + \hat{E}\frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t}$$
(V.40)

where $\alpha = 1/2$ is expected to provide second-order accurate prediction, and other seminal values are $\alpha = 1$ (the explicit case, which is expected to be stiff) and $\alpha = 0$ (the fully implicit case).

For a generic α , (V.40) looks implicit. However, thermodynamics has brought in an *ordinary* differential equation-type extension to the Hooke continuum, not a *partial* one, and a linear one, in fact. Thus, (V.40) can be rewritten in explicit form:

$$\sigma_n^{j+1} = \frac{1}{1 - \alpha + \frac{\tau}{\Delta t}} \left\{ \left(\frac{\tau}{\Delta t} - \alpha \right) \sigma_n^j + E \left[\alpha \varepsilon_n^j + (1 - \alpha) \varepsilon_n^{j+1} \right] + \hat{E} \frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} \right\}$$
(V.41)

assuming

$$1 - \alpha + \frac{\tau}{\Delta t} \neq 0. \tag{V.42}$$

Verifying the second-order accuracy of (V.41) for $\alpha = 1/2$ is then straightforward.

V.2.1 Stability

One may specify a space step Δx according to the given need, adjusted to the desirable spatial resolution. » In parallel, the time step Δt is reasonably chosen to be considerably smaller than the involved time scales $(e.g., \tau \text{ and } \hat{\tau} \text{ of our example system})$. Now, a finite difference scheme may prove to be unstable for the taken Δx and Δt , making numerical errors (which are generated unavoidably because of floating-point round-off) increase essentially exponentially and ruin the usefulness of what we have done. Therefore, first, a stability analysis is recommended, to explore the region of good pairs of Δx , Δt for the given scheme and system.

Now, a von Neumann investigation [145] is performed for the scheme presented above, where the idea is similar to the derivation of a dispersion relation where the time evolution of continuum Fourier modes was studied, while here we examine whether errors, expanded in modes with e^{ikx_n} space dependence, increase or not, during an iteration by one time step. For such linear situations as ours, when the iteration step means a multiplication by a matrix, such a mode may simply obtain a growth factor ξ (that is k-dependent but space-independent); in other words, the iteration matrix (frequently called the "transfer matrix") has these modes as eigenvectors with the corresponding eigenvalues ξ . Thus, $|\xi| < 1$ (for all k) ensures stability. Furthermore, $|\xi| = 1$ means stability if the algebraic multiplicity of ξ —its multiplicity as a root of the characteristic polynomial of the transfer matrix—equals its geometric

multiplicity—the number of linearly independent eigenvectors (eigenmodes), *i.e.*, the dimension of the eigensubspace [146, 59].

We find it important to emphasize the following. The stability of the corresponding physical model, the Poynting–Thomson–Zener body, is ensured by the second law of thermodynamics. Thus, asymptotic stability of the solutions is guaranteed. The numerical method, and thus the stability analysis, must reflect the thermodynamical (physical) requirements as well, together with the particular conditions related to the applied discretization method. In overall, these aspects are not independent of each other. Such a way of thinking is also emphasized in [147], in which a numerical method is developed for electrodynamical problems using staggered fields and expecting similar properties as in our case.

With boundary conditions specified, one can say more¹. Boundary conditions may allow only certain combinations of e^{ikx_n} as eigenmodes of the transfer matrix. Consequently, this type of analysis is more involved and is, therefore, usually omitted. As a general rule of thumb, one can expect that $|\xi| > 1$ for some e^{ikx_n} indicates instability for modes obeying the boundary conditions, while $|\xi| \leq 1$ for all e^{ikx_n} suggests stability for all modes allowed by the boundary conditions².

V.2.1.1 The Hooke case

In the Hooke case, the "plane wave modes" for the two bookkept quantities v, ε can, for later convenience, be written as

$$v_{n+1/2}^{j-1/2} = iA_v^j e^{ik\left(n+\frac{1}{2}\right)\Delta x}, \qquad \qquad \varepsilon_n^j = A_\varepsilon^j e^{ikn\Delta x}, \qquad \qquad k\Delta x \in [0, 2\pi), \qquad (V.43)$$

and the condition on k related to that k outside such a "Brillouin zone" makes the description redundant.

Realizing the iteration steps (V.39) as matrix products leads, for the amplitudes introduced in (V.43), to

$$\begin{pmatrix} A_v^{j+1} \\ A_\varepsilon^{j+1} \end{pmatrix} = \begin{pmatrix} 1 & 2c^2 \frac{\Delta t}{\Delta x} S \\ -2\frac{\Delta t}{\Delta x} S & 1 - 4c^2 \frac{\Delta t^2}{\Delta x^2} S^2 \end{pmatrix} \cdot \begin{pmatrix} A_v^j \\ A_\varepsilon^j \end{pmatrix} \equiv \mathsf{T} \cdot \begin{pmatrix} A_v^j \\ A_\varepsilon^j \end{pmatrix}$$
(V.44)

with

$$S = \sin \frac{k\Delta x}{2}, \qquad 0 \le S \le 1. \tag{V.45}$$

For space dependences (V.43),

$$v_{n+1/2}^{j+1/2} = \xi v_{n+1/2}^{j-1/2}, \quad \varepsilon_n^{j+1} = \xi \varepsilon_n^j \quad \text{lead to} \quad A_v^{j+1} = \xi A_v^j, \quad A_\varepsilon^{j+1} = \xi A_\varepsilon^j, \quad (V.46)$$

in other words, to the eigenvalue problem

$$\mathsf{T}y = \xi y \qquad \text{with} \qquad y = \begin{pmatrix} A_v^j \\ A_\varepsilon^j \end{pmatrix}.$$
 (V.47)

Let us introduce the notation

$$C = c \frac{\Delta t}{\Delta x} \tag{V.48}$$

for the Courant number of our scheme for the Hooke system. Comparing the characteristic polynomial of T,

$$P(\xi) = \xi^2 + \left(4C^2S^2 - 2\right)\xi + 1 \tag{V.49}$$

¹Actually, all continuum problems require boundary or asymptotic conditions—we also specify some in the forthcoming section on applications.

²Namely, the problem of differing multiplicities for $|\xi| = 1$ can be wiped out by the boundary conditions.

with its form written via its roots,

$$(\xi - \xi_{+}) (\xi - \xi_{-}) = \xi^{2} - (\xi_{+} + \xi_{-}) \xi + \xi_{+} \xi_{-},$$
(V.50)

reveals, on one side, that, in order to have both $|\xi_+| \le 1$ and $|\xi_+| \le 1$, both magnitudes have to be 1 (since their product is 1), which, on the other side, also implies

$$4C^2S^2 - 2 = -\xi_+ - \xi_- \le |\xi_+| + |\xi_-| \le 2 \qquad \Longrightarrow \qquad C^2S^2 \le 1, \quad CS \le 1,$$
(V.51)

as both C and S are non-negative.

If CS < 1, then the two roots,

$$\xi_{\pm} = 1 - 2C^2 S^2 \pm \sqrt{4C^2 S^2 \left(C^2 S^2 - 1\right)},\tag{V.52}$$

are complex, with a unit modulus, and are the complex conjugate of one another. Especially simple—and principally distinguished, as we see in the next sections—is the case C = 1. Thus,

$$\xi_{\pm} = \mathrm{e}^{\pm \mathrm{i}k\Delta x},\tag{V.53}$$

with the remarkable property that $\arg \xi_{\pm}$ linearly depends on k—which is to say that both branches of the discrete dispersion relation are linear.

In parallel, if CS = 1, then the two roots coincide, $\xi_{\pm} = -1$. The algebraic multiplicity 2 is accompanied with geometric multiplicity 1: only the multiples of

$$y = \begin{pmatrix} c \\ -1 \end{pmatrix} \tag{V.54}$$

are eigenvectors. If C = 1, then this affects only one mode, S = 1, $k = \frac{\pi}{k}$, and if that mode is prohibited by the boundary conditions, then the choice C = 1 ensures a stable scheme.

With C > 1, $CS \le 1$ would be violated by a whole interval for k (recall (V.45)), which may not be cured by boundary conditions, so the best candidate (the largest Δt for a fixed Δx , or the smallest possible Δx for fixed Δt) to have stability is C = 1.

V.2.1.2 Poynting–Thomson–Zener case

For the PTZ system, the von Neumann stability analysis of our discretization studies the modes

$$v_{n+1/2}^{j-1/2} = iA_v^j e^{ik\left(n+\frac{1}{2}\right)\Delta x}, \qquad \qquad \varepsilon_n^j = A_\varepsilon^j e^{ikn\Delta x}, \qquad \qquad \sigma_n^j = A_\sigma^j e^{ikn\Delta x}, \qquad (V.55)$$

on which iteration via

$$\sigma_n^{j+1} = \frac{1}{1 - \alpha + \frac{\tau}{\Delta t}} \left\{ \left(\frac{\tau}{\Delta t} - \alpha \right) \sigma_n^j + E \left[\alpha \varepsilon_n^j + (1 - \alpha) \varepsilon_n^{j+1} \right] + \hat{E} \frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} \right\},\tag{V.57}$$

gives

$$\begin{pmatrix} A_v^{j+1} \\ A_{\varepsilon}^{j+1} \\ A_{\sigma}^{j+1} \end{pmatrix} = \hat{\mathsf{T}} \begin{pmatrix} A_v^j \\ A_{\varepsilon}^j \\ A_{\sigma}^j \end{pmatrix}$$
(V.58)

with

$$\hat{\mathsf{T}} = \begin{pmatrix} 1 & 0 & 2\frac{\Delta t}{\varrho\Delta x}S \\ -2\frac{\Delta t}{\Delta x}S & 1 & -4\frac{\Delta t^2}{\varrho\Delta x^2}S^2 \\ -2\frac{E(1-\alpha)+\frac{\hat{E}}{\Delta t}}{(1-\alpha)+\frac{\tau}{\Delta t}} \cdot \frac{\Delta t}{\Delta x}S & \frac{E}{(1-\alpha)+\frac{\tau}{\Delta t}} & \frac{\tau}{(1-\alpha)+\frac{\tau}{\Delta t}} - 4\frac{E(1-\alpha)+\frac{\hat{E}}{\Delta t}}{(1-\alpha)+\frac{\tau}{\Delta t}} \cdot \frac{\Delta t^2}{\varrho\Delta x^2}S^2 \end{pmatrix}.$$
(V.59)

The characteristic polynomial is now

$$\hat{P}(\xi) = a_3 \xi^3 + a_2 \xi^2 + a_1 \xi + a_0, \qquad (V.60)$$

$$a_{0} = \frac{\alpha - \frac{\tau}{\Delta t}}{(1 - \alpha) + \frac{\tau}{\Delta t}}, \quad a_{1} = 3 - \frac{2 - 4\left(\alpha - \frac{\hat{\tau}}{\Delta t}\right)C^{2}S^{2}}{(1 - \alpha) + \frac{\tau}{\Delta t}}, \quad a_{2} = -3 + \frac{1 + 4\left[(1 - \alpha) + \frac{\hat{\tau}}{\Delta t}\right]C^{2}S^{2}}{(1 - \alpha) + \frac{\tau}{\Delta t}}, \quad a_{3} = 1$$
(V.61)

Three roots are considerably more difficult to directly analyze. One alternative is to use Jury's criteria [148] for whether the roots are within the unit circle of the complex plane, and another possibility is to apply the Möbius transformation $\xi = \frac{\eta+1}{\eta-1}$ on (V.60) and utilize the Routh–Hurwitz criteria to determine whether the mapped roots are within the left half plane. The two approaches provide the same result. Nevertheless, one criterion provided by one of these two methods may not directly be one criterion of the other method. It is only the combined result (the intersection of the conditions) that agrees. Accordingly, it can be beneficial to perform both investigations because it may be laboring to recognize a simple condition provided by one of the routes as a consequence of the conditions directly offered by the other route.

Jury's criteria, for our case, are as follows. First, $\hat{P}(1) > 0$ gives

$$\frac{4C^2S^2}{(1-\alpha) + \frac{\tau}{\Delta t}} > 0, \qquad \Longleftrightarrow \qquad (1-\alpha) + \frac{\tau}{\Delta t} > 0.$$
 (V.62)

Second, $(-1)^{3}\hat{P}(-1) > 0$ yields

$$8 - 8 \frac{\frac{1}{2} + \left[\left(\frac{1}{2} - \alpha \right) + \frac{\hat{\tau}}{\Delta t} \right] C^2 S^2}{(1 - \alpha) + \frac{\tau}{\Delta t}} > 0,$$
(V.63)

which, in light of (V.62), reduces to

$$\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t} > \left[\left(\frac{1}{2} - \alpha\right) + \frac{\hat{\tau}}{\Delta t}\right] C^2 S^2.$$
(V.64)

Third, the matrices $\begin{pmatrix} a_3 & a_2 \\ 0 & a_3 \end{pmatrix} \pm \begin{pmatrix} 0 & a_0 \\ a_0 & a_1 \end{pmatrix}$ have to be positive innerwise³. Now, the '+' branch leads to

$$\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t} > \frac{\hat{\tau} - \tau}{\Delta t} C^2 S^2, \tag{V.65}$$

which is weaker than (V.64) because there the rhs is larger by $\left[(1-\alpha) + \frac{\tau}{\Delta t}\right]C^2S^2$ (and cf. (V.62)). Meanwhile, the '-' branch induces condition

$$\hat{\tau} > \tau, \tag{V.66}$$

which we have already encountered in (V.28) as the thermodynamical requirement (V.26) at the continuum level, and which also induces, via (V.65),

$$\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t} > 0, \tag{V.67}$$

³Following Jury [148], a matrix is *positive innerwise* if the determinant of the matrix and its all inners are positive. Here, the *inner* Δ_{m-2} of an $m \times m$ matrix is formed by deleting its first and *m*th rows and columns. Inner Δ_{m-4} is the inner of Δ_{m-2} , and the procedure is continued until Δ_1 or Δ_2 is reached. Inners enter the picture only for $m \ge 3$ so, in our case, only positive definiteness of the matrices themselves is to be ensured.

which is stronger than (V.62). This also allows us to rearrange (V.64) and exploit it as

$$C^{2}S^{2} < \frac{\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t}}{\left(\frac{1}{2} - \alpha\right) + \frac{\hat{\tau}}{\Delta t}} < 1 \qquad \text{for all} \quad 0 \le S \le 1 \implies C^{2} < \frac{\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t}}{\left(\frac{1}{2} - \alpha\right) + \frac{\hat{\tau}}{\Delta t}} < 1.$$
(V.68)

Conditions (V.66)–(V.68) summarize the obtained stability requirements, the first referring to the constants of the continuum model only, the second relating α and Δt of the scheme, and the third limiting Δx (through C) in light of α and Δt .

If, instead of Jury's criteria, one follows the Routh–Hurwitz path on the Möbius transformed polynomial,

$$\hat{Q}(\eta) = (\eta - 1)^3 \hat{P}\left(\frac{\eta + 1}{\eta - 1}\right) = b_3 \eta^3 + b_2 \eta^2 + b_1 \eta + b_0,$$
(V.69)

$$b_0 = 8\varrho\Delta x^2 \left\{ \left[\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t} \right] - \left[\left(\frac{1}{2} - \alpha\right) + \frac{\hat{\tau}}{\Delta t} \right] C^2 S^2 \right\}, \quad b_1 = 4\varrho\Delta x^2 \left(1 - C^2 S^2\right) \Delta t, \quad (V.70)$$

$$b_2 = 8\left[\left(\frac{1}{2} - \alpha\right) + \frac{\tau}{\Delta t}\right] E \Delta t^2 S^2, \qquad b_3 = 4E \Delta t^3 S^2, \qquad (V.71)$$

then, having $b_3 > 0$, roots lie in the left half plane if all corner subdeterminants of $\begin{pmatrix} b_2 & b_0 & 0 \\ b_3 & b_1 & 0 \\ 0 & b_2 & b_0 \end{pmatrix}$ are positive; i.e. $b_2 > 0$, $b_1b_2 - b_0b_3 > 0$ and $b_0(b_1b_2 - b_0b_3) > 0$ (hence, $b_0 > 0$) are needed. As expected, these conditions prove to be equivalent to the ones obtained via Jury's criteria—we omit the details to avoid redundant repetition.

V.2.1.2.1 The Kelvin–Voigt model Although the focus of the present study is on the hyperbolic-like case corresponding to $\tau > 0$, the above calculations are valid for $\tau = 0$, the Kelvin–Voigt subfamily as well. As a brief analysis of this case, (V.66) is trivially satisfied with $\hat{\tau} > 0$. (V.67) gives the nontrivial condition $\alpha < 1/2^4$. Finally, (V.68) gives

$$\left(\frac{1}{2} - \alpha\right)\Delta t^2 + \hat{\tau}\Delta t < \frac{\frac{1}{2} - \alpha}{c^2}\Delta x^2,\tag{V.72}$$

which looks like some mixture of a stability condition for a scheme for a parabolic problem, such as Fourier heat conduction, and of a condition for a simple reversible wave propagation.

V.2.1.2.2 Beyond Kelvin–Voigt When $\tau > 0$, then

$$\hat{C} = \hat{c} \frac{\Delta t}{\Delta x} > C \tag{V.73}$$

becomes important [recall (V.30)].

The most interesting case is $\alpha = 1/2$, where the scheme yields second-order accurate predictions: (V.67) holds trivially, and (V.68) can be rewritten as

$$\hat{C} < 1. \tag{V.74}$$

With boundary conditions also present, one may extend this condition to

$$C \le 1. \tag{V.75}$$

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Considering the two other potentially interesting cases as well: If $\alpha = 1$, then (V.67) induces $\Delta t < 2\tau$, which is not a harsh requirement since the time step must usually be much smaller than the time scales of the system in order to obtain a physically acceptable numerical solution. In parallel, \hat{C} is limited from above by a number smaller than 1. On the other side, when $\alpha = 0$, then (V.67) is automatically true again, and now \hat{C} is limited from above by a number larger than 1. Since we may need $\Delta t \ll \tau$ for a satisfactory solution, this $\mathcal{O}\left(\frac{\Delta t}{\tau}\right)$ gain over 1 is not considerable.

⁴Together with boundary conditions, this may be weakened to $\alpha \leq 1/2$.

V.2.1.2.3 Hooke case It is worth looking back to the Hooke limit of (V.68): $\tau = \hat{\tau} = 0$ (with whatever α) tells C < 1. One can see that the $|\xi| < 1$ stability requirement yields conservative results and does not tell us how far the obtained inequalities are from equalities.

V.2.2 Numerical results and investigation of dissipation and dispersion errors

The calculations communicated here are carried out with zero v, ε, σ as initial conditions, and with stress boundary conditions: on one end of the sample, a cosine-shaped pulse is applied, while the other end is free (stress is zero). With τ_b denoting the temporal width of the pulse, the excitation is, hence,

$$\sigma(t,0) = \begin{cases} \frac{\sigma_{\rm b}}{2} \left[1 - \cos\left(2\pi \frac{t}{\tau_{\rm b}}\right) \right] & \text{if } 0 \le t \le \tau_{\rm b}, \\ 0 & \text{otherwise.} \end{cases}$$
(V.76)

Temperature is calculated via the discretized form of (V.27), with the natural choice that temperature values reside at the same place as stress and strain, but half-shifted in time $(T_n^{j-1/2} \text{ at } t^j - \frac{\Delta t}{2}, x_n)$.

When plotting, say, elastic energy of the whole sample at time t^j , a simple $\frac{E}{2} \sum_n (\varepsilon_n^j)^2 \Delta x$ type sum is used, with two adjustments. First, terms living at the outer endpoint of an outermost space cell, such as $(\varepsilon_0^j)^2$ and $(\varepsilon_N^j)^2$, are counted with weight $\frac{1}{2}$. Second, kinetic energy and thermal energy, both being based on quantities half-shifted in time, are calculated as a time average, their value at t^j taken as the average of their value at $t^j - \frac{\Delta t}{2}$ and $t^j + \frac{\Delta t}{2}$.

The numerical calculations are performed for dimensionless quantities. For making the quantities dimensionless, the following units are used: the length of the sample X, c (so a Hookean wave arrives at the other end during unit time), E, σ_b , and c_σ . Accordingly, dimensionless position, time, velocity, stress, strain, energy, temperature, and wave number are defined as

$$\tilde{x} = \frac{1}{X}x, \quad \tilde{t} = \frac{c}{X}t, \quad \tilde{v} = \frac{1}{c}v, \quad \tilde{\sigma} = \frac{1}{\sigma_{\rm b}}\sigma, \quad \tilde{\varepsilon} = \frac{E}{\sigma_{\rm b}}\varepsilon, \quad \tilde{e} = \frac{E^2}{c^2\sigma_{\rm b}^2}e, \quad \tilde{T} = \frac{E^2c_{\sigma}}{c^2\sigma_{\rm b}^2}T, \quad \tilde{k} = Xk.$$
(V.77)

The results are presented for dimensionless time constants

$$\tilde{\tau}_{\rm b} = 0.2, \qquad \qquad \tilde{\tau} = 1.25, \qquad \qquad \hat{\tau} = 5, \qquad (V.78)$$

the latter two implying $\hat{c}/c = 2$.

V.2.2.1 Hookean wave propagation

For the Hooke system, our scheme is symplectic, with very reliable long-time behavior. This is well visible in Figure V.5: the shape is nicely preserved, no numerical artefacts are visible in the spacetime picture, and the sum of elastic and kinetic energy is conserved.



Figure V.5: Left: Snapshot of the stress pulse right before its 15th bouncing back from the boundary. Middle: Spacetime picture of the wave propagation. Bouncing back from free ends makes stress change sign. Right: Elastic energy, kinetic energy, and their sum as functions of time. Calculation done with N = 200 space cells and C = 1.

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The Hooke system might appear as a simple introductory task for numerics. This is actually far from true. The Hooke case already displays both dissipation error and dispersion error if not treated with appropriate care (see the introductory part of this section). While the greatest danger, instability, is about an exponential exploding of error, dissipation error is "the opposite", *i.e.*, when the signal decreases in time, losing energy due to numerical artefact only. This type of error is related to $|\xi| < 1$ modes, which indicates that one should try to stay on the unit circle with ξ . On the other side, in addition to the modulus of ξ , its argument can also cause trouble: if $\arg \xi$ is not linear in k, then dispersion error is induced, which is observable as unphysical waves are generated numerically around signal fronts. These errors may be present, depending on settings, even for a symplectic scheme such as ours, as illustrated in Figure V.6. More insight is provided by Figure V.7.

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Figure V.6: Wavy dispersion error and decrease by dissipative error for the Hooke system when C = 1/2, with N = 100.



Figure V.7: Upper row: Case of C = 1; lower row: case of C = 1/2. Left: The two roots ξ_{\pm} in the complex plane; right: k dependence of the argument of ξ_{\pm} .

As a comparison, the same problem is solved via the finite element software COMSOL v5.3a (see Figures V.1, V.2 and V.3). COMSOL solutions are heavily dependent on the solution methods and their settings. However, since RK34 option proved the best, in order to test the mesh dependence of its solution, the $\tilde{\tau}_b = 0.04$ case is examined with 300 space cells ($\Delta \tilde{x} = \Delta \tilde{t} = 0.0033$) as well, for a longer process (100 bounces). For the simulations, a configuration of an i7-7700 CPU with 3.6 GHz and 16 GB RAM is used. COMSOL supports parallel computing, which is an option that has been exploited. Although the run time strongly depends on other factors, it provides a good picture for comparing the effectiveness of the commercial approach and the scheme presented above. With these settings, the developed scheme required 0.3 s in Matlab and shows no numerical artefact, while the COMSOL solution

took 9649 s and exhibits apparent dissipative error and mild but increasing dispersion error around the rear of the pulse (see Figure V.8).



Figure V.8: Rear-side velocity history in time, for pulse length $\tilde{\tau}_b = 0.04$, with 300 nodes. Left: solution by the scheme presented here; right: COMSOL RK34 result.

To summarize, compared to the developed scheme realized in Matlab, COMSOL run times are 100–1000–10,000 times larger, with large memory demand, and various settings have to be tuned to obtain a stable solution with moderate artificial dissipation and dispersion.

V.2.2.2 Poynting-Thomson-Zener Wave Propagation

For the PTZ system, the principally optimal choice of $\alpha = 1/2$ does outperform $\alpha = 0$ (with $\hat{C} = 1$). Figure V.9 shows such a comparison: $\alpha = 1/2$ produces a reliable signal shape quite independently of space resolution, while $\alpha = 0$ needs more than N = 1000 space cells to reach the same reliability.



Figure V.9: Upper row: $\alpha = 1/2$; Lower row: $\alpha = 0$ —calculation of the stress signal when it starts its 7th bouncing, with $\hat{C} = 1$. From left to right: N = 400, 800, 1600 space cells.

 $\alpha = 1/2$ suggests that realibility already at N = 50, and even N = 25, "does a decent job," as depicted in Figure V.10.



Figure V.10: The same $\alpha = 1/2$ prediction with N = 25, 50, 100 space cells, from left to right, respectively.



Figure V.11: $\alpha = 1/2$, $\hat{C} = 1$ spacetime picture and energy conservation, N = 200.

With $\alpha = 1/2$, the spacetime picture and total energy conservation are not less satisfactory, as visible in Figure V.11.

The physical explanation of the signal shape (Figures V.9–V.10) is that the fastest modes propagate with speed \hat{c} (recall Section 2), transporting the front of the signal, while slow modes travel with $c < \hat{c}$, gradually falling behind, and forming, little by little, a thickening tail.

In parallel, the spacetime picture shows that this tail effect is less relevant than the overall decrease of the signal, due to dissipation.

Concerning the energy results, the remarkable fact is that all ingredients $v, \varepsilon, \sigma, T$ are calculated via discretized time integration, so total energy conservation is not built in, but is a test of the quality of the whole numerical approach.

In case of a dissipative system such as the PTZ one, it is hard to detect the dissipative error, i.e. to distinguish it from the physical dissipation. The dispersion error remains visible, as Figure V.12 shows.



Figure V.12: The stress signal provided by the scheme with $\hat{C} = 1/2$, N = 200, for comparison with Figure V.10. (All other settings are the same.)

Usually, one would need to set Δt to be much smaller than τ , $\hat{\tau}$ (and τ_b) to obtain a physically »

acceptable approximation. Rewriting the coefficients (V.61) as

$$a_{0} = \frac{\alpha \frac{\Delta t}{\tau} - 1}{(1 - \alpha) \frac{\Delta t}{\tau} + 1} = -1 + \mathcal{O}\left(\frac{\Delta t}{\tau}\right), \quad a_{1} = 3 - \frac{2\frac{\Delta t}{\tau} - 4\left(\alpha \frac{\Delta t}{\tau} - \frac{\hat{\tau}}{\tau}\right)C^{2}S^{2}}{(1 - \alpha) \frac{\Delta t}{\tau} + 1} = 3 - 4\hat{C}^{2}S^{2} + \mathcal{O}\left(\frac{\Delta t}{\tau}\right), \quad (V.79)$$

$$a_{2} = -3 + \frac{\frac{\Delta t}{\tau} + 4\left[(1-\alpha)\frac{\Delta t}{\tau} + \frac{\dot{\tau}}{\tau}\right]C^{2}S^{2}}{(1-\alpha)\frac{\Delta t}{\tau} + 1} = -3 + 4\hat{C}^{2}S^{2} + \mathcal{O}\left(\frac{\Delta t}{\tau}\right), \qquad a_{3} = 1$$

in the limit $\frac{\Delta t}{\tau} \to 0$, the characteristic polynomial reduces to

$$\xi^{3} + \left(-3 + 4\hat{C}^{2}S^{2}\right)\xi^{2} + \left(3 - 4\hat{C}^{2}S^{2}\right)\xi - 1 = \left(\xi - 1\right)\left[\xi^{2} + \left(-2 + 4\hat{C}^{2}S^{2}\right)\xi + 1\right], \quad (V.80)$$

with roots satisfying $\xi_0 = |\xi_+| = |\xi_-| = 1$, excluding thus the dissipation error. Especially simple and distinguished is the case $\hat{C} = 1$, when the roots are

$$\xi_0 = 1, \qquad \xi_{\pm} = e^{\pm ik\Delta x},$$
 (V.81)

providing dispersion relations linear in k and, hence, getting rid of dispersion error as well.

With slightly nonzero $\frac{\Delta t}{\tau}$, these nice properties are detuned but only up to $\mathcal{O}(\frac{\Delta t}{\tau})$, as shown in Figures V.13–V.15 (prepared at a dimensionless time step value of 0.01; the detuning appears weaker for $\alpha = 1/2$ than for $\alpha = 0$).



Figure V.13: Visualization of the three branches $\xi_0(k), \xi_+(k), \xi_-(k)$ for $\hat{C} = 1$. Upper row: $\alpha = 1/2$; lower row: $\alpha = 0$.



Figure V.14: Same as Figure V.13, but with $\hat{C} = 1/2$.



Figure V.15: In Figures V.13–V.14, the roots are not exactly on the unit circle—here, Δt dependence of $|\xi_0|$ and $|\xi_{\pm}|$ is displayed, at a neutral value $k\Delta x = \pi/4$, for $\hat{C} = 1$ and $\alpha = 1/2$.

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V.3 The numerical scheme on a three spatial dimensional Cartesian grid

The 3D scheme is designed to keep the nice, second-order, behavior of the discretization both in spatial and in temporal direction. Achieving this is not so trivial—different components of vectors and of tensors are placed at different discretized positions to fulfill the aim. In parallel, the boundaries also pose a challenge: quantities must be placed in such a way that the set of equations becomes closed. A rule has been found for this, which is so general that it holds for both stress and displacement boundary conditions, even at edges where these two differ at the two joining sides of the 3D sample (see Figure V.16).



Figure V.16: Spatial arrangement of the discretized quantities (two-dimensional projection). Circles stand for diagonal tensor components, squares for offdiagonal ones, and triangles for vector components, different components with differently oriented triangles. Void quantities are prescribed by boundary condition (in case stress boundary conditions are considered, like here.)

In finding the arrangement of discretized quantities suggested here, the spacetime perspective has helped a lot. Specifically, on one side, thermodynamical balances in their differential form are four-divergences from the spacetime aspect, and have an integral counterpart which, via Gauss' theorem, helps one to find out where to represent which flux-type quantity. Also, knowing that, from the spacetime point of view, velocity is a timelike four-vector [149, 22] gives the information that velocity should be shifted not only spatially but temporally as well. Oppositely, stress is a spacelike tensor so no temporal shift is needed.

Let us take a Cartesian grid with spacings Δx , Δy , Δz , and time step Δt . Corresponding to the

continuum formula (V.2), we introduce the finite difference discretization

$$\varrho \frac{(v_x)_{l+1/2,m,n}^{j+1/2} - (v_x)_{l+1/2,m,n}^{j-1/2}}{\Delta t} = \frac{(\sigma_{xx})_{l+1,m,n}^j - (\sigma_{xx})_{l,m,n}^j}{\Delta x} + \frac{(\sigma_{xy})_{l+1/2,m+1/2,n}^j - (\sigma_{xy})_{l+1/2,m-1/2,n}^j}{\Delta y} + \frac{(\sigma_{xz})_{l+1/2,m,n+1/2}^j - (\sigma_{xz})_{l+1/2,m,n-1/2}^j}{\Delta z},$$
(V.82)

$$\varrho \frac{(v_y)_{l,m+1/2,n}^{j+1/2} - (v_y)_{l,m+1/2,n}^{j-1/2}}{\Delta t} = \frac{(\sigma_{yx})_{l+1/2,m+1/2,n}^j - (\sigma_{yx})_{l-1/2,m+1/2,n}^j}{\Delta x} + \frac{(\sigma_{yy})_{l,m+1,n}^j - (\sigma_{yy})_{l,m,n}^j}{\Delta y} + \frac{(\sigma_{yz})_{l,m+1/2,n+1/2}^j - (\sigma_{yz})_{l,m+1/2,n-1/2}^j}{\Delta z}, \quad (V.83)$$

$$\varrho \frac{(v_z)_{l,m,n+1/2}^{j+1/2} - (v_z)_{l,m,n+1/2}^{j-1/2}}{\Delta t} = \frac{(\sigma_{zx})_{l+1/2,m,n+1/2}^j - (\sigma_{zx})_{l-1/2,m,n+1/2}^j}{\Delta x} + \frac{(\sigma_{zy})_{l,m+1/2,n+1/2}^j - (\sigma_{zy})_{l,m-1/2,n+1/2}^j}{\Delta y} + \frac{(\sigma_{zz})_{l,m,n+1}^j - (\sigma_{zz})_{l,m,n}^j}{\Delta z}, \quad (V.84)$$

where the time index j refers to a value at $t^j = j \cdot \Delta t$, j + 1/2 to a value at $t^{j+1/2} = (j + 1/2) \cdot \Delta t$, the space index l refers to a value at $x_l = l \cdot \Delta x$, m is the space index in the y direction, and n in the z direction. Accordingly, stress (and strain) values reside at integer time instants, while velocity ones are shifted in time by half; diagonal stress (and strain) components reside at integer positions, offdiagonal ones are shifted in the two directions matching with the two Cartesian indices; and velocity components are shifted only in the direction matching with their Cartesian index. From these formulae, the j + 1/2 indexed velocities can be expressed explicitly (as functions of earlier quantities).

This same pattern—distribution of quantities—is used for the discretization of (V.2):

$$\frac{(\varepsilon_{xx})_{l,m,n}^{j+1} - (\varepsilon_{xx})_{l,m,n}^{j}}{\Delta t} = \frac{(v_x)_{l+1/2,m,n}^{j+1/2} - (v_x)_{l-1/2,m,n}^{j+1/2}}{\Delta x},$$
(V.85)

$$\frac{(\varepsilon_{yy})_{l,m,n}^{j+1} - (\varepsilon_{yy})_{l,m,n}^{j}}{\Delta t} = \frac{(v_y)_{l,m+1/2,n}^{j+1/2} - (v_y)_{l,m-1/2,n}^{j+1/2}}{\Delta x},$$
(V.86)

$$\frac{(\varepsilon_{zz})_{l,m,n}^{j+1} - (\varepsilon_{zz})_{l,m,n}^{j}}{\Delta t} = \frac{(v_z)_{l,m,n+1/2}^{j+1/2} - (v_z)_{l,m,n-1/2}^{j+1/2}}{\Delta x},$$
(V.87)

$$\frac{(\varepsilon_{xy})_{l+1/2,m+1/2,n}^{j+1} - (\varepsilon_{xy})_{l+1/2,m+1/2,n}^{j}}{\Delta t} = \frac{1}{2} \left\{ \frac{(v_x)_{l+1/2,m+1,n}^{j+1/2} - (v_x)_{l+1/2,m,n}^{j+1/2}}{\Delta y} + \frac{(v_y)_{l+1,m+1/2,n}^{j+1/2} - (v_y)_{l,m+1/2,n}^{j+1/2}}{\Delta x} \right\}, \quad (V.88)$$

$$\frac{(\varepsilon_{xz})_{l+1/2,m,n+1/2}^{j+1} - (\varepsilon_{xz})_{l+1/2,m,n+1/2}^{j}}{\Delta t} = \frac{1}{2} \left\{ \frac{(v_x)_{l+1/2,m,n+1}^{j+1/2} - (v_x)_{l+1/2,m,n}^{j+1/2}}{\Delta z} + \frac{(v_z)_{l+1,m,n+1/2}^{j+1/2} - (v_z)_{l,m,n+1/2}^{j+1/2}}{\Delta x} \right\}, \quad (V.89)$$

$$\frac{(\varepsilon_{yz})_{l,m+1/2,n+1/2}^{j+1} - (\varepsilon_{yz})_{l,m+1/2,n+1/2}^{j}}{\Delta t} = \frac{1}{2} \left\{ \frac{(v_y)_{l,m+1/2,n+1}^{j+1/2} - (v_y)_{l,m+1/2,n}^{j+1/2}}{\Delta z} + \frac{(v_z)_{l,m+1,n+1/2}^{j+1/2} - (v_z)_{l,m,n+1/2}^{j+1/2}}{\Delta y} \right\}, \quad (V.90)$$

from which formulae the j + 1 indexed strains can be expressed explicitly, and for the discretized version of (V.4),

$$\begin{aligned} \alpha \left(\sigma_{pq}^{d}\right)_{l',m',n'}^{j} + (1-\alpha) \left(\sigma_{pq}^{d}\right)_{l',m',n'}^{j+1} + \frac{\left(\sigma_{pq}^{d}\right)_{l',m',n'}^{j+1} - \left(\sigma_{pq}^{d}\right)_{l',m',n'}^{j}}{\Delta t} \\ &= E^{d} \left[\alpha \left(\varepsilon_{pq}^{d}\right)_{l',m',n'}^{j} + (1-\alpha) \left(\varepsilon_{pq}^{d}\right)_{l',m',n'}^{j+1}\right] + \hat{E}^{d} \frac{\left(\varepsilon_{pq}^{d}\right)_{l',m',n'}^{j+1} - \left(\varepsilon_{pq}^{d}\right)_{l',m',n'}^{j}}{\Delta t}, \quad (V.91) \\ \alpha \left(\sigma_{pq}^{s}\right)_{l',m',n'}^{j} + (1-\alpha) \left(\sigma_{pq}^{s}\right)_{l',m',n'}^{j+1} + \frac{\left(\sigma_{pq}^{s}\right)_{l',m',n'}^{j+1} - \left(\sigma_{pq}^{s}\right)_{l',m',n'}^{j}}{\Delta t} \\ &= E^{s} \left[\alpha \left(\varepsilon_{pq}^{s}\right)_{l',m',n'}^{j} + (1-\alpha) \left(\varepsilon_{pq}^{s}\right)_{l',m',n'}^{j+1}\right] + \hat{E}^{s} \frac{\left(\varepsilon_{pq}^{s}\right)_{l',m',n'}^{j+1} - \left(\varepsilon_{pq}^{s}\right)_{l',m',n'}^{j}}{\Delta t}, \quad (V.92) \\ &p, q = x, y, z, \quad l', m', n' = \text{integers or half-integers depending on } p, q, \end{aligned}$$

where $\alpha = 1/2$ ensures second-order accuracy of the whole scheme, from which—together with $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{d} + \boldsymbol{\sigma}^{s}$ —the (j + 1)-indexed stresses can be expressed explicitly, except for stress boundary locations where we express strain, instead (and know stress from the boundary condition).

Actually, concerning boundary conditions, the rule is found for both stress boundary condition and velocity (or displacement) boundary condition is that if a quantity is missing for determining another boundary quantity then that missing quantity is to be added *outside* the boundary. This works for mixed boundary conditions as well, with different ones meeting at edges of a rectangular sample, for example. In the next subsection an examples for stress boundary conditions (relevant, *e.g.*, for a wide class of rock mechanical applications) is presented.

The pattern of which quantity to reside where—at integer or half-integer space and time indices could also be conjectured from the structure of the equations but, as noted earlier, the spacetime viewpoint helps a lot to find this arrangement a geometrically—spacetime geometrically—natural one.

In the reversible special case of the Hooke system, this scheme is symplectic. It is actually the symplectic Euler method (which is, in words: 'new₁ from old_1 and old_2 , new₂ from new₁ and old_2 '). The improvement is the interpretation: here, new₁ and new₂ are shifted in time with respect to each other so second-order accuracy is achieved, while the conventional interpretation of the symplectic Euler method is first-order only. In parallel, since mechanical energy (the Hamiltonian) is a velocity dependent term plus a strain dependent term (stress becomes a simple linear function of strain), the scheme is explicit. This remains true at the PTZ level as well so one can expect—and find, actually—a fast-running program code.

For the aspects of thermodynamics, equation (V.15) with (V.10), explicitly expressing the j + 1/2 indexed temperature values from

$$\frac{T_{l,m,n}^{j+1/2} - T_{l,m,n}^{j-1/2}}{\Delta t} = \frac{1}{\varrho c_{\sigma}} \left\{ \frac{1}{\hat{I}^{\mathsf{d}}} \operatorname{tr} \left(\hat{\sigma}^{\mathsf{d}^2} \right)_{l,m,n}^j + \frac{1}{\hat{I}^{\mathsf{s}}} \operatorname{tr} \left(\hat{\sigma}^{\mathsf{s}^2} \right)_{l,m,n}^j \right\},\tag{V.93}$$

where the notation (V.5) is utilized, and the traces are to be expanded in Cartesian components and the terms containing offdiagonal components—which reside at half space-shifted locations in two indices—are averaged around the location l, m, n, first neighbours only.

V.3.1 Numerical solutions and the role of total energy

The example on which the scheme is demonstrated is a square cross-sectioned long beam, treated thus as a plane-strain problem. Initially, the beam is in relaxed/equilibrium state (zero stress, strain and velocity, and homogeneous temperature). Then, on one of its sides, a single normal stress pulse is applied, with

$$\sigma_{yy}(t, x, 0, z) = \begin{cases} \sigma_{b} \left\{ \frac{1}{2} \left[1 - \cos\left(2\pi \frac{t}{\tau_{b}}\right) \right] \cdot \frac{1}{2} \left[1 - \cos\left(2\pi \frac{x - X/2}{W_{b}}\right) \right] \right\} & \text{if } 0 \le t \le \tau_{b} \text{ and} \\ \frac{X - W_{b}}{2} \le x \le \frac{X + W_{b}}{2}, \quad (V.94) \\ 0 & \text{otherwise}, \end{cases}$$

where τ_b is the duration of the pulse, σ_b is its amplitude, W_b is its spatial width, and X is the width of the beam. On the other sides, normal stress is constantly zero (free surfaces).

A 50 × 50 grid is considered in the x-y plane, for 240 time steps, where the time step is the largest at which stability is maintained. Notably, stability investigation is fairly involved for this problem and would require a separate whole study. Further settings (in appropriate units) are $\rho = 1$, $E^{d} = 4$, $E^{s} = 10$, $\tau_{b} = 0.3$, $\sigma_{b} = 5$, $W_{b}/X = 0.6$, $\hat{E}^{d} = 1.4$, $\tau^{d} = 0.2$, $c_{\sigma} = 0.001$, $T^{0} = 0.1$, $\alpha = 1/2$.

Simulation results for Hooke-elastic material can be found in [48], the scheme proved to provide satisfactory and reliable solutions, which is almost trivial, since the scheme is a second order generalization of the symplectic Euler method.

In a PTZ medium, the solution of the analogous problem is similarly good. Snapshots are presented in Figures V.17 and V.18, which display the Huber–Mises–Hencky or von Mises equivalent stress⁵ $\sqrt{\operatorname{tr}(\hat{\sigma}^{d^2})}$ and temperature *T*. Dissipation is nicely indicated via temperature.

⁵Aside from the multiplier $\sqrt{\frac{3}{2}}$.



Figure V.17: Snapshots of the distribution of the stress invariant $\sqrt{\operatorname{tr}\left(\hat{\boldsymbol{\sigma}}^{d^2}\right)}$ (left column) and of temperature (right column) at various instants, in the PTZ case. From top to bottom: snapshots at instants $(1/2)\tau_{\rm b}, \tau_{\rm b}, (3/2)\tau_{\rm b}, 2\tau_{\rm b}$, respectively.



Figure V.18: Continuation of Figure V.17: Snapshots of the distribution of the stress invariant $\sqrt{\operatorname{tr}\left(\hat{\boldsymbol{\sigma}}^{d^2}\right)}$ (left column) and of temperature (right column) at various instants, in the PTZ case. From top to bottom: snapshots at instants $(5/2)\tau_{\rm b}, 3\tau_{\rm b}, (7/2)\tau_{\rm b}, 4\tau_{\rm b}$, respectively.

In a movie format, it is more spectacular how reliably the simulation performs.

- Furthermore, it is not only the eye that could judge the reliability: with the help of thermodynamics, total energy proves to be a useful diagnostic tool:
 - If it explodes then there is instability.

»

- If it deviates from a constant then there is dissipation error.
- If it is wavy/oscillating then there is dispersion error.

The scheme presented here functions satisfactorily in this aspect as well, as displayed in Figure V.19. For energy, we perform summation, over the integer centred discrete cells, of the energy terms discretized along the above lines, including that averages like for (V.93) are taken wherever necessary, also in the time direction (for kinetic energy).



Figure V.19: Total energy and the various energy types as functions of time, for the PTZ case.

V.4 Discussion

Choosing a good finite difference numerical scheme for a continuum thermodynamical problem is not easy. The numerical scheme presented here, due to its symplectic root, second-order accuracy, and the equation-friendly and spacetime geometry friendly arrangement of discretized quantities (*i.e.*, staggered arrangement of quantities by half space and time steps, suited to balances, to the kinematic equations, to the Onsagerian equations, *etc.*), has been found to provide reliable results in a fast and resource-friendly way. Being a finite difference scheme, it is not very flexible to simulate arbitrary shaped samples but already the extension of the Cartesian formulae to cylindrical and spherical geometries promises useful applications, including the various wave-based measurement methods used in rock mechanics (see, *e.g.*, [150]), many of which rely on simple and easily treatable sample shapes. Fitting a rheological model on experimental data may require many runs so good finite difference schemes find their applicability.

Even with all such preparations, instability is a key property to ensure. When all these are settled, dissipative and dispersive errors can invalidate our calculation, which may not be recognized when the continuum system is dissipative or when it allows wave propagation.

Notably, there is a principal difference between the stability problems of a numerical method and the stability issues for a continuum phenomenon itself. The former are induced by the approximations and depend on the type of approximation, while the original continuum system may be fine regarding stability—for example, ensured by thermodynamical consistence. It is interesting to realize that, nevertheless, these two types of instability are not completely independent. In one of the directions, the stability investigation of a numerical scheme may provide information for the underlying continuum phenomenon as well. An example for this has been provided by equation (V.66) above, which is a condition that is independent of the time step, of the space step, of the parameter α that parametrizes the scheme, and of any other aspect of the scheme. Rather, it is a thermodynamical condition as one of the stability requirements imposed by thermodynamical consistency, seen at (V.28). This example illustrates that, in more complicated problems, it is also worth investigating the stability conditions of the numerical method and trying to distill *scheme-independent information* on the continuum system from them. In parallel, the other direction is when the stability of a continuum system can be used *to devise stable numerical methods*. One such example is the case of symplectic numerical schemes, which are actually exact integrators of a certain Hamiltonian system—a slightly different one from the original system. The generalization of this way of thinking to nonconservative systems is a promising research direction. Concerning the future prospects of the study provided here, the following are the main tasks:

concerning the future prospects of the study provided here, the following are the main tasks.

- The solutions presented here can be supplemented by comparison with analytical solutions and further finite element calculations, performed for the whole PTZ system.
- Regarding the thermodynamical system to be investigated, the whole Kluitenberg–Verhás family—which the present PTZ model is a subclass of—could be studied. The presence of the second derivative of strain, and actually already the Kelvin–Voigt subfamily, brings in the aspect of parabolic characteristics, so useful implications may be gained for other thermodynamical areas such as non-Fourier heat conduction.
- Reliable numerical methods for thermodynamical systems, which avoid all the various pitfalls, are an important direction for future research. In the presented investigations, balance of internal energy is decoupled from the mechanical equations, thus after solving these mechanical equations and knowing the mechanical quantities (velocity, stress and strain), the thermal quantities (temperature, various kinds of energy, entropy, entropy production rate density) can be calculated automatically. However, when thermal and mechanical processes are coupled (*e.g.*, in the presence of heat conduction or thermal expansion) and take place simultaneously, then the balance of internal energy should be time stepped together with the mechanical equations. Calculation of such problems and application of the presented scheme is a nice challenge in the direction of unification and is already in progress.
- The investigation of stability and of dissipative and dispersion error is expected to be much more involved than in the corresponding one space dimensional situation. Nevertheless, it is an important task for the future because the outcomes support efficient applications of the scheme.
- It is an interesting challenge to apply the presented scheme for other dissipative situations (like [151], just to mention one example).
- If the spacetime background is strengthened further, by using four-quantities, four-equations on them, and formulating discretization in a fully four-geometrical way then a systematic and general framework could be obtained, beneficial for other purposes as well. It would, for example, help in building connection to a finite element—spacetime finite element—approach, along which way objects of general shape could also be treated. Notably, the current finite element paradigm has deficiencies and probably needs to be renewed, as indicated by results found here as well as in earlier works [27].
- In addition, utilizing the thermodynamical full description of a system for monitoring and controlling numerical artefacts during a computer simulation is a promising perspective. The steps made here: recognizing the usefulness of total energy and its various parts, and of entropy production rate density, are hoped to contribute to a future routine in numerical environments of how thermodynamics is taken advantage of.
- Currently, the scheme is applicable only for stable state of the material [cf. the physical condition (V.28) with the numerical stability requirement (V.66)]. A possible direction of further developments, which is also motivated by engineering, is to generalize the scheme for material stability loss—*e.g.*, taking the plastic deformations into account.
Chapter VI

Analytical solutions of rheological processes in the force-equilibrium approximation

A possibility to investigate the rheological behavior of solids is the studying of solutions. Assuming homogeneity in the force-equilibrial approximation, solutions explain experimental results and can be applied for fitting the material coefficients [1]. In the previous chapter a dynamical problem, namely, wave propagation in rheological media was studied. Now, a technically important case, space dependent rheological processes in the force-equilibrial approximations are investigated. Such processes can be induced via time dependent boundary conditions (*e.g.*, drilling or pressurizing/depressurizing can modeled).

As reported in Chapter I, illustrative examples for time dependent processes are observable in tunneling (see Figure I.11), polymer technique or even for steels operated at high temperature (*e.g.*, power plant steam pipes, turbine blades). The appropriate development, design, establishment and operation of such facilities and components requires accurate calculations.

A general treatment of linear rheological problems is given in integral equation formulation [152, 153, 154, 155]. This also includes Volterra's principle [156], which in a nutshell says that the solution of a linear rheological problem can be derived from the solution of the corresponding elastic one. The integral equation based approach has been utilized to find various numerical solutions, however, obtaining analytical solutions is less straightforward since an operator inverse should be calculated analytically. Furthermore, [152] presents only a general treatment without application examples, [153] generalizes only Young's modulus and assumes Poisson's ratio to remain a constant, and the assumptions of [155] for mathematical convenience are usually not fulfilled in applications.

While the scope of analytical solutions is limited, the discretization-based numerical methods face at problems. Solutions obtained by such methods may considerably depend on the resolution of the applied discretization. Furthermore, for complex three-dimensional problems, calculation times are large. These disadvantages already occur in the force-equilibrial approximation. In addition to the fact that analytical solutions can be used to validate numerical solutions, the analytical solution of a simplified version of the problem can provide a reasonable first approximation and can highlight useful qualitative relationships.

Motivated by the advantages of analytical solutions over numerical ones, an analytical solution method has been developed [157], which takes the advantage of the possibilities offered by Volterra's principle. In this chapter, analytical solutions for practically important examples are presented obtained via this method.

This chapter is based on the publications [158, 159, 160]. The author's contributions are as follows:

- Applying the general solution method on several concrete problems. The obtained solutions are presented together with analysis and interpretation.
- Based on the obtained solutions an unprecedented phenomenon is identified, which is invisible in elasticity and in one spatial dimension. In addition to damping and delaying effects, rheology can lead to motions of the medium with varying direction dependence.

VI.1 The method of four elastic spatial pattern sets demonstrated on a concrete example

This section presents a method for determination of rheological processes in the force-equilibrial approximation. The method is developed by Tamás Fülöp. Here, instead of the general treatment given in [157], the steps of the method are described on a concrete example.

The method is based on Volterra's principle and, accordingly, the rheological solution is obtained from the *known* elastic one. The final version of the method has had a long evolution. In the first variant, the elasticity coefficients were replaced by unknown time-dependent functions in the elastic solution, which functions are determined from temporal ordinary differential equations generated by the rheological operators [158, 160]. This approach—called the *method of elasticity constants made time dependent*—can easily be applied, however, the range of problems that can be solved this way is too narrow. As the next evolutionary step, the elastic stress solution is decomposed into linearly independent spatial patterns [159, 160]. Replacing the constant coefficients of these spatial patterns by unknown time-dependent functions and determining them, the solution for the rheological problem can be obtained. This method—called the *method of elastic spatial patterns*—expanded the range of applicability, however, some problems that can be solved via the firs approach are out of scope for this second one. Finally, as a common generalization, the *method of four elastic spatial patterns set* has been born [157], which will be presented below and proves general enough for numerous practical applications.

VI.1.1 Equations of elasticity and rheology in the force-equilibrial approximation

In this chapter, purely mechanical problems of homogeneous and isotropic solids are considered in the small-strain regime. The investigations are performed in the force-equilibrial approximation, *i.e.*, acceleration¹ is neglected and, accordingly, the balance of linear momentum (II.21) reduces to

$$\boldsymbol{\sigma} \cdot \overleftarrow{\nabla} = -\varrho \mathbf{g},\tag{VI.1}$$

where ρg is the volumetric force density (assumed to be time independent). In this so-called quasistationary treatment, the strain ε has to fulfill the geometry-originated compatibility equation

$$\vec{\nabla} \times \boldsymbol{\varepsilon} \times \overleftarrow{\nabla} = \mathbf{0},$$
 (VI.2)

which means from a mathematical point of view that there exists a so-called Cauchy vector potential $\mathbf{u}^{\text{Cauchy}}$ from which $\boldsymbol{\varepsilon}$ can be obtained as

$$\boldsymbol{\varepsilon} = \left(\mathbf{u}^{\text{Cauchy}} \otimes \boldsymbol{\nabla} \right)^{\text{S}}. \tag{VI.3}$$

The Cauchy vector potential can be determined from ε via Cesàro's formula [161]

$$\mathbf{u}^{\text{Cauchy}}(t,\mathbf{r}) = \mathbf{u}_0(t) + \mathbf{\Omega}(t)\left(\mathbf{r} - \mathbf{r}_0\right) + \int_{\mathbf{r}_0}^{\mathbf{r}} \left\{ \boldsymbol{\varepsilon}(t,\tilde{\mathbf{r}}) + 2\left[\boldsymbol{\varepsilon}(t,\tilde{\mathbf{r}})\otimes\tilde{\nabla}\right]^{A_{1,3}}\left(\mathbf{r} - \tilde{\mathbf{r}}\right) \right\} \mathrm{d}\tilde{\mathbf{r}}, \qquad (\text{VI.4})$$

where $A_{1,3}$ denotes antisymmetrization in the first and third tensorial indices, and the position vector \mathbf{r}_0 and the path of integration are arbitrary. The Cauchy vector potential is indeterminate up to an arbitrary vector function $\mathbf{u}_0(t)$ and an arbitrary antisymmetric tensor function $\Omega(t)$, which are related to rigidbody translations and rotations, respectively. To obtain the displacement field **u**—which is one among the possible Cauchy vector potentials—, these uncertainties have to be fixed (*e.g.*, via symmetry arguments and other physically plausible considerations) [162].

¹Accordingly, wave phenomena are out of scope here.

Stress and strain are connected through the constitutive equation, which in case of linear elasticity is Hooke's law

$$\sigma^{d} = E^{d} \varepsilon^{d}, \qquad \sigma^{s} = E^{s} \varepsilon^{s}$$
 (VI.5)

and, in case of linear rheological models, it can be expressed as

$$S^{d}\sigma^{d} = \mathcal{E}^{d}\varepsilon^{d}, \qquad \qquad S^{s}\sigma^{s} = \mathcal{E}^{s}\varepsilon^{s}$$
(VI.6)

with the linear differential operators

$$\mathcal{S}^{d} = 1 + \tau_{1}^{d} \frac{\partial}{\partial t} + \tau_{2}^{d} \frac{\partial^{2}}{\partial t^{2}} + \cdots, \qquad \qquad \mathcal{E}^{d} = E_{0}^{d} + E_{1}^{d} \frac{\partial}{\partial t} + E_{2}^{d} \frac{\partial^{2}}{\partial t^{2}} + \cdots, \qquad (\text{VI.7})$$

$$\mathcal{S}^{s} = 1 + \tau_{1}^{s} \frac{\partial}{\partial t} + \tau_{2}^{s} \frac{\partial^{2}}{\partial t^{2}} + \cdots, \qquad \qquad \mathcal{E}^{s} = E_{0}^{s} + E_{1}^{s} \frac{\partial}{\partial t} + E_{2}^{s} \frac{\partial^{2}}{\partial t^{2}} + \cdots, \qquad (\text{VI.8})$$

where the coefficients $\tau_i^{d}, \tau_i^{s}, E_k^{d}, E_l^{s}$ are assumed to be constants.

Considering elasticity, equations (VI.1), (VI.2) and (VI.5) form a closed system of equations, which, together with appropriate boundary conditions, can be solved.

When treating the rheological problem, equations (VI.1), (VI.2) and (VI.6) form a closed system of equations. Since the constitutive equation (VI.6) contains time derivatives, in addition to boundary conditions (which may be time dependent in general) initial conditions are also required to solve the problem. In this case, all equations and boundary conditions have to be fulfilled at all time instants.

When one deals with the above-described rheological generalization of the problem then, in addition to (VI.1), (VI.2), (VI.6) and the boundary conditions (which may be time dependent in general), initial conditions are also required to ensure uniqueness of the solution, since the constitutive equations contain time derivatives [see (VI.7) and (VI.8)]. In the rheological case, all fields are functions of both time and space, and all equations and boundary conditions have to be satisfied for all time instants.

Inspired by Volterra's principle, since the elastic solution satisfies all the *spatial* requirements, the presented method relies strongly on the *known* elastic solution and reduces the rheological problem—formulated by (VI.1), (VI.2), (VI.6) and the initial and boundary conditions—to solving a system of *temporal* differential equations.

Here, the aim is to determine the displacement field u, the strain field ε and the stress field σ .

VI.1.2 Preparations

First, such time independent fields $\bar{\sigma}$ and $\bar{\varepsilon}$ —the effect of the force density, called hereafter as primary fields—are separated that satisfy the equations

$$\bar{\boldsymbol{\sigma}} \cdot \stackrel{\leftarrow}{\nabla} = -\varrho \mathbf{g},\tag{VI.9}$$

$$\vec{\nabla} \times \bar{\boldsymbol{\varepsilon}} \times \overleftarrow{\nabla} = \mathbf{0},$$
 (VI.10)

$$\bar{\boldsymbol{\sigma}}^{\mathrm{d}} = E_0^{\mathrm{d}} \bar{\boldsymbol{\varepsilon}}^{\mathrm{d}}, \qquad \bar{\boldsymbol{\sigma}}^{\mathrm{s}} = E_0^{\mathrm{s}} \bar{\boldsymbol{\varepsilon}}^{\mathrm{s}}.$$
 (VI.11)

For the time independent fields $\bar{\sigma}$ and $\bar{\varepsilon}$, (VI.6) gets simplified to Hooke's law with $E^{d} = E_{0}^{d}$, $E^{s} = E_{0}^{s}$, thus equation (VI.11) remains valid for the rheological case [cf. (VI.7)–(VI.8)] as well. As a consequence, the difference fields $\hat{\sigma} := \sigma - \bar{\sigma}$ and $\hat{\varepsilon} := \varepsilon - \bar{\varepsilon}$ satisfy the homogeneous equations

$$\hat{\boldsymbol{\sigma}} \cdot \nabla = \mathbf{0},$$
 (VI.12)

$$\vec{\nabla} \times \hat{\boldsymbol{\varepsilon}} \times \overleftarrow{\nabla} = \mathbf{0},$$
 (VI.13)

$$S^{d}\hat{\sigma}^{d} = \mathcal{E}^{d}\hat{\varepsilon}^{d}, \qquad S^{s}\hat{\sigma}^{s} = \mathcal{E}^{s}\hat{\varepsilon}^{s}.$$
 (VI.14)

In general, this decomposition detunes the initial and boundary conditions, which has to be taken into account during the calculations.

For each problem considered here, the spatial domain filled by the medium has only one nonzero boundary condition. In general, when in a problem more than one boundary conditions are nonzeros, then the problem can be divided into such subproblems in which only one boundary condition is nonzero. Since the treated problem is linear, the sum of such subsolutions yields solution for the whole problem.

In the considered problems, the normal component of stress is prescribed at the boundaries of the domain. From the point of view of applications, via such boundary conditions, models of bores, tunnels, pipes, cavities and tanks are obtained. In general, the boundary condition can be time dependent and, actually, it is this time dependence that induces the nontrivial rheological changes. In what follows, we restrict ourselves to such time dependencies where the boundary condition is rescaled via a time-dependent function $\lambda(t)$, which must be sufficiently many times differentiable. For modeling the process of drilling or loading/unloading of pipes or tanks, this function can be chosen simply as

$$\lambda(t) = \begin{cases} 0 & \text{if } t \leq t_1, \\ 1 & \text{if } t \geq t_2, \\ \text{smooth in between.} \end{cases}$$
(VI.15)

Naturally, then the solution of the *elastic* problem also gets rescaled homogeneously by this factor $\lambda(t)$.

Based on dimensional reasoning, when stress boundary conditions are considered, the elastic solution depends only the ratio of E^{d} and E^{s} (in notation $\eta := \frac{E^{d}}{E^{s}}$, and its connection to Poisson's ratio ν is $\nu = \frac{1-\eta}{2+\eta}$) and not individually on the elasticity coefficients.

In such situations, instead of strain ε , a so-called stress-dimensioned strain $\zeta := E^s \varepsilon$ is recommended to use. Naturally, then $\overline{\zeta} = E^s \overline{\varepsilon}$ and $\hat{\zeta} = E^s \hat{\varepsilon}$. Correspondingly, the compatibility equation for $\hat{\zeta}$ is

$$\vec{\nabla} \times \hat{\boldsymbol{\zeta}} \times \vec{\nabla} = \mathbf{0},$$
 (VI.16)

Hooke's law reduces to

$$\hat{\boldsymbol{\sigma}}^{\mathrm{d}} = \eta \hat{\boldsymbol{\zeta}}^{\mathrm{d}}, \qquad \hat{\boldsymbol{\sigma}}^{\mathrm{s}} = \hat{\boldsymbol{\zeta}}^{\mathrm{s}}, \qquad (\mathrm{VI.17})$$

and the rheological constitutive equation is

$$\mathcal{S}^{d}\hat{\boldsymbol{\sigma}}^{d}(t,\mathbf{r}) = \mathcal{Z}^{d}\hat{\boldsymbol{\zeta}}^{d}(t,\mathbf{r}), \qquad \qquad \mathcal{S}^{s}\hat{\boldsymbol{\sigma}}^{s}(t,\mathbf{r}) = \mathcal{Z}^{s}\hat{\boldsymbol{\zeta}}^{s}(t,\mathbf{r}) \qquad \qquad (\text{VI.18})$$

with

$$\mathcal{Z}^{d} = \eta + \frac{E_{1}^{d}}{E_{0}^{s}} \frac{\partial}{\partial t} + \frac{E_{2}^{d}}{E_{0}^{s}} \frac{\partial^{2}}{\partial t^{2}} + \cdots, \qquad \mathcal{Z}^{s} = 1 + \frac{E_{1}^{s}}{E_{0}^{s}} \frac{\partial}{\partial t} + \frac{E_{2}^{s}}{E_{0}^{s}} \frac{\partial^{2}}{\partial t^{2}} + \cdots.$$
(VI.19)

VI.1.3 The method of four elastic spatial pattern sets

In order to present and demonstrate the method of four elastic spatial pattern sets, a "simple but complicated enough" example is chosen. Namely, the rheological process induced by boring in a semi-infinite domain loaded by its own weight is considered. This example is practically also relevant, for example, in tunnel construction.

First, the elastic solution for the fully opened bore is presented [163, 164, 165]. In general, this problem is investigated for arbitrary values of the lateral pressure coefficient k. This coefficient plays an important role in the design of geotechnical structures, among others. Three theoretical values of k are usually investigated:

• When initially a hydrostatic pressure distribution can be assumed in the medium then k = 1.

- When the dilatation of the medium is laterally inhibited then $k = \frac{\nu}{1-\nu} = \frac{1-\eta}{1+2\eta}$.
- When the dilatation of the medium is laterally free then k = 0.

Hereafter, the case of initial hydrostatic pressure distribution (*i.e.*, k = 1) is investigated.



Figure VI.1: Outline, coordinate systems and notation for the considered problem.

As boundary conditions, zero normal stress is prescribed for the contour of the cylinder (after the drilling) and for the plane surface. For modeling the drilling, the first one will be rescaled by (VI.15). In general, the elastic solution is given in infinite-sum form [163], however, when a large-depth approximation is considered, *i.e.*, d/R > 1.5 (where d is the depth of the center of the bore and R is the radius of the cylinder, see Figure VI.1) then the solution is well approximated by the leading-order term [164, 165], which is

$$\sigma_{rr} = \frac{\gamma R}{4} \left(4\frac{r}{R} - \frac{4+5\eta}{1+2\eta} \frac{R}{r} - \frac{3\eta}{1+2\eta} \frac{R^3}{r^3} \right) \sin \varphi - \gamma d \left(1 - \frac{R^2}{r^2} \right),$$
(VI.20)

$$\sigma_{\varphi\varphi} = \frac{\gamma R}{4} \left(4\frac{r}{R} + \frac{3\eta}{1+2\eta} \frac{R}{r} + \frac{1+\eta}{1+2\eta} \frac{R^3}{r^3} \right) \sin\varphi - \gamma d\left(1 + \frac{R^2}{r^2}\right), \qquad (VI.21)$$

$$\sigma_{r\varphi} = \frac{\gamma R}{4} \left(\frac{3\eta}{1+2\eta} \frac{R}{r} + \frac{1+\eta}{1+2\eta} \frac{R^3}{r^3} \right) \cos\varphi, \tag{VI.22}$$

$$\sigma_{zz} = \frac{\gamma R}{2} \left(2\frac{r}{R} - \frac{1-\eta}{1+2\eta} \frac{R}{r} \right) \sin \varphi - \gamma d \left(1 + 2\frac{1-\eta}{2+\eta} \frac{R^2}{r^2} \cos 2\varphi \right), \tag{VI.23}$$

$$\sigma_{rz} = \sigma_{\varphi z} = 0, \tag{VI.24}$$

where $\gamma = \varrho g$ describes the homogeneous force density. The time-independent primary field

$$\bar{\boldsymbol{\sigma}}_{(x,y,z)} = \gamma(y-d)\mathbf{1}, \qquad \bar{\boldsymbol{\sigma}}_{(r,\varphi,z)} = \gamma(r\sin\varphi - d)\mathbf{1}$$
(VI.25)

can be separated, and the remaining field with elements

$$\hat{\sigma}_{rr} = \frac{\gamma R}{4} \left(-\frac{4+5\eta}{1+2\eta} \frac{R}{r} - \frac{3\eta}{1+2\eta} \frac{R^3}{r^3} \right) \sin \varphi + \gamma d \frac{R^2}{r^2}, \qquad (VI.26)$$

$$\hat{\sigma}_{\varphi\varphi} = \frac{\gamma R}{4} \left(\frac{3\eta}{1+2\eta} \frac{R}{r} + \frac{1+\eta}{1+2\eta} \frac{R^3}{r^3} \right) \sin\varphi - \gamma d\frac{R^2}{r^2}, \qquad (\text{VI.27})$$

$$\hat{\sigma}_{r\varphi} = \frac{\gamma R}{4} \left(\frac{3\eta}{1+2\eta} \frac{R}{r} + \frac{1+\eta}{1+2\eta} \frac{R^3}{r^3} \right) \cos\varphi, \qquad (VI.28)$$

$$\hat{\sigma}_{zz} = \frac{\gamma R}{2} \left(-\frac{1-\eta}{1+2\eta} \frac{R}{r} \right) \sin \varphi - 2\gamma d \frac{1-\eta}{2+\eta} \frac{R^2}{r^2} \cos 2\varphi, \qquad (VI.29)$$

$$\hat{\sigma}_{rz} = \hat{\sigma}_{\varphi z} = 0 \tag{VI.30}$$

»

is the complementary one, which is at the focus of the investigation. This elastic stress solution with the corresponding stress-dimensioned strain solution satisfies equations (VI.12), (VI.16) and the boundary conditions for any *allowable* η . The idea is to seek for the rheological solution in the form of a *time-* « *dependent* linear combination of elastic solutions with different η 's.

Let us decompose the elastic stress solution into a finite sum² in such a way that η dependence and r are separated:

$$\hat{\boldsymbol{\sigma}}_{\rm el}(\boldsymbol{\eta}, \mathbf{r}) = \sum_{i=1}^{I} a_i(\boldsymbol{\eta}) \, \boldsymbol{\alpha}_i(\mathbf{r}), \qquad (\text{VI.31})$$

where *I* is an integer, and $a_i(\eta)$'s and $\alpha_i(\mathbf{r})$'s are linearly independent coefficient functions and space » dependencies—the latter called hereafter 'spatial patterns'. This decomposition for the currently investigated problem is

$$\hat{\boldsymbol{\sigma}}_{el}(\eta, \mathbf{r}) = \boldsymbol{\alpha}_1(\mathbf{r}) + \frac{1-\eta}{1+2\eta} \boldsymbol{\alpha}_2(\mathbf{r})$$
(VI.32)

with $I=2, a_1(\eta)=1$ $a_2(\eta)=\frac{1-\eta}{1+2\eta}$ and

$$\boldsymbol{\alpha}_{1}(\mathbf{r}) = \begin{pmatrix} -\frac{\gamma R}{4} \left(3\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \sin\varphi + \gamma d\frac{R^{2}}{r^{2}} & \frac{\gamma R}{4} \left(-\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \cos\varphi & 0\\ \frac{\gamma R}{4} \left(-\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \cos\varphi & \frac{\gamma R}{4} \left(\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \sin\varphi - \gamma d\frac{R^{2}}{r^{2}} & 0\\ 0 & 0 & 0 \end{pmatrix}, \quad (VI.33)$$

$$\boldsymbol{\alpha}_{2}(\mathbf{r}) = \begin{pmatrix} \frac{\gamma R}{4} \left(-\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \sin \varphi & \frac{\gamma R}{4} \left(\frac{R}{r} - \frac{R^{3}}{r^{3}}\right) \cos \varphi & 0\\ \frac{\gamma R}{4} \left(\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \cos \varphi & -\frac{\gamma R}{4} \left(\frac{R}{r} + \frac{R^{3}}{r^{3}}\right) \sin \varphi & 0\\ 0 & 0 & -\frac{\gamma R}{2} \frac{R}{r} \sin \varphi \end{pmatrix}.$$
 (VI.34)

« The elastic stress-dimensioned strain solution and its deviatoric and spherical parts are also analogously decomposed, as

$$\hat{\boldsymbol{\zeta}}_{\rm el}(\eta, \mathbf{r}) = \sum_{j=1}^{J} b_j(\eta) \boldsymbol{\beta}_j(\mathbf{r}), \quad \hat{\boldsymbol{\zeta}}_{\rm el}^{\rm d}(\eta, \mathbf{r}) = \sum_{k=1}^{K} c_k(\eta) \boldsymbol{\gamma}_k(\mathbf{r}), \quad \hat{\boldsymbol{\zeta}}_{\rm el}^{\rm s}(\eta, \mathbf{r}) = \sum_{l=1}^{L} d_l(\eta) \boldsymbol{\delta}_l(\mathbf{r}), \quad (\text{VI.35})$$

with the finite integers J (not necessarily equal to I), K, L, linearly independent coefficient functions $b_j(\eta)$ [not necessarily the same ones as $a_i(\eta)$], $c_k(\eta)$, $d_l(\eta)$ and the linearly independent spatial patterns $\beta_j(\mathbf{r})$ [not necessarily the same ones as $\alpha_i(\mathbf{r})$], $\gamma_k(\mathbf{r})$, $\delta_l(\mathbf{r})$. From Hooke's law, the deviatoric and spherical parts of stress can be given with these as

$$\hat{\boldsymbol{\sigma}}_{\rm el}^{\rm d}(\eta, \mathbf{r}) = \sum_{k=1}^{K} \eta c_k(\eta) \boldsymbol{\gamma}_k(\mathbf{r}), \qquad \hat{\boldsymbol{\sigma}}_{\rm el}^{\rm s}(\eta, \mathbf{r}) = \sum_{l=1}^{L} d_l(\eta) \boldsymbol{\delta}_l(\mathbf{r}).$$
(VI.36)

» Then, for the investigated problem, the deviatoric part of the elastic stress solution is

$$\hat{\boldsymbol{\sigma}}_{el}^{d}(\eta, \mathbf{r}) = \boldsymbol{\gamma}_{1}(\mathbf{r}) + \frac{1-\eta}{1+2\eta} \boldsymbol{\gamma}_{2}(\mathbf{r})$$
(VI.37)

with K = 2, $c_1(\eta) = \frac{1}{\eta}$, $c_2(\eta) = \frac{1-\eta}{\eta(1+2\eta)}$, $\gamma_1(\mathbf{r}) = \boldsymbol{\alpha}_1^{d}(\mathbf{r})$ and $\gamma_2(\mathbf{r}) = \boldsymbol{\alpha}_2^{d}(\mathbf{r})$, and its spherical part is

$$\hat{\boldsymbol{\sigma}}_{el}^{s}(\eta, \mathbf{r}) = \frac{3}{1+2\eta} \boldsymbol{\delta}_{1}(\mathbf{r})$$
(VI.38)

²The generalization for such problems, in which this decomposition only in infinite sum can be given, is plan for the future.

with L = 1, $d_1(\eta) = \frac{3}{1+2\eta}$ and $\delta_1(\mathbf{r}) = 2\boldsymbol{\alpha}_1^{s}(\mathbf{r}) = \boldsymbol{\alpha}_2^{s}(\mathbf{r})$. Correspondingly, stress-dimensioned strain is

$$\hat{\boldsymbol{\zeta}}_{\rm el}(\eta, \mathbf{r}) = \frac{1}{\eta} \left[\boldsymbol{\gamma}_1(\mathbf{r}) + 2\boldsymbol{\gamma}_2(\mathbf{r}) \right] + \frac{3}{1+2\eta} \left[-\boldsymbol{\gamma}_2(\mathbf{r}) + \boldsymbol{\delta}_1(\mathbf{r}) \right], \qquad (\text{VI.39})$$

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with J = 2, $b_1(\eta) = \frac{1}{\eta}$, $b_2(\eta) = \frac{3}{1+2\eta}$, $\beta_1(\mathbf{r}) = \gamma_1(\mathbf{r}) + 2\gamma_2(\mathbf{r})$ and $\beta_2(\mathbf{r}) = -\gamma_2(\mathbf{r}) + \delta_1(\mathbf{r})$. Next, let us see the case when the boundary condition is multiplied by $\lambda(t)$. Then the elastic solution

Next, let us see the case when the boundary condition is multiplied by $\lambda(t)$. Then the elastic solution gets rescaled accordingly:

$$\hat{\boldsymbol{\sigma}}_{\mathrm{el},\lambda}(t,\eta,\mathbf{r}) = \lambda(t)\,\hat{\boldsymbol{\sigma}}_{\mathrm{el}}(\eta,\mathbf{r}), \qquad \hat{\boldsymbol{\zeta}}_{\mathrm{el},\lambda}(t,\eta,\mathbf{r}) = \lambda(t)\,\hat{\boldsymbol{\zeta}}_{\mathrm{el}}(\eta,\mathbf{r}). \tag{VI.40}$$

As it has already been mentioned, the solution of the rheological problem $(\hat{\sigma}_{\text{rheol}}(t, \mathbf{r}), \hat{\zeta}_{\text{rheol}}(t, \mathbf{r}))$ is sought for as a time-dependent linear combination of different elastic solutions (because such solutions trivially satisfy all spatial requirements, thus one can focus on the time dependency). Let us fix *I* values $\eta_1, \eta_2, \ldots, \eta_m, \ldots, \eta_I$ for the stress solution such that $\hat{\sigma}_{\text{el}}(\eta_m, \mathbf{r})$ are linearly independent, and expand the range of freedom spanned by the possible $\hat{\sigma}_{\text{el}}(\eta, \mathbf{r})$'s and, analogously, *J* values $\eta_1, \eta_2, \ldots, \eta_n, \ldots, \eta_J$ for the stress-dimensioned strain solution with the same requirement. The sequence $\eta_1, \eta_2, \ldots, \eta_m, \ldots, \eta_{\text{max}(I,J)}$ can be chosen arbitrarily: if the rheological solution is fixed by the initial conditions uniquely then it will be invariant under the choice of the η sequence. It means that the rheological solution is sought for in the form of

$$\hat{\boldsymbol{\sigma}}_{\text{rheol}}(t,\mathbf{r}) \stackrel{(VI.31)}{=} \sum_{m=1}^{I} \varphi_m(t) \,\hat{\boldsymbol{\sigma}}_{\text{el}}(\eta_m,\mathbf{r}) = \sum_{m,i=1}^{I} \varphi_m(t) \,a_i(\eta_m) \,\boldsymbol{\alpha}_i(\mathbf{r}), \quad (VI.41)$$

$$\hat{\boldsymbol{\zeta}}_{\text{rheol}}(t,\mathbf{r}) \stackrel{(VI.35)}{=} \sum_{n=1}^{J} \psi_n(t) \hat{\boldsymbol{\zeta}}_{\text{el}}(\eta_n,\mathbf{r}) = \sum_{n,j=1}^{J} \psi_n(t) b_j(\eta_n) \boldsymbol{\beta}_j(\mathbf{r}), \quad (VI.42)$$

which satisfy equations (VI.12) and (VI.16), while the requirement

$$\sum_{m=1}^{I} \varphi_m(t) = \lambda(t) \tag{VI.43}$$

ensures the fulfillment of the boundary condition. All that is left is to derive relationships among the unknown coefficient functions $\varphi_m(t)$, $\psi_n(t)$ based on (VI.18). The constitutive equation (VI.18) is given in deviatoric–spherical decomposition, hence, $\hat{\sigma}_{el}(\eta, \mathbf{r})$ in (VI.41) and $\hat{\zeta}_{el}(\eta, \mathbf{r})$ in (VI.42) also have to be given in the isotropic decomposition. In general, $\alpha_i^d(\mathbf{r})$'s, $\alpha_i^s(\mathbf{r})$'s, $\beta_j^d(\mathbf{r})$'s and $\beta_j^s(\mathbf{r})$'s may not be linearly independent [see the vicinity of equations (VI.37)–(VI.39)], but $\gamma_k(\mathbf{r})$'s and $\delta_l(\mathbf{r})$'s are, thus the former spatial patterns have to be expressed by these latter ones, *i.e.*, $\alpha_i^d(\mathbf{r}) = \sum_{k=1}^{K} A_{ik} \gamma_k(\mathbf{r})$, $\beta_j^d(\mathbf{r}) = \sum_{k=1}^{K} B_{jk} \gamma_k(\mathbf{r})$, $\alpha_i^s(\mathbf{r}) = \sum_{l=1}^{L} C_{il} \delta_l(\mathbf{r})$ and $\beta_j^s(\mathbf{r}) = \sum_{l=1}^{L} D_{jl} \delta_l(\mathbf{r})$ with appropriate matrices A_{ik}, B_{jk}, C_{il} and D_{jl} . These matrices, for the current investigated problem, are

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 2 \\ 0 & -1 \end{pmatrix}, \qquad C = \begin{pmatrix} \frac{1}{2} \\ 1 \end{pmatrix}, \qquad D = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$
 (VI.44)

Substituting these matrices into the deviatoric and spherical parts of (VI.41) and (VI.42), then from « (VI.18) equations

$$\mathcal{S}^{\mathsf{d}} \sum_{m,i=1}^{I} \sum_{k=1}^{K} \varphi_m(t) a_i(\eta_m) A_{ik} \boldsymbol{\gamma}_k(\mathbf{r}) = \mathcal{Z}^{\mathsf{d}} \sum_{n,j=1}^{J} \sum_{k=1}^{K} \psi_n(t) b_j(\eta_n) B_{jk} \boldsymbol{\gamma}_k(\mathbf{r}), \quad k = 1, \dots, K, \quad (\mathsf{VI.45})$$

$$\mathcal{S}^{\mathsf{s}} \sum_{m=1}^{I} \sum_{k=1}^{L} (\varphi_m(t) a_i(\eta_m) C_{ik} \boldsymbol{\delta}_k(\mathbf{r})) = \mathcal{Z}^{\mathsf{s}} \sum_{m=1}^{J} \sum_{k=1}^{L} \psi_n(t) b_i(\eta_m) D_{ik} \boldsymbol{\delta}_k(\mathbf{r}), \quad l = 1, \dots, K, \quad (\mathsf{VI.45})$$

$$\mathcal{S}^{s} \sum_{m,i=1} \sum_{l=1} \varphi_{m}(t) a_{i}(\eta_{m}) C_{il} \boldsymbol{\delta}_{l}(\mathbf{r}) = \mathcal{Z}^{s} \sum_{n,j=1} \sum_{l=1} \psi_{n}(t) b_{j}(\eta_{n}) D_{jl} \boldsymbol{\delta}_{l}(\mathbf{r}), \quad l = 1, \dots, L \quad (VI.46)$$

are obtained, from which—because of linear independency of $\gamma(\mathbf{r})$'s and $\delta(\mathbf{r})$'s—the system of linear temporal differential equations

$$\sum_{m,i=1}^{I} \mathcal{S}^{\mathsf{d}} \varphi_m(t) \, a_i(\eta_m) \, A_{ik} = \sum_{n,j=1}^{J} \mathcal{Z}^{\mathsf{d}} \psi_n(t) \, b_j(\eta_n) \, B_{jk}, \qquad k = 1, \dots, K, \tag{VI.47}$$

$$\sum_{m,i=1}^{I} \mathcal{S}^{s} \varphi_{m}(t) a_{i}(\eta_{m}) C_{il} = \sum_{n,j=1}^{J} \mathcal{Z}^{s} \psi_{n}(t) b_{j}(\eta_{n}) D_{jl}, \qquad l = 1, \dots, L.$$
(VI.48)

are derived for $\varphi_m(t)$'s and $\psi_n(t)$'s. The functions

$$\Phi_{k}^{d}(t) = \sum_{m,i=1}^{I} \varphi_{m}(t) a_{i}(\eta_{m}) A_{ik}, \qquad \Phi_{l}^{s}(t) = \sum_{m,i=1}^{I} \varphi_{m}(t) a_{i}(\eta_{m}) C_{il}, \qquad (VI.49)$$

$$\Psi_{k}^{d}(t) = \sum_{n,j=1}^{J} \psi_{n}(t) b_{j}(\eta_{n}) B_{jk}, \qquad \Psi_{l}^{s}(t) = \sum_{n,j=1}^{J} \psi_{n}(t) b_{j}(\eta_{n}) D_{jl} \qquad (VI.50)$$

are the time dependent factors of the spatial patterns $\gamma_k(\mathbf{r})$ and $\delta_l(\mathbf{r})$ [cf. with (VI.45)–(VI.46)]. Although there is arbitrariness in the choice of η_k 's, these functions do not contain any arbitrariness.

Finally, for our concrete investigated problem, the resulting deviatoric rheological equations are

$$\mathcal{S}^{d}\left\{a_{1}(\eta_{1})\varphi_{1}(t)+a_{1}(\eta_{2})\varphi_{2}(t)\right\}=\mathcal{Z}^{d}\left\{b_{1}(\eta_{1})\psi_{1}(t)+b_{1}(\eta_{2})\psi_{2}(t)\right\},$$
(VI.51)

$$\mathcal{S}^{\mathsf{d}}\left\{a_{2}(\eta_{1})\varphi_{1}(t)+a_{2}(\eta_{2})\varphi_{2}(t)\right\}=\mathcal{Z}^{\mathsf{d}}\left\{\left[b_{1}(\eta_{1})-b_{2}(\eta_{1})\right]\psi_{1}(t)+\left[b_{1}(\eta_{2})-b_{2}(\eta_{2})\right]\psi_{2}(t)\right\},\quad(\text{VI.52})$$

the spherical equation is

»

«

$$\mathcal{S}^{s}\left\{\left[\frac{1}{2}a_{1}(\eta_{1})+a_{2}(\eta_{1})\right]\varphi_{1}(t)+\left[\frac{1}{2}a_{1}(\eta_{2})+a_{2}(\eta_{2})\right]\varphi_{1}(t)\right\}=\mathcal{Z}^{s}\left\{b_{2}(\eta_{1})\psi_{1}(t)+b_{2}(\eta_{2})\psi_{2}(t)\right\},$$
(VI.53)

and the boundary condition imposes

$$\varphi_1(t) + \varphi_2(t) = \lambda(t), \qquad (VI.54)$$

which means four linear temporal differential equations on the four unknown functions φ_1 , φ_2 , ψ_1 and ψ_2 , which with corresponding initial conditions can be determined, thus together with the spatial patterns the rheological solutions for stress and stress-dimensioned strain are given.

Finally, the displacement field—displacement understood with respect to the primary initial state of the continuum—can be calculated via Cesàro's formula (VI.4), *i.e.*,

$$\mathbf{u}(t,\mathbf{r}) = \mathbf{u}_{0}(t) + \mathbf{\Omega}(t)\left(\mathbf{r} - \mathbf{r}_{0}\right) + \frac{1}{E^{s}} \sum_{k=1}^{K} \Psi_{k}^{d}(t) \int_{\mathbf{r}_{0}}^{\mathbf{r}} \left\{ \boldsymbol{\gamma}_{k}(\tilde{\mathbf{r}}) + 2\left[\boldsymbol{\gamma}_{k}(\tilde{\mathbf{r}}) \otimes \boldsymbol{\nabla}\right]^{\mathbf{A}_{1,3}}(\mathbf{r} - \tilde{\mathbf{r}}) \right\} \mathrm{d}\tilde{\mathbf{r}} \\ + \frac{1}{E^{s}} \sum_{l=1}^{L} \Psi_{l}^{s}(t) \int_{\mathbf{r}_{0}}^{\mathbf{r}} \left\{ \boldsymbol{\delta}_{l}(\tilde{\mathbf{r}}) + 2\left[\boldsymbol{\delta}_{l}(\tilde{\mathbf{r}}) \otimes \boldsymbol{\nabla}\right]^{\mathbf{A}_{1,3}}(\mathbf{r} - \tilde{\mathbf{r}}) \right\} \mathrm{d}\tilde{\mathbf{r}}. \quad (\text{VI.55})$$

Here, we remark that the rigid-body like displacement-and-rotation freedom has to be fixed³.

VI.2 Practical applications

» The following examples are solved via the method of four elastic spatial patterns set:

³For infinite domains, one can prescribe $\mathbf{u} \to \mathbf{0}$ for asymptotically distant points while, for semi-infinite domains like the one in question, by the heuristically analogous condition that the highest points of the "ground level"—see Figure VI.1—have no vertical displacement. Here, this latter requirement has been applied.

- Cylindrical bore and spherical hollow opened in infinite, homogeneous and isotropic stress field;
- Pressurizing of thick-walled tube and spherical tank;
- Cylindrical bore opened in infinite, homogeneous and anisotropic stress field;
- Cylindrical bore opened in homogeneous medium loaded by its self weight:
 - Hydrostatic initial stress state, *i.e.*, k = 1;
 - No lateral deformations in the initial stress state, *i.e.*, $k = \frac{\nu}{1-\nu} = \frac{1-\eta}{1+2\eta}$;
 - Free lateral deformations in the initial stress state, *i.e.*, k = 0.

Among these examples, the bold texted ones are demonstrated in what follows, with figures that demonstrate the typical behavior.

For modeling drilling—a gradual removal of the material—, the function

$$\lambda(t) = \begin{cases} 0 & \text{if } t \le t_1, \\ \frac{1}{2} \left[1 + \sin\left(\pi \frac{t - \frac{t_1 + t_2}{2}}{t_2 - t_1} \right) \right] & \text{if } t_1 \le t \le t_2, \\ 1 & \text{if } t_2 \le t \end{cases}$$
(VI.56)

is chosen [cf. (VI.15)]. In this regard, three practically interesting different cases are considered:

- when the switch-on $\lambda(t)$ is very slow compared to the rheological time scales,
- when the switch-on time scale $t_2 t_1$ is comparable to the rheological time scales,
- when the switch-on $\lambda(t)$ is very fast compared to the rheological time scales.

According to experience, rheological behavior is usually recognized in the deviatoric part, thus in our investigations Hooke's elasticity model is assumed for the spherical part, while in the deviatoric part the simplest rheological model, namely, the Kelvin model⁴ is considered. In case of this so-called Kelvin – Hooke (deviatorically Kelvin – spherically Hooke) model

$$\boldsymbol{\sigma}^{\mathrm{d}} = \eta \boldsymbol{\zeta}^{\mathrm{d}} + (E_1^{\mathrm{d}}/E^{\mathrm{s}}) \dot{\boldsymbol{\zeta}}^{\mathrm{d}}, \qquad \boldsymbol{\sigma}^{\mathrm{s}} = \boldsymbol{\zeta}^{\mathrm{s}}, \qquad (\mathrm{VI.57})$$

the rheological time scale is $\frac{E_1^d/E^s}{\eta}$, which is applied as the unit of time. Slow switch-on of the boundary condition is represented by $t_2 - t_1 = 5$, the medium case by $t_2 - t_1 = 1$, and fast switch-on by $t_2 - t_1 = 0.1$. The plots are calculated with $\eta = E^d/E^s = E_0^d/E^s = 0.4$ [to which the Poisson's ratio $\nu = 0.25$ corresponds].

Coloring conventions of the following plots are displayed in Figure VI.2.

$$--- \Phi_1^{\rm d}(t), \Psi_1^{\rm d}(t) --- \Phi_2^{\rm d}(t), \Psi_2^{\rm d}(t) --- \Phi_3^{\rm d}(t), \Psi_3^{\rm d}(t) --- \Phi_1^{\rm s}(t), \Psi_1^{\rm s}(t) --- \Phi_2^{\rm s}(t), \Psi_2^{\rm s}(t)$$

Figure VI.2: Colour codes of the coefficient functions in the figures below.

In all the following figures, the outline and typical results for different arrangements are presented. In the upper right corner, the time evolution tendency of the displacement field for a fast opening is illustrated (displacements are enlarged for visibility), while the second and third rows show the time evolution of the coefficient functions for slow (left column), medium-speed (middle column) and fast (right column) openings.

⁴Remarkably, already the deviatoric Kelvin model leads to a Poynting–Thomson–Zener behavior in uniaxial loadings, exhibiting creep and stress relaxation.



Figure VI.3: Cylindrical bore opened in an infinite, homogeneous and isotropic stress field. In this simplest problem, nothing surprising is visible.



Figure VI.4: Cylindrical bore opened in an infinite and homogeneous but anisotropic stress field. In addition to the anisotropic distortion of the contours, note the nontrivial time dependencies depicted by the greenish lines in the middle and right columns: they start with opposite sign with respect to the later and asymptotically taken sign.



Figure VI.5: Cylindrical bore opened in homogeneous medium loaded by its self weight, with hydrostatic initial stress state (k = 1). The observable nontrivial time dependencies resemble the ones seen for the anisotropic problem (see Figure VI.4). Plausibly, self-weight qualitatively acts as a kind of anisotropy.



Figure VI.6: Cylindrical bore opened in homogeneous medium loaded by its self weight, with no lateral deformations allowed in the primary field $(k = \frac{\nu}{1-\nu} = \frac{1-\eta}{1+2\eta})$. The more elaborate initial condition yields a richer structure of spatial patterns, some of which start with opposite sign compared to the asymptotic equilibrial one.



Figure VI.7: Cylindrical bore opened in homogeneous medium loaded by its self weight, with free lateral deformations in the primary field (k = 0). A remarkable difference from the previous two examples is that, here, the contour of the tunnel expands in the horizontal direction.

Demonstrating the applicability of the method for general linear rheological models, Figure VI.8 presents time evolution of coefficient functions with respect to Kluitenberg–Verhás – Hooke model, *i.e.*,

$$\boldsymbol{\sigma}^{\mathrm{d}} = \eta \boldsymbol{\zeta}^{\mathrm{d}} + (E_1^{\mathrm{d}}/E^{\mathrm{s}}) \dot{\boldsymbol{\zeta}}^{\mathrm{d}} + (E_2^{\mathrm{d}}/E^{\mathrm{s}}) \ddot{\boldsymbol{\zeta}}^{\mathrm{d}}, \qquad \boldsymbol{\sigma}^{\mathrm{s}} = \boldsymbol{\zeta}^{\mathrm{s}}.$$
(VI.58)

For simplicity, the coefficient of $\dot{\sigma}^{d}$ is choosen to be zero, thus the index of inertia (see [43]) is necessarily positive so, accordingly, (damped) rheological oscillation will be present. Again, $\eta = 0.4$ and the time unit $\frac{E_{1}^{d}/E^{s}}{\eta}$ are used. Regarding the coefficient of the second time derivative term, $\frac{E_{2}^{d}/E^{s}}{\eta} = 1$ is taken.



Figure VI.8: Time dependencies when the settings of Figure VI.6 are applied to the Kluitenberg–Verhás model (VI.58). Strong and slowly decreasing oscillations are observable.

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VI.3 Conclusions

Analytical solutions provide a first and qualitatively useful insight for several problems and, depending on situation, quantitative results can also be obtained.

As conclusion, the solutions presented above testify that rheology means not only delayed and damped response but—even in the simplest 'deviatoric Kelvin – spherical Hooke' case—it can lead to direction dependent and temporarily counter-intuitive motion.

The importance of rheological behavior is well-known in civil engineering and in mine industry. A hollow opened in an underground stone block often takes its eventual shape only years after the drilling. Accordingly, a freshly opened underground tunnel needs initially only a temporary—relatively weak—support, and the eventual support is enough to be established only later, when most of displacements have already been occured, allowing thus a much cheaper eventual support. The presented solutions also illustrate the phenomena of convergence, tunnel squeezing and rotation of the cross section (see Figures VI.4, VI.5, VI.6 and VI.7).

Further investigations are planned in the future. First, to explore the possibilities of generalization of the solution method itself, a method for infinitely many expansion terms (see such problems in [163, 166]) would be welcome. In parallel, a numerical approach based on the presented method can widen the range of applicability.

Chapter VII

Summary and theses

This dissertation investigates non-Fourier heat conduction and rheology of solids in two frameworks of irreversible thermodynamics, namely, Internal Variable Methodology and the GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) formulation. This chapter presents the author's scientific results.

First, the effect of thermal expansion on heat conduction is investigated, and its possible consequences in room temperature heat pulse experiments is anaysed. The performed investigations justify that the reason of the measured non-Fourier like behavior at room temperature is not thermal expansion.

<u>Thesis 1:</u>

Based on the basic equations of thermoelasticity, the effect of thermal expansion on heat conduction can be summarized in a non-Fourier-like heat conduction equation on temperature T solely, *i.e.*,

$$rac{1}{c_{\parallel}^2}\partial_t^2(arrho c_arepsilon\partial_t T-\lambda\Delta T)=\Delta(arrho c_{ ext{eff}}\partial_t T-\lambda\Delta T),$$

where ∂_t and Δ are the partial time derivative and the Laplace operator, respectively, c_{\parallel} is the longitudinal elastic wave propagation velocity, ρ is the density, λ is the thermal conductivity, c_{ε} is the constant-strain specific heat capacity and c_{eff} is an effectively measurable specific heat capacity, which includes the effects of thermal expansion and elastic wave propagation.

At room temperature (293 K), thermal expansion modifies the thermal diffusivity $a_{\varepsilon} = \frac{\lambda}{\varrho c_{\varepsilon}}$ to an effective one $a_{\text{eff}} = \frac{\lambda}{\varrho c_{\text{eff}}}$, which causes a deviation of 1% for steel, 2% for copper, 3% for aluminum, and for granite and PA6 this effect is practically negligible. At a length scale denoted by ℓ and the corresponding 'effective' Fourier-time scale $\frac{\ell^2}{a_{\text{eff}}}$, the left-hand side of the above equation is, to a rough estimate, $\frac{1}{\ell}$ times a heat conduction equation, while its right-hand side is $\frac{1}{\left(\frac{\ell^2}{a_{\text{eff}}}\right)^2 c_{\parallel}^2}$ times the nearly same heat conduction equation. Otherwise, the left-hand side of the equation provides a contribution to the right-hand side via a dimensionless factor $\frac{a_{\text{eff}}}{\ell^2} c_{\parallel}^2$. In heat-pulse experiments for samples with a size of $\ell = 3$ mm, this factor is about 10^{-15} to 10^{-10} for the above-mentioned materials. Therefore, the deviation from Fourier heat conduction measured at room-temperature heat-pulse experiments cannot be explained by thermal expansion.

Corresponding publication: [T1] ([23]). Corresponding section: III.1.

The previous investigation pointed out that the reason of non-Fourier behavior cannot be connected to thermal expansion in room-temperature heat-pulse experiments. Different branches of irreversible thermodynamics have their own methodologies to derive equations and hence to model phenomena beyond Fourier heat conduction. However, the connections of these methodologies as well as the physical interpretations are insufficient. Similarly to the case of internal variables, physical background and interpretation of entropy current multipliers (also known as Nyíri multipliers) remain hidden. Applying simultaneously the methodologies of internal variables and GENERIC, a possible physical interpretation for the entropy current multipliers can be given. This recognition can open a way towards the unification of the microscopic and macroscopic theories of heat conduction, and may lead to novel numerical simulation approaches (hyperbolic vs. parabolic equation to solve).

Thesis 2:

In the theory of non-Fourier heat conduction, Nyíri multipliers can be interpreted as generalizations of higher-order thermodynamical state variables. When the tensorial order of the highest tensorial order state variable is smaller than the tensorial order of the highest tensorial order entropy current multiplier, the Nyíri multiplier can be treated as a relaxed state variable. That is, after fast relaxation, the time dependence of a state variable with the same tensorial order as the highest tensorial order current multiplier becomes restricted by the variables with lower tensorial orders, thus explicit time dependence of this variable disappears. In this case, a non-local parabolic extension of the constitutive equations is obtained.

Corresponding publication: [T2] ([114]). Corresponding section: III.2.

The internal variable approach of irreversible thermodynamics, with a symmetric tensorial internal variable, provides a general and distinguished model family—the Kluitenberg–Verhás model family (covering as special cases Hooke's elasticity, the Kelvin–Voigt and Poynting–Thomson–Zener models, and also the Maxwell and Jeffreys models)—for the rheology of solids. This family has proved significant not only from a theoretical perspective but also for experimental and engineering applications. In parallel, the GENERIC formulation motivates efficient and high-precision numerical methods, thus it is recommended and beneficial to study how a model derived by the internal variable methodology suits the frame of GENERIC. An analysis is performed how the internal variable formulation leading to the Kluitenberg–Verhás model family can be represented in GENERIC and how the two frameworks are related to each other. Furthermore, GENERIC derivation ensures a simple way to generalize the Kluitenberg–Verhás model family to incorporate thermal expansion. An opportunity to enlarge numerical advantages is investigated, namely, how and under what conditions the irreversibility-originated but entropy-preserving terms can be represented in a symplectic structure.

Thesis 3:

Rheology of isotropic solids based on a single second-order tensorial internal variable can be implemented in the framework of GENERIC via specific-entropy based set of state variables. Through variable transformation into temperature-based set of state variables, the equivalence with the Kluitenberg–Verhás rheological model family of solids can be demonstrated. The derivations are presented and the fulfilment of GENERIC requirements are proved in the isotropic decomposition of second-order tensors, treating the deviatoric and spherical parts as independent state variables, which simplifies the constitutive equations, helping numerical realizations. The established description also proves to enable incorporating thermal expansion into the model family.

Assuming constant coefficients in the linear Onsagerian equations, the irreversibility-originated but entropy-preserving terms can be represented in the symplectic structure, for which the fulfillment of the Jacobi identity is proved.

Corresponding publication: [T3,T4] ([138, 139]). Corresponding chapter: IV.

A direct numerical realization of the above GENERIC implementation is investigating wave propagation in a rheological solid, namely, in a Poynting–Thomson–Zener medium (which is a special case of the Kluitenberg–Verhás model family). Applying a finite-difference discretization with half space and time shifts with appropriate implicitness factor (*i.e.*, $\alpha = 1/2$), the scheme turns out to be as a secondorder generalization of the symplectic Euler method. A von Neumann investigation is performed for the scheme. Analyzing the roots of the so-called transfer matrix stability, dispersion and dissipation errors are analyzed. These artificial numerical errors can lead to numerical violation of conservation of total energy. This behavior is also investigated, and a natural three spatial dimensional generalization based on an appropriate half space shift of the vectorial and tensorial components on a cubic Cartesian grid has proved to numerically preserve total energy.

Thesis 4:

One spatial dimensional wave propagation in a Poynting–Thomson–Zener medium is investigated via the set of difference equations

$$\begin{split} v_{n+1/2}^{j+1/2} &= v_{n+1/2}^{j-1/2} + \frac{\Delta t}{\varrho \Delta x} \left(\sigma_{n+1}^j - \sigma_n^j \right), \\ \varepsilon_n^{j+1} &= \varepsilon_n^j + \frac{\Delta t}{\Delta x} \left(v_{n+1/2}^{j+1/2} - v_{n-1/2}^{j+1/2} \right), \\ \sigma_n^{j+1} &= \frac{1}{1 - \alpha + \frac{\tau}{\Delta t}} \left\{ \left(\frac{\tau}{\Delta t} - \alpha \right) \sigma_n^j + E \left[\alpha \varepsilon_n^j + (1 - \alpha) \varepsilon_n^{j+1} \right] + \hat{E} \frac{\varepsilon_n^{j+1} - \varepsilon_n^j}{\Delta t} \right\}, \end{split}$$

where v, σ and ε are the velocity, stress and strain fields, respectively, ρ is the mass density, E is Young's modulus, and \hat{E} and τ are rheological parameters, furthermore Δt and Δx denotes time and space steps, and α is the measure of implicitness.

The stability of the scheme proves to be ensured via the inequalities

$$(1-lpha)+rac{ au}{\Delta t}>0, \qquad \qquad \left(rac{1}{2}-lpha
ight)+rac{ au}{\Delta t}>\left[\left(rac{1}{2}-lpha
ight)+rac{E}{E}
ight]C^2S^2, \ rac{\hat{E}}{E}> au, \qquad \qquad \left(rac{1}{2}-lpha
ight)+rac{ au}{\Delta t}>0$$

where $C:=\sqrt{rac{E}{arrho}}rac{\Delta t}{\Delta x}$ is the Courant number, $S:=\sinrac{k\Delta x}{2}$ and k denotes the wave number.

The numerics-originated dispersive errors can be eliminated if $\alpha = \frac{1}{2}$ and the value of the rheological Courant number $\hat{C} = \sqrt{\frac{E_{\text{dyn}}}{\varrho}} \frac{\Delta t}{\Delta x}$ calculated with the dynamical Young's modulus $E_{\text{dyn}} := \frac{\hat{E}}{\tau}$ is 1, since the argument of the eigenvalues of the transfer matrix of the scheme is linear in $k\Delta x$.

The numerics-originated dissipation errors are quantifiably small even for large time steps if $\alpha = \frac{1}{2}$ and $\hat{C} = 1$: the error is caused by a deviation from 1 of the absolute value of the eigenvalues of the transfer matrix, which for the nondimensional time step $\Delta \tilde{t} \leq 0.05$ is under 1.5%.

The natural generalization of the one spatial dimensional scheme to a three spatial dimensional cubic Cartesian grid proves to numerically preserve the total energy for the case of $\alpha = \frac{1}{2}$.

Corresponding publication: [T5,T6] ([44, 48]). Corresponding sections: V.2.1, V.2.2 and V.3.1.

Numerical solutions have to be validated, for which known analytical solutions can be used. In case of rheology, there are only very few known analytical solutions, even in the case of force-equilibrial approximation (acceleration neglected, thus wave propagation phenomena omitted). For such problems, inspired by Volterra's principle, an exact analytical method (the method of four elastic spatial pattern sets) has been developed by Tamás Fülöp. According to this method, the elastic stress and strain solutions are decomposed into linearly independent spatial patterns and, replacing the constant coefficients of

these spatial patterns by unknown time-dependent functions and determining them, the solution for the rheological problem can be obtained. Via this method, analytical solutions for six practically important problems have been given. Analyzing the solutions, two unprecedented phenomena are identified, which are invisible in elasticity and in one spatial dimension: in addition to damping and delaying effects, rheology can induce motions of the medium with varying direction dependence, and transient motion patterns with opposite sign with respect to the large-time values. The method and results can be applied in tunneling for both qualitative and quantitative understanding of processes.

Thesis 5:

Via the method of four elastic spatial pattern sets, the time and space dependence of the stress, strain and displacement fields are determined

- around cylindrical bore and spherical hollow opened in infinite, homogeneous and isotropic stress field;
- around cylindrical bore opened in infinite, homogeneous and anisotropic stress field;
- around cylindrical bore opened in homogeneous medium loaded by its self weight for arbitrary lateral pressure factor $-\frac{1}{2} < k \leq 1$, more exactly:
 - for hydrostatic initial stress state, *i.e.*, k = 1,
 - when no lateral deformations in the initial stress state are allowed, *i.e.*, $k = \frac{\nu}{1-\nu}$ (here ν denotes Poisson's ratio),
 - when free lateral deformations in the initial stress state are allowed, *i.e.*, k = 0;
- for pressurizing of thick-walled tubes and spherical tanks.

The solutions show that rheology is more than damped and delayed elastic behavior: it can lead to motions of the medium with varying direction dependence, and to transients with opposite signs to the asymptotic time tendencies. The results illustrate such well-known phenomena in tunneling as convergence, tunnel squeezing and rotations of the cross sections.

Corresponding publications: [T7, T8, T9, T10] ([158, 159, 160, 157]). Corresponding sections: VI.1.3 and VI.2.

Publications corresponding to theses:

- [T1] T. Fülöp, R. Kovács, Á. Lovas, Á. Rieth, T. Fodor, M. Szücs, P. Ván, and G. Gróf. Emergence of non-Fourier hierarchies. *Entropy*, vol. 20, no. 11, p. 832, 2018.
- [T2] M. Szücs, M. Pavelka, R. Kovács, T. Fülöp, P. Ván, and M. Grmela. A case study of non-Fourier heat conduction using internal variables and GENERIC. Journal of Non-Equilibrium Thermodynamics, vol. 47, no. 1, pp. 31–60, 2022.
- [T3] M. Szücs. Szilárd közegek reológiája a GENERIC nemegyensúlyi termodinamikai leírásban [Rheology of solids in the nonequilibrium thermodynamical framework GENERIC]. In Tamás Fülöp, editor, *Nemegyensúlyi termodinamika és szilárd közegeke [Nonequilibrium thermodynamics and solids]*, Mérnökgeológia–Kőzetmechanika Kiskönyvtár [Book Series on Engineering Geology and Rock Mechanics] 22, pp. 181–240, Budapest: Egyesület a Tudomány és Technológia Egységéért, 2018.
- [T4] **M. Szücs** and *T. Fülöp*. Kluitenberg–Verhás rheology of solids in the GENERIC framework. *Journal of Non-Equilibrium Thermodynamics*, vol. 44, no. 3, pp. 247–259, 2019.

- [T5] T. Fülöp, R. Kovács, M. Szücs, and M. Fawaier. Thermodynamical extension of a symplectic numerical scheme with half space and time shifts demonstrated on rheological waves in solids. *Entropy*, vol. 20, no. 11, p. 832, 2018.
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