

**Weierstraß-Institut**  
**für Angewandte Analysis und Stochastik**  
**Leibniz-Institut im Forschungsverbund Berlin e. V.**

Preprint

ISSN 2198-5855

**A general thermodynamical model for finitely-strained continuum  
with inelasticity and diffusion, its GENERIC derivation in Eulerian  
formulation, and some application**

Alexander Mielke<sup>1</sup>, Tomáš Roubíček<sup>2</sup>

submitted: May 6, 2024

<sup>1</sup> Weierstrass Institute  
Mohrenstr. 39  
10117 Berlin  
Germany  
E-Mail: alexander.mielke@wias-berlin.de

<sup>2</sup> Mathematical Institute  
Charles University  
Sokolovská 83  
186 75 Praha 8  
Czech Republic  
and  
Institute of Thermomechanics  
Czech Academy of Sciences  
Dolejšková 5  
182 00 Praha 8  
Czech Republic  
E-Mail: tomas.roubicek@mff.cuni.cz

No. 3107  
Berlin 2024



---

2020 *Mathematics Subject Classification.* 35Q74, 74L05, 74F05, 74N25, 76A10, 80A19, 86A99.

*Key words and phrases.* Eulerian mechanics, visco-elastodynamics, Jeffreys rheology, plasticity, poroelasticity, GENERIC, Lie derivatives, Poisson operator, Onsager operator, phase transitions in rocks, martensitic phase transitions.

A.M. acknowledges partial support by the Deutsche Forschungsgemeinschaft through Collaborative Research Center SFB 1114 “Scaling Cascades in Complex Systems” (Project Number 235221301). T.R. acknowledges hospitality and a support from the Weierstrass Institute Berlin. This research was also supported from the CSF project no. 23-06220S, and from the institutional support RVO: 61388998 (ČR).

Edited by  
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)  
Leibniz-Institut im Forschungsverbund Berlin e. V.  
Mohrenstraße 39  
10117 Berlin  
Germany

Fax: +49 30 20372-303  
E-Mail: [preprint@wias-berlin.de](mailto:preprint@wias-berlin.de)  
World Wide Web: <http://www.wias-berlin.de/>

# A general thermodynamical model for finitely-strained continuum with inelasticity and diffusion, its GENERIC derivation in Eulerian formulation, and some application

Alexander Mielke, Tomáš Roubíček

## Abstract

A thermodynamically consistent visco-elastodynamical model at finite strains is derived that also allows for inelasticity (like plasticity or creep), thermal coupling, and poroelasticity with diffusion. The theory is developed in the Eulerian framework and is shown to be consistent with the thermodynamic framework given by General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC). For the latter we use that the transport terms are given in terms of Lie derivatives. Application is illustrated by two examples, namely volumetric phase transitions with dehydration in rocks and martensitic phase transitions in shape-memory alloys. A strategy towards a rigorous mathematical analysis is only very briefly outlined.

## 1 Introduction

In this article, we give a systematic derivation of a fairly general visco-elastodynamical model with possibly certain internal variables at large strains (also called finite strain) in the Eulerian setting. The mechanical attributes can be summarized as follows:

- (i) hyperelasticity for the elastostatic part (i.e. the conservative part of the Cauchy stress comes from a free energy  $\psi$ ),
- (ii) Jeffreys' rheology (also called anti-Zenner rheology) with the multiplicative decomposition of the deformation gradient into the elastic and the inelastic (plastic/creep) distortions,
- (iii) Fick-type diffusion of an intensive variable (like phase field),
- (iv) Fick-type diffusion of an extensive variable (like a conserved chemical species),
- (iv) and the heat equation (either as an energy- or an entropy-balance equation).

Our goal is to devise a model in the Eulerian formulation, consistent with sound thermodynamical principles of energy conservation, entropy entropy-production balance, an non-negativity of temperature. These properties might still be satisfied by various other models, hence we show that our class of models also fits into the so-called GENERIC framework, which is the acronym standing for *General Equation for Non-Equilibrium Reversible-Irreversible Coupling*. This name which was introduced in [21] but this class of models has its origins in the metriplectic theory developed in [45, 46], cf. the survey [47]. Over the last decade, the GENERIC framework has proved to be a versatile modeling

tool for various complex coupled models for fluids and solids, see e.g. [4, 16, 26, 35, 36, 42, 54–56, 76] and the references therein. We also refer to [43] for a derivation of a dissipative GENERIC system from (non-dissipative) Hamiltonian systems.

The plan of this paper is as follows: In Sect. 2 we recall the standard Eulerian kinematics in continuum mechanics with Eulerian velocity  $\boldsymbol{v}$ . Sect. 3 is devoted to the formulation of a rather general model for compressible thermo-visco-elastodynamics with inelasticity motivated by the multiplicative split  $\boldsymbol{F} = \boldsymbol{F}_e \boldsymbol{F}_p$  but replaced by the kinematic equation

$$\dot{\boldsymbol{F}}_e = (\nabla \boldsymbol{v}) \boldsymbol{F}_e - \boldsymbol{F}_e \boldsymbol{L}_p,$$

where the elastic part  $\boldsymbol{F}_e \in \mathbb{R}^{d \times d}$  of the deformation will be a state variable while the inelastic distortion rate tensor  $\boldsymbol{L}_p$  will be given in terms of a flow rule involving the Mandel tensor. Additionally, we allow for the diffusion of an intensive variable or extensive variable  $z$ . The model is phrased in the classical mechanical approach using the heat equation in terms of the absolute temperature  $\theta > 0$  and the referential free energy  $\psi(\boldsymbol{F}_e, z, \theta)$ .

To give a physically more sound justification, in Sect. 4 we do a step aside and derive a quite similar general continuum model, but start from a completely different angle. Instead of studying balance equations and constitutive laws, we follow the philosophy of GENERIC where the model is determined by an energy and an entropy functionals  $\mathcal{E}$  and  $\mathcal{S}$  as well as geometric operators  $\mathbb{J}$  and  $\partial \mathcal{R}^*$  describing the Hamiltonian and the dissipative parts of the evolution, namely

$$\frac{\partial}{\partial t} q = \mathbb{J}(q) D\mathcal{E}(q) + \partial_{\xi} \mathcal{R}^*(q, D\mathcal{S}(q)).$$

A particular advantage of this theory is that it easily allows for coordinate changes and consistent coupling of different effects, see [26, 42, 54–56, 76]. In particular, it is useful that one is able to choose an arbitrary thermodynamical variable  $w$  (e.g. the internal energy  $e$ , the entropy  $s$ , the temperature  $\theta$ , or its inverse  $1/\theta$ ) when deriving the energy balance or the entropy imbalance. Using  $e = E(\boldsymbol{F}_e, z, w)$  and  $s = S(\boldsymbol{F}_e, z, w)$  one has

$$\theta = \Theta(\boldsymbol{F}_e, z, w) = \frac{E'_w(\boldsymbol{F}_e, z, w)}{S'_w(\boldsymbol{F}_e, z, w)} \quad \text{and} \quad \Sigma_{\text{Cauchy}} = [ (E'_{\boldsymbol{F}_e} - \Theta S'_{\boldsymbol{F}_e}) \boldsymbol{F}_e^{\top} + (E - \Theta S) \mathbb{I} ]_{(\boldsymbol{F}_e, z, w)}$$

for all choices of  $w$ . As a natural by-product, the GENERIC structure reveals in a transparent way which source terms appear in the energy equation and which ones in the entropy equation. To the best of our knowledge, this provides the first complete treatment of Eulerian elasticity in GENERIC.

In Sect. 5, we study the impact of the GENERIC formulation on the model developed in Sect. 3 formulated in terms of temperature and referential free energy. In Sect. 6, we illustrate the possible application on two examples involving volumetric and spherical phase transitions, namely Earth's mantle dynamics with (de)hydration and martensitic phase transition with plasticity and possibly also a metal-hybrid phase transition. Finally, we comment (mostly very technical) analytical aspects very briefly and only conceptually in Sect. 7.

For readers' convenience, let us summarize the basic notation used in what follows:

$\mathbf{y}$ deformation,	$J = \det \mathbf{F}$ Jacobian = determinant of $\mathbf{F}$ ,
$\mathbf{v}$ velocity,	$p_{\text{heat}}$ heat production rate,
$\mathbf{L} = \nabla \mathbf{v}$ velocity gradient,	$p_{\text{mech}}$ mechanical power,
$\rho$ mass density,	$\sigma_{\text{prod}}$ entropy production rate,
$\Sigma_{\text{Cauchy}}$ the Cauchy stress,	$\mathbf{j}_{\text{ener}}$ energy flux,
$\Sigma_{\text{Mandel}}$ the Mandel stress,	$\mathbf{j}_{\text{entr}}$ entropy flux,
$\Sigma_{\text{dissip}}$ the dissipative stress,	$\mathbb{K}_{\text{heat}}$ heat conductivity,
$\mathbf{F}$ deformation gradient,	$\mathbb{K}_{\text{diff}}$ diffusivity/mobility ( $\mathbb{A}_{\text{diff}}$ or $\mathbb{B}_{\text{diff}}$ ),
$\mathbf{F}_e$ elastic strain,	$R_{\text{plast}}$ inelastic entropy-production potential,
$\mathbf{F}_p$ inelastic strain,	$A_{\text{source}}$ source of intensive variable $\alpha$ ,
$\mathbf{L}_p$ inelastic distortion rate,	$\text{tr}(\cdot)$ trace of a matrix,
$z$ content of diffusant ( $\alpha$ or $\beta$ ),	$\text{dev}(\cdot)$ deviatoric part of a matrix
$\mu$ chemical potential,	$\mathbb{R}_{\text{sym}}^{d \times d}$ set of symmetric matrices,
$\theta$ temperature,	$\mathbb{R}_{\text{dev}}^{d \times d} = \{A \in \mathbb{R}_{\text{sym}}^{d \times d}; \text{tr} A = 0\}$ ,
$e$ internal energy ( $= \psi + \theta s$ ),	$\mathbb{J}$ Poisson operator in GENERIC,
$\psi$ free energy (actual),	$\mathbb{K}$ Onsager operator in GENERIC,
$\Psi$ free energy (referential),	$w$ general thermal variable (e.g. $e, \theta, 1/\theta, s$ ),
$s$ entropy,	$E(\mathbf{F}_e, \alpha, \beta, w)$ internal energy as function,
$\xi$ return mapping,	$S(\mathbf{F}_e, \alpha, \beta, w)$ entropy as function,
$\mathbf{D} = \text{sym} \mathbf{L} = (\mathbf{L}^\top + \mathbf{L})/2$ ,	$\mathcal{L}_v \square$ Lie derivative w.r.t. the vector field $\mathbf{v}$ ,
$\rho_R$ referential mass density,	$\square$ a general placeholder (or the end of proofs).
$\mathbf{g}$ gravity acceleration,	

Table 1. Summary of the basic notation used.

## 2 Kinematics

In the finite-strain (also called large-strain) continuum mechanics, the basic geometrical concept is a *deformation*  $\mathbf{y} : \Omega \rightarrow \mathbb{R}^d$  as a mapping from a reference configuration  $\Omega \subset \mathbb{R}^d$  into the physical space  $\mathbb{R}^d$ . The inverse motion  $\xi = \mathbf{y}^{-1} : \mathbf{y}(\Omega) \rightarrow \Omega$ , if it exists, is called a *return* (or sometimes a *reference*) *mapping*. We will denote by  $\mathbf{X}$  and  $\mathbf{x}$  the reference (Lagrangian) and the actual (Eulerian) point coordinates, respectively. The other basic geometrical object is the (referential) *deformation gradient*  $\mathbf{F}_R(\mathbf{X}) = \nabla_{\mathbf{X}} \mathbf{y}$ .

If evolving in time,  $\mathbf{x} = \mathbf{y}(t, \mathbf{X})$  is sometimes called a “motion”. The important quantity is the (referential) velocity  $\mathbf{v}_R = \frac{d}{dt} \mathbf{y}(t, \mathbf{X})$  with  $d/dt$  the derivative with respect to time of a time dependent function. When composed with the return mapping  $\xi$ , we obtain the Eulerian representations

$$\mathbf{F}(t, \mathbf{x}) = \mathbf{F}_R(t, \xi(\mathbf{x})) \quad \text{and} \quad \mathbf{v}(t, \mathbf{x}) = \mathbf{v}_R(t, \xi(\mathbf{x})). \quad (2.1)$$

The Eulerian velocity  $\mathbf{v}$  is employed in the convective time derivative

$$(\cdot)^{\cdot} = \frac{\partial}{\partial t}(\cdot) + (\mathbf{v} \cdot \nabla)(\cdot) \quad (2.2)$$

with  $\nabla$  taken with respect to actual coordinates, to be used for scalars and, component-wise, for vectors or tensors.

Then the velocity gradient  $\nabla \mathbf{v} = \nabla_{\mathbf{X}} \mathbf{v} \nabla_{\mathbf{x}} \mathbf{X} = \dot{\mathbf{F}} \mathbf{F}^{-1}$ , where we used the chain-rule calculus and  $\mathbf{F}^{-1} = (\nabla_{\mathbf{X}} \mathbf{x})^{-1} = \nabla_{\mathbf{x}} \mathbf{X}$ . This gives the *transport-and-evolution equation* (the so-called *kinematic equation*) for the deformation gradient as

$$\dot{\mathbf{F}} = \mathbf{L} \mathbf{F} \quad \text{with } \mathbf{L} := \nabla \mathbf{v}. \quad (2.3)$$

From this, we also obtain the kinematic equation for  $\det \mathbf{F}$  as  $\overline{\det \mathbf{F}} = (\operatorname{div} \mathbf{v}) \det \mathbf{F}$ .

Introducing a (generally non-symmetric) *inelastic distortion* tensor  $\mathbf{F}_p$ , a conventional large-strain plasticity is based on Kröner-Lie-Liu [31, 37] *multiplicative decomposition*

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p. \quad (2.4)$$

Here  $\mathbf{F}_e = \mathbf{F} \mathbf{F}_p^{-1}$  is the *elastic distortion*. The interpretation of  $\mathbf{F}_p$  is a transformation of the reference configuration into an intermediate stress-free configuration, and then  $\mathbf{F}_e$  transforms this intermediate configuration into the current actual configuration.

Applying the material derivative on (2.4) and using (2.3), we obtain  $\mathbf{L} \mathbf{F} = \dot{\mathbf{F}} = \dot{\mathbf{F}}_e \mathbf{F}_p + \mathbf{F}_e \dot{\mathbf{F}}_p$  and, multiplying it by  $\mathbf{F}^{-1} = \mathbf{F}_p^{-1} \mathbf{F}_e^{-1}$ , we eventually obtain

$$\mathbf{L} = \underbrace{\dot{\mathbf{F}}_e \mathbf{F}_e^{-1}}_{\substack{\text{elastic} \\ \text{distortion} \\ \text{rate}}} + \underbrace{\mathbf{F}_e \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \mathbf{F}_e^{-1}}_{\substack{\text{inelastic} \\ \text{distortion} \\ \text{rate} =: \mathbf{L}_p}}, \quad (2.5)$$

which is used mostly in connection to plasticity, cf. e.g. [3, 14, 22, 23, 29, 38, 58]; the term “distortion rates” is due to [22, 23] while sometimes  $\mathbf{L}_p$  is called a “plastic dissipation tensor” [3] or “velocity gradient of purely plastic deformation” in [38], etc. By the algebraic manipulation, we can eliminate  $\dot{\mathbf{F}}_p$  and see that (2.5) is equivalent to the *kinematic equation* for  $\mathbf{F}_e$ :

$$\dot{\mathbf{F}}_e = \mathbf{L} \mathbf{F}_e - \mathbf{F}_e \mathbf{L}_p. \quad (2.6)$$

In principle, if one is interested also in the inelastic distortion itself, we can reconstruct  $\mathbf{F}_p$  from (2.5) when re-arranging it to the plastic-distortion evolution rule  $\dot{\mathbf{F}}_p = \mathbf{L}_p \mathbf{F}_p$  and by prescribing an initial condition  $\mathbf{F}_p|_{t=0}$ .

### 3 A thermo-visco-elastodynamics with diffusion

To come straight to a quite general model, which represents a concrete motivation for the next section. We first formulate it in a manner which is quite common in engineering and physics, specifically using a *free energy* from which one can read both the internal energy and the entropy. Moreover, it is quite standard to use the *referential free energy*  $\psi = \psi(\mathbf{F}_e, z, \theta)$  considered in  $\text{J/m}^{-3} = \text{Pa}$ , i.e. a specific energy per referential volume, and the heat equation formulated in terms of temperature. For another, also a standard setting involves a referential free energy considered in  $\text{J/kg}$ , see Remark 5.1 below.

The other ingredient is the dissipation potential  $r = r(z, \theta; \cdot, \cdot) : \mathbb{R}^{d \times d} \times \mathbb{R}_{\text{dev}}^{d \times d} \rightarrow \mathbb{R}$  acting on the velocity gradient  $\mathbf{L}$  (or here rather only on its symmetric part) and the inelastic distortion rate  $\mathbf{L}_p$ .

For the sake of generality, we distinguish two cases concerning the content or concentration variable  $z$ : *extensive* or *intensive*, later in Section 4 denoted respectively by  $\alpha$  and  $\beta$ , the former case leading to some additional terms. To write the equations more “compactly” for both cases, we will use the “switch”

$$\mathfrak{s}_{\text{EXT}} = \begin{cases} 1 & \text{if } z \text{ is intensive,} \\ 0 & \text{if } z \text{ is extensive.} \end{cases} \quad (3.1)$$

This affects the conservative Cauchy stress  $\Sigma_{\text{Cauchy}}$  in (3.2b) and the diffusion equation (3.2d) as well as the temperature equation (3.2f) below. The system for the six-tuple  $(\varrho, \mathbf{v}, \mathbf{F}_e, z, \mathbf{L}_p, w)$  is composed from the six equations, namely the mass-density continuity equation, the momentum equation, the kinematic equation (2.6), the diffusion equation, the inelastic flow rule, and the heat equation:

$$\frac{\partial \varrho}{\partial t} + \text{div}(\varrho \mathbf{v}) = 0 \quad (3.2a)$$

$$\frac{\partial}{\partial t}(\varrho \mathbf{v}) + \text{div}(\varrho \mathbf{v} \otimes \mathbf{v}) = \varrho \mathbf{g} + \text{div}(\Sigma_{\text{Cauchy}} + \Sigma_{\text{dissip}}) \quad \text{with } \Sigma_{\text{dissip}} = [r^*]_{\mathbf{D}}'(z, \theta; \mathbf{D}, \mathbf{L}_p)$$

$$\text{and } \Sigma_{\text{Cauchy}} = \frac{\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) \mathbf{F}_e^\top - \mathfrak{s}_{\text{EXT}} z \psi'_z(\mathbf{F}_e, z, \theta) \mathbb{I}}{\det \mathbf{F}_e}, \quad (3.2b)$$

$$\dot{\mathbf{F}}_e = (\nabla \mathbf{v}) \mathbf{F}_e - \mathbf{F}_e \mathbf{L}_p, \quad (3.2c)$$

$$\dot{z} + \mathfrak{s}_{\text{EXT}} z \text{div } \mathbf{v} = \text{div}(\mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta}) \quad \text{with } \mu = \frac{\psi'_z(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e}, \quad (3.2d)$$

$$r'_{\mathbf{L}_p}(z, \theta; \mathbf{D}, \mathbf{L}_p) = \text{dev } \Sigma_{\text{Mandel}} \quad \text{with } \Sigma_{\text{Mandel}} = \frac{\mathbf{F}_e^\top \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e}, \quad (3.2e)$$

$$c(\mathbf{F}_e, z, \theta) \dot{\theta} = p_{\text{heat}} - \text{div}(\mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta}) + \theta \frac{\psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta) \mathbf{F}_e^\top}{\det \mathbf{F}_e} : \nabla \mathbf{v} - \theta \frac{\mathbf{F}_e^\top \psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e} : \mathbf{L}_p \\ - \frac{\psi'_z(\mathbf{F}_e, z, \theta) - \theta \psi''_{z\theta}(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e} \dot{z} - \mathfrak{s}_{\text{EXT}} \frac{z \psi'_z(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e} \text{div } \mathbf{v}$$

$$\text{with the heat production rate } p_{\text{heat}} = \Sigma_{\text{dissip}} : \mathbf{D} + r'_{\mathbf{L}_p}(z, \theta; \mathbf{D}, \mathbf{L}_p) : \mathbf{L}_p$$

$$\text{and the heat capacity } c(\mathbf{F}_e, z, \theta) = -\theta \frac{\psi''_{\theta\theta}(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e}, \quad (3.2f)$$

where  $\mathbb{K}_{\text{diff}} = \mathbb{K}_{\text{diff}}(\mathbf{F}_e, z, \theta)$  and  $\mathbb{K}_{\text{heat}} = \mathbb{K}_{\text{heat}}(\mathbf{F}_e, z, \theta)$  are the (symmetric positive definite) matrices of diffusivity (mobility) and heat conductivity coefficients, and where  $r^*(z, \theta; \cdot, \cdot)$  denotes the convex conjugate to the dissipation potential  $r(z, \theta; \cdot, \cdot)$ . This system will be derived and thermodynamically justified in Section 5 by exploiting a universal tool in the next Section 4.

To ensure non-negativity of temperature (sometimes called the 0<sup>th</sup> law of thermodynamics), the  $\psi'_z(\mathbf{F}_e, z, \theta) \dot{z}$ -term suggests the restriction  $\psi'_z(\mathbf{F}_e, z, 0) = 0$ . A particular and perhaps physically most relevant ansatz to satisfy  $\psi'_z(\mathbf{F}_e, z, 0) = 0$  is

$$\psi(\mathbf{F}_e, z, \theta) = \theta \eta(\mathbf{F}_e, z) + \phi(\mathbf{F}_e, \theta). \quad (3.3)$$

With this ansatz, the term  $(\psi'_z(\mathbf{F}_e, z, \theta) - \theta \psi''_{z\theta}(\mathbf{F}_e, z, \theta)) \dot{z}$  vanishes identically and also the heat capacity  $c(\mathbf{F}_e, z, \theta) = -\theta \psi''_{\theta\theta}(\mathbf{F}_e, z, \theta) / \det \mathbf{F}_e = -\theta \phi''_{\theta\theta}(\mathbf{F}_e, \theta) / \det \mathbf{F}_e$  becomes independent of

$z$ , so that the diffusant content does not affect the heat capacity and, altogether, the diffusion does not directly affect the heat equation at all. Anyhow, there is some experience that, in some situations, diffusion can directly generate heat so that the ansatz (3.3) may be not entirely universal.

## 4 A general setup of the model for GENERIC

We consider a viscoelastoplastic material in an Eulerian domain  $\Omega$ , which is further characterized by the local temperature  $\theta$ , an intensive variable  $\alpha$  (like damage or aging or concentration of a diffusant) and an extensive variable  $\beta$  (like a content of a diffusant). The material properties are encoded in the *actual free-energy density*

$$\psi = \psi(\mathbf{F}_e, \alpha, \beta, \theta) \quad (4.1)$$

which is related with the referential free energy  $\Psi$  used in Section 3 by

$$\psi(\mathbf{F}_e, z, \theta) = \frac{\Psi(\mathbf{F}_e, z, \theta)}{\det \mathbf{F}_e}. \quad (4.2)$$

Both  $\psi$  and  $\Psi$  are in the physical unit Pa, i.e. J/m<sup>3</sup>, but m<sup>3</sup> is meant as an actual volume vs a referential volume, respectively. The latter option can alternatively be considered in J/kg, cf. Remark 5.1 below. For consistency with GENERIC to be studied below, we introduce the entropy density  $S$  and the internal-energy density  $E$  via

$$S(\mathbf{F}_e, \alpha, \beta, \theta) = -\psi'_\theta(\mathbf{F}_e, \alpha, \beta, \theta) \quad \text{and} \quad E(\mathbf{F}_e, \alpha, \beta, \theta) = \psi(\mathbf{F}_e, \alpha, \beta, \theta) + \theta S(\mathbf{F}_e, \alpha, \beta, \theta).$$

The system we want to study will be formulated in terms of the state  $q = (\mathbf{p}, \mathbf{F}_e, \alpha, \beta, \theta)$ , where  $\mathbf{p} = \varrho \mathbf{v}$  is the linear momentum and

$$\varrho = \frac{\rho_R}{\det \mathbf{F}_e}. \quad (4.3)$$

Here  $\mathbf{F}_e$  is the elastic part of the deformation-gradient tensor  $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$ , viz (2.3), but  $\mathbf{F}_p$  is not needed while only the inelatic distortion rate  $\mathbf{L}_p$  will appear, viz (2.5)–(2.6).

Assuming  $\text{tr} \mathbf{L}_p = 0$ , the system for  $(\mathbf{v}, \mathbf{F}_e, \alpha, \beta, \theta)$  takes the following form:

$$\frac{\partial}{\partial t}(\varrho \mathbf{v}) + \text{div}(\varrho \mathbf{v} \otimes \mathbf{v}) = \text{div}(\boldsymbol{\Sigma}_{\text{Cauchy}} - \beta \psi'_\beta \mathbb{I} + \mathbb{D}_{\text{visc}}(q) \mathbf{D}), \quad (4.4a)$$

$$\frac{\partial \mathbf{F}_e}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{F}_e = (\nabla \mathbf{v}) \mathbf{F}_e - \mathbf{F}_e \mathbf{L}_p, \quad (4.4b)$$

$$\frac{\partial \alpha}{\partial t} + \mathbf{v} \cdot \nabla \alpha = \text{div} \left( \mathbb{A}_{\text{diff}} \nabla \frac{\mu^\alpha}{\theta} \right) - A_{\text{source}} \frac{\mu^\alpha}{\theta} \quad (4.4c)$$

$$\frac{\partial \beta}{\partial t} + \text{div}(\beta \mathbf{v}) = \text{div} \left( \mathbb{B}_{\text{diff}} \nabla \frac{\mu^\beta}{\theta} \right) \quad (4.4d)$$

$$\frac{\partial e}{\partial t} + \text{div}(e \mathbf{v}) = (\boldsymbol{\Sigma}_{\text{Cauchy}} - \beta \psi'_\beta \mathbb{I} + \mathbb{D}_{\text{visc}} \mathbf{D}) : \mathbf{D} - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \right), \quad (4.4e)$$

where we have

$$\boldsymbol{\Sigma}_{\text{Cauchy}} = \psi'_{\mathbf{F}_e} \mathbf{F}_e^\top + \psi \mathbb{I}, \quad \mathbf{D} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^\top), \quad \mu^\alpha = \psi'_\alpha, \quad \mu^\beta = \psi'_\beta, \quad (4.4f)$$

$$\mathbf{L}_p = \theta \mathbb{M}^* \partial_{\eta \mathbf{F}_e} R_{\text{plast}}^*(q, \mathbb{M}(q) \boldsymbol{\Sigma}_{\text{Mandel}}) \quad \text{with } \boldsymbol{\Sigma}_{\text{Mandel}} = \mathbf{F}_e^\top \psi'_{\mathbf{F}_e}, \quad \text{and} \quad (4.4g)$$

$$e = E(\mathbf{F}_e, \alpha, \beta, \theta), \quad \text{and} \quad \varrho = \rho_R / \det \mathbf{F}_e \quad \text{as in (4.3)}. \quad (4.4h)$$

On the left-hand sides of (4.4a-e), we can see the appropriate convective derivatives, which are in fact Lie derivatives, see Proposition 4.2. The coefficient  $A_{\text{source}} = A_{\text{source}}(\mathbf{F}_e, z, \theta)$  in the intensive-variable evolution (4.4c) can be used for modeling damage- or aging-type processes.

The aim of the following section is to show that this system can be cast in the GENERIC framework.

## 4.1 The principles of GENERIC

We consider states  $q$  in a state space  $\mathcal{Q}$  which is either a flat space or a smooth manifold. A GENERIC system is a quintuple  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ , where the energy  $\mathcal{E}$  and the entropy  $\mathcal{S}$  are differentiable functions on  $\mathcal{Q}$  with differentials  $D\mathcal{E}(q), D\mathcal{S}(q) \in T_q^* \mathcal{Q}$ . The geometric structures are the Poisson operator  $\mathbb{J}$  for Hamiltonian dynamics and the Onsager operator  $\mathbb{K}$  for dissipative dynamics, which maps  $T^* \mathcal{Q}$  to  $T \mathcal{Q}$ . The evolution equation then takes the form

$$\frac{\partial q}{\partial t} = \mathbb{J}(q) D\mathcal{E}(q) + \mathbb{K}(q) D\mathcal{S}(q).$$

The Poisson operator is defined by being skew-symmetric and satisfying the Jacobi identity, i.e.

$$\langle \zeta_1, D\mathbb{J}(q)[\mathbb{J}(q)\zeta_2]\zeta_3 \rangle + \text{cycl. perm.} \equiv 0 \quad \text{for all } \zeta_1, \zeta_2, \zeta_3 \in T_q^* \mathcal{Q}. \quad (4.5)$$

The Onsager operators are defined by the conditions of symmetry and positive semi-definiteness, namely  $\mathbb{K}(q)^* = \mathbb{K}(q) \geq 0$ .

The main condition for GENERIC are the so-called *non-interaction conditions*, namely

$$\mathbb{J}(q) D\mathcal{S}(q) \equiv 0 \quad \text{and} \quad \mathbb{K}(q) D\mathcal{E}(q) \equiv 0. \quad (4.6)$$

Using the chain rule, a simple consequence of the second condition is energy conservation along solutions, i.e.  $\frac{d}{dt} \mathcal{E}(q(t)) = 0$ , while the second condition implies entropy increase, namely  $\frac{d}{dt} \mathcal{S}(q(t)) = \langle D\mathcal{S}(q), \mathbb{K}(q) D\mathcal{S}(q) \rangle \geq 0$ . See [42, Sec. 2.2] and [53] for further properties of GENERIC systems.

In fact, often the linear kinetic relation  $\zeta \mapsto \mathbb{K}(q)\zeta$  for the dissipative part needs to be generalized to allow for nonlinear relations. In such cases, one uses the dual dissipation potential  $\mathcal{R}^* : T^* \mathcal{Q} \rightarrow [0, \infty]$ , where  $\mathcal{R}^*(q, \cdot) : T_q^* \rightarrow [0, \infty]$  is a lower semicontinuous and convex functional satisfying  $0 = \mathcal{R}^*(q, 0) \leq \mathcal{R}^*(q, \zeta)$ . In the linear form it takes the form  $\mathcal{R}^*(q, \zeta) = \frac{1}{2} \langle \zeta, \mathbb{K}(q)\zeta \rangle$ . Then, the kinetic relation takes the form  $\zeta \mapsto \partial_\zeta \mathcal{R}^*(q, \zeta) \subset T \mathcal{Q}$ , where  $\partial_\zeta \mathcal{R}^*$  is the (possibly multi-valued) convex subdifferential. The GENERIC evolution equation then reads

$$\frac{\partial q}{\partial t} = \mathbb{J}(q) D\mathcal{E}(q) + \mathbb{K}(q) D\mathcal{S}(q),$$

and the second non-interaction condition is replaced by

$$\mathcal{R}^*(q, \lambda D\mathcal{E}(q)) \equiv 0 \quad \text{for all } \lambda \in \mathbb{R}.$$

By convexity, the latter condition implies  $\mathcal{R}^*(q, \zeta + \lambda D\mathcal{E}(q)) = \mathcal{R}^*(q, \zeta)$  for all  $(q, \zeta) \in T^* \mathcal{Q}$  and  $\lambda \in \mathbb{R}$ . Again, energy conservation and entropy increase follow.

## 4.2 Arbitrary thermal variable and stress tensors

Using the generalization of [42] (see also the recent usages in [4, 5]), we work with a general scalar thermodynamic variable  $w$  that can denote either the temperature  $\theta$ , the internal energy  $e$ , the entropy  $s$ , or other. The only restriction is that both functions  $e = E(\mathbf{F}_e, \alpha, \beta, w)$  and  $s = S(\mathbf{F}_e, \alpha, \beta, w)$  satisfy the relation

$$\theta = \Theta(\mathbf{F}_e, \alpha, \beta, w) = \frac{\partial_w E(\mathbf{F}_e, \alpha, \beta, w)}{\partial_w S(\mathbf{F}_e, \alpha, \beta, w)} > 0, \quad (4.7)$$

where  $\theta$  is the absolute temperature.

Since the derivatives of the free energy with respect to  $\mathbf{F}_e$ ,  $\alpha$ , and  $\beta$  at constant temperature play a crucial role as thermodynamical driving forces, we recall from [42, Eqn. (2.13)] the important relations

$$\psi'_{\mathbf{F}_e}(\mathbf{F}_e, \alpha, \beta, \theta) \Big|_{\theta=\Theta(\mathbf{F}_e, \alpha, \beta, w)} = E'_{\mathbf{F}_e}(\mathbf{F}_e, \alpha, \beta, w) - \Theta(\mathbf{F}_e, \alpha, \beta, w) S'_{\mathbf{F}_e}(\mathbf{F}_e, \alpha, \beta, w) \quad \text{and} \quad (4.8a)$$

$$\psi'_\zeta(\mathbf{F}_e, \alpha, \beta, \theta) \Big|_{\theta=\Theta(\mathbf{F}_e, \alpha, \beta, w)} = E'_\zeta(\mathbf{F}_e, \alpha, \beta, w) - \Theta(\mathbf{F}_e, \alpha, \beta, w) S'_\zeta(\mathbf{F}_e, \alpha, \beta, w) \quad (4.8b)$$

for  $\zeta = \alpha, \beta$ . For general choices of the thermal variable  $w$ , the free energy is always given by  $\psi(\mathbf{F}_e, \zeta, w) = E(\mathbf{F}_e, \zeta, w) - \Theta(\mathbf{F}_e, \zeta, w)S(\mathbf{F}_e, \zeta, w)$ . Note that, in view of (4.8a), the first Piola-Kirchhoff tensor can be calculated by the same formula  $E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e}$  independent of the choice of  $w$ , whereas the formula  $\psi'_{\mathbf{F}_e}$  gives the first Piola-Kirchhoff tensor only for the choice  $w = \theta$ . Similarly, (4.8b) says that the chemical potentials can always be calculated by  $\mu^\zeta = E'_\zeta - \Theta S'_\zeta$ , but the formula  $\mu^\zeta = \psi'_\zeta$  only holds for  $w = \theta$ .

Our densities  $E$  and  $S$  are defined with respect to the actual Eulerian volume  $d\mathbf{x}$ . The first Piola-Kirchhoff tensor  $\mathbf{T}$  is obtained by the derivative of the free energy (at fixed  $\theta$ ) when taking with respect to the material (i.e. Lagrangian) volume measure  $d\mathbf{X}$ . Using  $d\mathbf{x} = \det \mathbf{F}_e d\mathbf{X}$  (recall  $\det \mathbf{F}_p = 1$ ) we have  $\mathbf{T} = (\det \mathbf{F}_e \psi)'_{\mathbf{F}_e}$ . The actual stress tensor in the Eulerian setting is the Cauchy stress tensor  $\boldsymbol{\Sigma}_{\text{Cauchy}}$  which is related to  $\mathbf{T}$  via  $\boldsymbol{\Sigma}_{\text{Cauchy}} = (1/\det \mathbf{F}_e)\mathbf{T}\mathbf{F}_e^\top$ , see e.g. [23, Eqn. (48.2)]. Thus, exploiting  $(\det \mathbf{F}_e)'_{\mathbf{F}_e} = \text{Cof } \mathbf{F}_e = (\det \mathbf{F}_e) \mathbf{F}_e^{-\top}$  and (4.8a) provides us with the formula

$$\boldsymbol{\Sigma}_{\text{Cauchy}} = \frac{1}{\det \mathbf{F}_e} \left( (E \det \mathbf{F}_e)'_{\mathbf{F}_e} - \Theta (S \det \mathbf{F}_e)'_{\mathbf{F}_e} \right) \mathbf{F}_e^\top = (E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e}) \mathbf{F}_e^\top + (E - \Theta S) \mathbb{I}. \quad (4.9)$$

## 4.3 The Hamiltonian part of Eulerian thermoelastoplasticity

We follow ideas from [27] for the Hamiltonian part of thermoelasticity in the Eulerian setting based on the state variables  $(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, \mathbf{F}_e, \theta)$ , see also [55] for a related form involving  $\varrho$  as an additional state variable.

Using that  $\varrho = \rho_r / \det \mathbf{F}_e$ , the total energy and total entropy can be written as

$$\mathcal{E}(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, w) = \int_{\Omega} \left( \frac{|\mathbf{p}|^2}{2\varrho} + E(\mathbf{F}_e, \alpha, \beta, w) \right) d\mathbf{x} \quad \text{and} \quad \mathcal{S}(\mathbf{F}_e, \alpha, \beta, w) = \int_{\Omega} S(\mathbf{F}_e, \alpha, \beta, w) d\mathbf{x}.$$

For generality we have introduced two scalar variables  $\alpha$  and  $\beta$ , which are assumed to be intensive and extensive, respectively. See [76] for the importance of treating intensive and extensive variables

accordingly. Here,  $E$  and  $S$  are the energy and entropy densities with respect to the actual Eulerian volume.

Taking into account  $\mathbf{p} = \varrho \mathbf{v}$  with  $\varrho = \varrho(\mathbf{F}_e)$  from (4.3) so that  $\varrho'_{\mathbf{F}_e} = -\varrho \mathbf{F}_e^{-\top}$ , the differentials of  $\mathcal{E}$  and  $\mathcal{S}$  take the form

$$D\mathcal{E}(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, w) = \begin{pmatrix} \mathbf{v} \\ E'_{\mathbf{F}_e} + \frac{\varrho |\mathbf{v}|^2}{2} \mathbf{F}_e^{-\top} \\ E'_\alpha \\ E'_\beta \\ E'_w \end{pmatrix} \quad \text{and} \quad D\mathcal{S}(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, w) = \begin{pmatrix} 0 \\ S'_{\mathbf{F}_e} \\ S'_\alpha \\ S'_\beta \\ S'_w \end{pmatrix}. \quad (4.10)$$

In GENERIC, the Hamiltonian (or reversible) part of the evolution is given in the form

$$\frac{\partial q}{\partial t} = \mathbb{J}(q) D\mathcal{E}(q),$$

where  $\mathbb{J}$  satisfies three conditions:

$$\text{skew symmetry: } \mathbb{J}(q)^* = -\mathbb{J}(q); \quad (4.11a)$$

$$\text{Jacobi's identity: } \langle \zeta_1, D\mathbb{J}(q)[\mathbb{J}(q)\zeta_2]\zeta_3 \rangle + \text{cycl.perm} \equiv 0; \quad (4.11b)$$

$$\text{first non-interaction condition: } \mathbb{J}(q) D\mathcal{S}(q) \equiv 0. \quad (4.11c)$$

We construct a suitable  $\mathbb{J}$  with the block structure

$$\mathbb{J}(q) = \begin{pmatrix} \mathbb{J}^{pp} & \mathbb{J}^{p\mathbf{F}_e} & \mathbb{J}^{p\alpha} & \mathbb{J}^{p\beta} & \mathbb{J}^{pw} \\ \mathbb{J}^{\mathbf{F}_e p} & 0 & 0 & 0 & 0 \\ \mathbb{J}^{\alpha p} & 0 & 0 & 0 & 0 \\ \mathbb{J}^{\beta p} & 0 & 0 & 0 & 0 \\ \mathbb{J}^{wp} & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.12)$$

We set

$$\begin{aligned} \mathbb{J}^{pp}(q)\zeta &= -\text{div}(\mathbf{p} \otimes \zeta) - (\nabla \zeta)^\top \mathbf{p}, & \mathbb{J}^{\mathbf{F}_e p}(q)\zeta &= -(\zeta \cdot \nabla) \mathbf{F}_e + (\nabla \zeta) \mathbf{F}_e, \\ \mathbb{J}^{\alpha p}(q)\zeta &= -\zeta \cdot \nabla \alpha, & \mathbb{J}^{\beta p}(q)\zeta &= -\text{div}(\beta \zeta). \end{aligned}$$

Here  $\mathbb{J}^{pp}(q)$  is different from the canonical co-symplectic structure for the incompressible Euler equation (cf. [27, 55]); for the compressible case we follow [76]. The operator  $\mathbb{J}^{\mathbf{F}_e p}$  is chosen for the transport of the tensor  $\mathbf{F}_e$ , giving  $\frac{\partial}{\partial t} \mathbf{F}_e + (\mathbf{v} \cdot \nabla) \mathbf{F}_e = (\nabla \mathbf{v}) \mathbf{F}_e$ . In the lower line,  $\mathbb{J}^{\alpha p}$  and  $\mathbb{J}^{\beta p}$  give the simple transport of an intensive and an extensive scalar, respectively. The operator  $\mathbb{J}^{wp}$  for the transport of  $w$  will be more complicated, as it has to be compatible with the transport of the extensive variable  $s = S(\mathbf{F}_e, \alpha, \beta, w)$ , where  $w$  may be neither intensive (like  $w = \theta$ ) or extensive (like for  $w \in \{e, s\}$ ). The proof of the validity of Jacobi's identity in Theorem 4.1 relies heavily on the fact that the operators  $\mathbb{J}^{pp}$ ,  $\mathbb{J}^{\mathbf{F}_e p}$ ,  $\mathbb{J}^{\alpha p}$ , and  $\mathbb{J}^{\beta p}$  are given by classical Lie derivatives of tensors in the direction of the vector field  $\mathbf{v} = \zeta$ .

In view of the desired skew symmetry (4.11a) we define

$$\mathbb{J}^{p\mathbf{F}_e}(q)\boldsymbol{\Xi} = \nabla \mathbf{F}_e : \boldsymbol{\Xi} + \text{div}(\boldsymbol{\Xi} \mathbf{F}_e^\top), \quad \mathbb{J}^{p\alpha}(q)a = a \nabla \alpha, \quad \mathbb{J}^{p\beta}(q)b = -\beta \nabla b.$$

To find  $\mathbb{J}^{pw}$ , we use the first non-interaction condition (4.11c) and observe that because of  $D_p \mathcal{S}(q) = 0$  we only have to satisfy the relation

$$\mathbb{J}^{pF_e}(q)S'_{F_e} + \mathbb{J}^{p\alpha}(q)S'_\alpha + \mathbb{J}^{p\beta}(q)S'_\beta + \mathbb{J}^{pw}(q)S'_w \equiv 0.$$

Obviously, this is satisfied by the choice

$$\mathbb{J}^{pw}(q)\omega = -S\nabla\left(\frac{\omega}{S'_w}\right) - \mathbb{J}^{pF_e}\left(\frac{\omega}{S'_w}S'_{F_e}\right) - \mathbb{J}^{p\alpha}\left(\frac{\omega}{S'_w}S'_\alpha\right) - \mathbb{J}^{p\beta}\left(\frac{\omega}{S'_w}S'_\beta\right).$$

Finally, defining  $\mathbb{J}^{wp}(q) = -\mathbb{J}^{pw}(q)^*$  we find

$$\begin{aligned} \mathbb{J}^{wp}(q)\zeta &= -\frac{1}{S'_w}\operatorname{div}(S\zeta) + \frac{1}{S'_w}S'_{F_e}:\mathbb{J}^{F_e p}\zeta + \frac{1}{S'_w}S'_\alpha\mathbb{J}^{\alpha p}\zeta + \frac{1}{S'_w}S'_\beta\mathbb{J}^{\beta p}\zeta \\ &= -\frac{1}{S'_w}\left(\operatorname{div}(S\zeta) + S'_{F_e}:(\zeta\cdot\nabla)F_e - (\nabla\zeta)F_e\right) + S'_\alpha\zeta\cdot\nabla\alpha + S'_\beta\operatorname{div}(\beta\zeta). \end{aligned}$$

Thus, we have  $\mathbb{J}^* = -\mathbb{J}$  and the full skew symmetry (4.11a) is established.

Moreover, assuming purely Hamiltonian flow with  $\frac{\partial}{\partial t}(F_e, \alpha, \beta, w) = (\mathbb{J}^{F_e p}, \mathbb{J}^{\alpha p}, \mathbb{J}^{\beta p}, \mathbb{J}^{wp})\mathbf{v}$ , we find

$$\frac{\partial}{\partial t}(S(F_e, \alpha, \beta, w)) = S'_{F_e}:\frac{\partial F_e}{\partial t} + S'_\alpha\frac{\partial\alpha}{\partial t} + S'_\beta\frac{\partial\beta}{\partial t} + S'_w\frac{\partial w}{\partial t} = -\operatorname{div}(S(F_e, \alpha, \beta, w)\mathbf{v}), \quad (4.13)$$

which shows that the entropy density is transported as an extensive variable.

**Theorem 4.1 (Poisson structure.)** *The operator  $\mathbb{J}$  defined above is a Poisson structure satisfying the conditions (4.11).*

For the readers convenience we give an explicit and self-contained proof of the validity of the Jacobi identity (4.5), however proofs for various restricted operators  $\mathbb{J}$  exist in the literature, see e.g. [27, 53, 55, 76]. Our proof will be based on two observations: (i)  $\mathbb{J}$  has the block structure (4.12), which will be analyzed in Appendix A, and (ii) that the components of  $\mathbb{J}$  are given in terms of Lie derivatives of tensors with respect to the underlying velocity field  $\mathbf{v}$ .

For a general vector field  $\mathbf{w}$  and a tensor field  $\mathbf{T}$ , the Lie derivative is defined by taking the derivative of  $\mathbf{T}$  along the flow of the  $\mathbf{w}$ . The important property of Lie derivatives is the commutator relation

$$\mathcal{L}_v(\mathcal{L}_w\mathbf{T}) - \mathcal{L}_w(\mathcal{L}_v\mathbf{T}) = \mathcal{L}_{[[v,w]]}\mathbf{T}, \quad (4.14)$$

where the commutator between vector fields is given by

$$[[v, w]] := \mathcal{L}_v w = -\mathcal{L}_w v = (v\cdot\nabla)w - (w\cdot\nabla)v = (\nabla w)v - (\nabla v)w.$$

The identity (4.14) cannot be found easily in the literature, but it is an easy consequence of its validity for functions, vectors, and co-vectors (1-forms) and of the well-known derivation rule  $\mathcal{L}_v(\mathbf{T}\otimes\mathbf{S}) = (\mathcal{L}_v\mathbf{T})\otimes\mathbf{S} + \mathbf{T}\otimes(\mathcal{L}_v\mathbf{S})$  by doing induction over the rank of the tensors.

**Proposition 4.2 (Lie derivatives)** *We have the following identities*

$$-\mathbb{J}^{pp}(\mathbf{q})\mathbf{v} = \mathfrak{L}_v^{(d-1)\text{-fo}} \mathbf{q} = \operatorname{div}(\mathbf{q} \otimes \mathbf{v}) + (\nabla \mathbf{v})^\top \mathbf{q}, \quad (4.15a)$$

$$-\mathbb{J}^{F_e p}(\mathbf{G})\mathbf{v} = \mathfrak{L}_v^{\text{vec}} \mathbf{G} = (\mathbf{v} \cdot \nabla) \mathbf{G} - (\nabla \mathbf{v}) \mathbf{G}, \quad (4.15b)$$

$$-\mathbb{J}^{\alpha p}(a) = \mathfrak{L}_v^{0\text{-fo}} a = (\mathbf{v} \cdot \nabla) a = \mathbf{v} \cdot \nabla a, \quad (4.15c)$$

$$-\mathbb{J}^{\beta p}(b) = \mathfrak{L}_v^{d\text{-fo}} b = \operatorname{div}(b\mathbf{v}), \quad (4.15d)$$

where  $\mathfrak{L}_v^{n\text{-fo}}$  denotes the Lie derivatives of an  $n$ -form, where intensive variables are 0-forms (simple functions) and extensive variables are  $d$ -forms (densities of volume forms with respect to the Lebesgue measure).

*Proof.* The relations in (4.15c) and (4.15d) are in all textbooks on tensor calculus, see e.g. [41, Sec. 4.3]. The same holds for (4.15b), if we observe that  $\mathbf{G} \mapsto \mathbb{J}^{F_e p}(\mathbf{G})\mathbf{v}$  acts on the columns of  $\mathbf{G}$ , i.e. we interpret  $\mathbf{G}$  as a collection of column vectors.

To obtain (4.15a) we can use the duality between  $(d-1)$ -forms and vectors. With  $\mathfrak{L}_v^{1\text{-fo}} \xi = (\mathbf{v} \cdot \nabla) \xi + (\nabla \mathbf{v})^\top \xi$  we find

$$\begin{aligned} \int_{\Omega} \mathbf{w} \cdot \mathfrak{L}_v^{(d-1)\text{-fo}}(\mathbf{q}) \, d\mathbf{x} &:= - \int_{\Omega} \mathbf{q} \cdot \mathfrak{L}_v^{\text{vec}} \mathbf{w} \, d\mathbf{x} = \int_{\Omega} \mathbf{q} \cdot ((\mathbf{v} \cdot \nabla) \mathbf{w} - (\nabla \mathbf{v}) \mathbf{w}) \, d\mathbf{x} \\ &= \int_{\Omega} \mathbf{w} \cdot (\operatorname{div}(\mathbf{q} \otimes \mathbf{v}) + (\nabla \mathbf{v})^\top \mathbf{q}) \, d\mathbf{x}, \end{aligned} \quad (4.16)$$

which is the desired result.  $\square$

We are now ready to complete the

*Proof of Theorem 4.1.* The conditions (4.11a) and (4.11c) are satisfied by construction.

To show the Jacobi identity (4.11b), there are two classical ways: (i) one simply uses the definition and evaluates the tri-linear form defined in (4.11b) or (ii) one uses the invariance of the Jacobi identity under the coordinate transformation.

We choose the latter one and consider the new variables  $\bar{q} = (\mathbf{p}, \mathbf{F}_e, \alpha, \beta, s)$  with  $s = S(\mathbf{F}_e, \alpha, \beta, w)$ . By (4.7) we know that this mapping is invertible to obtain  $w = W(\mathbf{F}_e, \alpha, \beta, s)$  back again. The new form of the energy density is  $\bar{E}(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, s) = E(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, W(\mathbf{F}_e, \alpha, \beta, s))$  and the entropy density is  $\bar{S}(\mathbf{p}, \mathbf{F}_e, \alpha, \beta, s) = s$ . In particular, using  $\bar{S}'_{\mathbf{F}_e} = 0$ ,  $\bar{S}'_{\alpha} = S'_{\beta} = 0$ , and  $\bar{S}'_s = 1$ , the operator  $\mathbb{J}$  transforms into

$$\mathbb{J}(q) = \begin{pmatrix} -\mathfrak{L}_{\square}^{(d-1)\text{-fo}}(\mathbf{p}) & \mathbb{J}^{p F_e}(\mathbf{F}_e) & \square \nabla \alpha & -\beta \nabla \square & -s \nabla \square \\ -\mathfrak{L}_{\square}^{\text{vec}}(\mathbf{F}_e) & 0 & 0 & 0 & 0 \\ -\mathfrak{L}_{\square}^{0\text{-fo}}(\alpha) & 0 & 0 & 0 & 0 \\ -\mathfrak{L}_{\square}^{d\text{-fo}}(\beta) & 0 & 0 & 0 & 0 \\ -\mathfrak{L}_{\square}^{d\text{-fo}}(s) & 0 & 0 & 0 & 0 \end{pmatrix},$$

where we already inserted the results from Proposition 4.2.

Finally, we apply Proposition A.1 with  $n \in \{1, \dots, N\}$  replaced by  $\mathbf{a} \in \{\mathbf{p}, \mathbf{F}_e, \alpha, \beta, s\}$ , i.e.  $\mathbf{p}$  plays the special role of  $n = 1$  in the block structure. We first observe that all the operators  $\mathbf{a} \mapsto \mathbb{J}^{ap}(\mathbf{a})$  are linear, such that

$$D\mathbb{J}^{ap}(\mathbf{a})[\mathbb{J}^{ap}(\mathbf{a})\mathbf{v}]\mathbf{w} = \mathbb{J}^{ap}(\mathbb{J}^{ap}(\mathbf{a})\mathbf{v})\mathbf{w} = \mathfrak{L}_{\mathbf{w}}^{\mathbf{a}}(\mathfrak{L}_{\mathbf{v}}^{\mathbf{a}}\mathbf{a}),$$

where  $\mathfrak{L}_v^a$  stands for  $\mathfrak{L}_v^{(d-1)\text{-fo}}$ ,  $\mathfrak{L}_v^{\text{vec}}$ ,  $\mathfrak{L}_v^{0\text{-fo}}$ ,  $\mathfrak{L}_v^{d\text{-fo}}$ , and  $\mathfrak{L}_v^{d\text{-fo}}$ , respectively.

To establish the Jacobi identity for  $\mathbb{J}^{pp}$  we use that  $\mathfrak{L}_{v_2}^{\text{vec}} \mathbf{w} = [[\mathbf{v}, \mathbf{w}]]$  satisfies it (see e.g. [41, p. 143]) and dualize:

$$\begin{aligned} \langle \mathbf{v}_1, \mathbb{J}^{pp}(\mathbb{J}^{pp}(\mathbf{p})\mathbf{v}_2)\mathbf{v}_3 \rangle + \text{cycl. perm.} &= \langle \mathbf{v}_1, \mathfrak{L}_{v_2}^p \mathfrak{L}_{v_3}^p \mathbf{p} \rangle + \text{cycl. perm.} \\ &= \langle \mathfrak{L}_{v_3}^{\text{vec}} \mathfrak{L}_{v_2}^{\text{vec}} \mathbf{v}_1, \mathbf{p} \rangle + \text{cycl. perm.} = \langle [[\mathbf{v}_3, [[\mathbf{v}_2, \mathbf{v}_1]]] + \text{cycl. perm.}, \mathbf{p} \rangle = \langle 0, \mathbf{p} \rangle = 0. \end{aligned}$$

Thus, (A.3a) and (A.3b) are established. To obtain (A.3c) for  $\mathbf{a} \in \{\mathbf{F}_e, \alpha, \beta, s\}$  we use the commutator property (4.14) for Lie derivatives.

$$\begin{aligned} \langle \zeta_a, \mathbb{J}^{ap}(\mathbb{J}^{ap}(\mathbf{a})\mathbf{v})\mathbf{w} - \mathbb{J}^{ap}(\mathbb{J}^{ap}(\mathbf{a})\mathbf{w})\mathbf{v} \rangle &= \langle \zeta_a, \mathfrak{L}_w^a \mathfrak{L}_v^a \mathbf{a} - \mathfrak{L}_v^a \mathfrak{L}_w^a \mathbf{a} \rangle \\ &\stackrel{(4.14)}{=} \langle \zeta_a, \mathfrak{L}_{[[\mathbf{w}, \mathbf{v}]]}^a \mathbf{a} \rangle_{X_a} = -\langle \zeta_a, -\mathbb{J}^{ap}(\mathbf{a})[[\mathbf{v}, \mathbf{w}]] \rangle_{X_a} = -\langle [[\mathbf{v}, \mathbf{w}]], \mathbb{J}^{pa}(\mathbf{a})\zeta_a \rangle_{X_p} \\ &= -\langle \mathfrak{L}_v^{\text{vec}} \mathbf{w}, \mathbb{J}^{pa}(\mathbf{a})\zeta_a \rangle_{X_p} \stackrel{(4.16)}{=} \langle \mathbf{w}, \mathfrak{L}_v^{(d-1)\text{-fo}} \mathbb{J}^{pa}(\mathbf{a})\zeta_a \rangle_{X_p} = \langle \mathbf{w}, \mathbb{J}^{pp}(\mathbb{J}^{pa}(\mathbf{a})\zeta_a)\mathbf{v} \rangle. \end{aligned}$$

Thus, (A.3c) is established as well and the proof is complete.  $\square$

We now discuss the terms arising from of the Hamiltonian part of the dynamics, namely  $\frac{\partial q}{\partial t} = \mathbf{V}_{\text{Ham}}(q) = \mathbb{J}(q)\text{D}\mathcal{E}(q)$ . Using (4.10) we obtain the following system of equations

$$\mathbf{V}_{\text{Ham}}(q) = \mathbb{J}(q)\text{D}\mathcal{E}(q) = \begin{pmatrix} -\text{div}(\varrho \mathbf{v} \otimes \mathbf{v}) + \text{div}(\boldsymbol{\Sigma}_{\text{Cauchy}} - p^{(\beta)} \mathbb{I}) \\ -\mathbf{v} \cdot \nabla \mathbf{F}_e + (\nabla \mathbf{v}) \mathbf{F}_e \\ -\mathbf{v} \cdot \nabla \alpha \\ -\text{div}(\beta \mathbf{v}) \\ -\frac{1}{S'_w} \text{div}(S \mathbf{v}) - \frac{1}{S'_w} \left( S'_{\mathbf{F}_e} : \frac{\partial \mathbf{F}_e}{\partial t} + S'_\alpha \frac{\partial \alpha}{\partial t} + S'_\beta \frac{\partial \beta}{\partial t} \right) \end{pmatrix}, \quad (4.17)$$

where the Cauchy stress tensor  $\boldsymbol{\Sigma}_{\text{Cauchy}}$  is defined via the free-energy density  $\psi = E - \Theta S$  as follows

$$\boldsymbol{\Sigma}_{\text{Cauchy}} = \widetilde{\boldsymbol{\Sigma}} \mathbf{F}_e^\top + \psi \mathbb{I} \quad \text{with} \quad \widetilde{\boldsymbol{\Sigma}} = E'_{\mathbf{F}_e}(\mathbf{F}_e, \alpha, \beta, w) - \Theta(\mathbf{F}_e, \alpha, \beta, w) S'_{\mathbf{F}_e}(\mathbf{F}_e, \alpha, \beta, w),$$

see Section 4.2. Moreover, the extensive variable  $\beta$  generates the additional pressure

$$p^{(\beta)} = \beta (E'_\beta - \Theta S'_\beta),$$

see also [55, Eqn. (2.15e)].

All terms in (4.17) are clear except for the first one involving the Cauchy stress tensor. To obtain the given compact form, we start from the definition

$$\begin{aligned} \mathbf{V}_{\text{Ham}}^p(q) &= \mathbb{J}^{pp} \text{D}_p \mathcal{E} + \mathbb{J}^{p\mathbf{F}_e} \text{D}_{\mathbf{F}_e} \mathcal{E} + \mathbb{J}^{p\alpha} \text{D}_\alpha \mathcal{E} + \mathbb{J}^{p\beta} \text{D}_\beta \mathcal{E} + \mathbb{J}^{pw} \text{D}_w \mathcal{E} \\ &= \mathbb{J}^{pp}(\mathbf{p})\mathbf{v} + \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \left( E'_{\mathbf{F}_e} + \frac{\varrho |\mathbf{v}|^2}{2} \mathbf{F}_e^{-\top} \right) + E'_\alpha \nabla \alpha - \beta \nabla (E'_\beta) \\ &\quad - S \nabla \left( \frac{E'_w}{S'_w} \right) - \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \left( \frac{E'_w}{S'_w} S'_{\mathbf{F}_e} \right) - \left( \frac{E'_w}{S'_w} S'_\alpha \right) \nabla \alpha - \beta \nabla \left( \frac{E'_w}{S'_w} S'_\beta \right). \end{aligned}$$

For the terms involving  $\mathbf{v}$ , we use  $\mathbf{p} = \varrho \mathbf{v}$  and find an important cancellation (see also [76, Eqn. (4.6)]):

$$\mathbb{J}^{pp}(\mathbf{p})\mathbf{v} + \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \left( \frac{\varrho |\mathbf{v}|^2}{2} \mathbf{F}_e^{-\top} \right) = -\text{div}(\varrho \mathbf{v} \otimes \mathbf{v}) - (\nabla \mathbf{v})^\top (\varrho \mathbf{v}) + \frac{\varrho |\mathbf{v}|^2}{2} \mathbf{F}_e^{-\top} : \nabla \mathbf{F}_e + \text{div} \left( \frac{\varrho |\mathbf{v}|^2}{2} \mathbb{I} \right)$$

$$= -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) - \varrho \nabla \left( \frac{|\mathbf{v}|^2}{2} \right) + \frac{\varrho |\mathbf{v}|^2}{2 \det \mathbf{F}_e} \nabla \det \mathbf{F}_e + \nabla \left( \varrho \frac{|\mathbf{v}|^2}{2} \right) = -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}),$$

because  $\varrho = \rho_r / \det \mathbf{F}_e$  implies  $\nabla \varrho = -(\varrho / \det \mathbf{F}_e) \nabla \det \mathbf{F}_e$ ; here we rely on that  $\rho_r$  is assumed constant in space.

Setting  $\widetilde{\boldsymbol{\Sigma}} = E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e}$  and using  $\Theta = E'_w / S'_w$  (note that  $\psi'_{\mathbf{F}_e} = \widetilde{\boldsymbol{\Sigma}} - S\Theta'_{\mathbf{F}_e} \neq \widetilde{\boldsymbol{\Sigma}}$ ) and  $\psi = E - \Theta S$ , we can also simplify the other terms and find

$$\begin{aligned} \mathbf{V}_{\text{Ham}}^p(q) &= -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) + \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} + (\psi'_\alpha + S\Theta'_\alpha) \nabla \alpha - \beta \nabla (\psi'_\beta + S\Theta'_\beta) - S \nabla \Theta \\ &= -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) + \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} + \psi'_\alpha \nabla \alpha - \beta \nabla \psi'_\beta \\ &\quad + S\Theta'_\alpha \nabla \alpha - \beta \nabla (S\Theta'_\beta) - S(\Theta'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + \Theta'_\alpha \nabla \alpha + \Theta'_\beta \nabla \beta + \Theta'_w \nabla w) \\ &= -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) + \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} - S\Theta'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + \psi'_\alpha \nabla \alpha - \beta \nabla \psi'_\beta - \nabla (S\beta\Theta'_\beta) + \psi'_w \nabla w, \end{aligned}$$

where, for the last term, we used the definition of  $\psi$  and  $\Theta$  to find  $\psi'_w = -S\Theta'_w$ . On the other hand we have

$$\begin{aligned} \operatorname{div}(\widetilde{\boldsymbol{\Sigma}} \mathbf{F}_e^\top + \psi \mathbb{I}) &= \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} - \widetilde{\boldsymbol{\Sigma}} : \nabla \mathbf{F}_e + \nabla \psi \\ &= \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} - E'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + \Theta S'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + (E - \Theta S)'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + \psi'_\alpha \nabla \alpha + \psi'_\beta \nabla \beta + \psi'_w \nabla w \\ &= \mathbb{J}^{p\mathbf{F}_e}(\mathbf{F}_e) \widetilde{\boldsymbol{\Sigma}} - S\Theta'_{\mathbf{F}_e} : \nabla \mathbf{F}_e + \psi'_\alpha \nabla \alpha + \psi'_\beta \nabla \beta + \psi'_w \nabla w. \end{aligned}$$

Combining the last two relations and exploiting  $\psi'_\beta + S\theta'_\beta = E'_\beta - \Theta S'_\theta$  yields

$$\mathbf{V}_{\text{Ham}}^p(q) = -\operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) + \operatorname{div} \left( \widetilde{\boldsymbol{\Sigma}} \mathbf{F}_e^\top + (\psi - \beta(E'_\beta - \Theta S'_\theta)) \mathbb{I} \right), \quad (4.18)$$

which shows the additional pressure correction  $\beta(E'_\beta - \Theta S'_\theta)$  for the extensive variable  $\beta$ .

With this the form of  $\mathbf{V}_{\text{Ham}}$  given in (4.17) is established. It can be checked easily, that when omitting  $\alpha$  and  $\beta$  and choosing  $\theta = w = \Theta(\mathbf{F}_e, w)$  we exactly obtain the equations derived in [27, Sec. 3].

#### 4.4 The dissipative part of Eulerian thermoelastoplasticity

As explained in [53, Sec. 2.3.2] (following [17]) and [42, Sec. 4.3], suitable nonlinear dissipation potentials  $\mathcal{R}$  or linear Onsager operators  $\mathbb{K}$  are constructed by collecting the building blocks of the dissipative mechanics and then combining them with a nontrivial operator  $N_{\mathcal{E}}$  in the form

$$\mathcal{R}^*(q, \boldsymbol{\zeta}) = \mathcal{R}_{\text{simple}}^*(q, N_{\mathcal{E}}(q)^* \boldsymbol{\zeta}) \quad \text{or} \quad \mathbb{K}(q) = N_{\mathcal{E}}(q) \mathbb{K}_{\text{simple}}(q) N_{\mathcal{E}}(q)^*.$$

In our model we can have five different dissipative processes:

- (A) viscoelastic dissipation induced by  $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^\top)$ ,
- (B) inelastic (or plastic) dissipation induced by  $\mathbf{L}_p = \mathbf{F}_e^{-1}((\nabla \mathbf{v}) \mathbf{F}_e - \frac{\partial}{\partial t} \mathbf{F}_e - (\mathbf{v} \cdot \nabla) \mathbf{F}_e)$ ,
- (C) diffusion and growth/decay for the intensive variable  $\alpha$ ,
- (D) diffusion for the extensive variable  $\beta$ ,
- (E) heat flow induced by  $\nabla(1/\theta)$ .

Thus, we can find a suitable dual dissipation potential in the additive form

$$\mathcal{R}_{\text{simple}}^* = \mathcal{R}_A^* + \mathcal{R}_B^* + \mathcal{R}_C^* + \mathcal{R}_D^* + \mathcal{R}_E^*.$$

However, we emphasize that this simplistic assumption is by far not necessary. Of course, it is possible to construct much more general thermodynamically consistent models where there is a strong interaction of the different dissipation mechanics (e.g. like cross diffusion). Nevertheless, we will restrict our approach to the case of a simple block structure.

The advantage of using an operator  $N_{\mathcal{E}}$  is three-fold. First, it is used guarantee the second non-interaction condition by asking

$$N_{\mathcal{E}}(q)^* D\mathcal{E}(q) = (0, \dots, 0, 1)^\top \quad \text{and} \quad \mathcal{R}_{\text{simple}}^*(q, (0, \dots, 0, \lambda)^\top) = 0 \quad \text{for all } \lambda \in \mathbb{R}. \quad (4.19)$$

Here  $\lambda \in \mathbb{R}$  stand for the constant (reciprocal of the) temperature  $1/\theta$ , which does not generate any dissipation.

The second advantage is the fundamental observation in [42, Sec. 4.3] that now the dissipative (a.k.a. irreversible) driving forces are now given by

$$\boldsymbol{\eta} = N_{\mathcal{E}}(q)^* D\mathcal{S}(q),$$

which contains already information on  $\mathcal{E}$  in a specific way because of (4.19).

Finally, the operator  $N_{\mathcal{E}}$  acting from the left on  $\partial\mathcal{R}_{\text{simple}}^*$  will encoded the dissipative terms that generate the energy conservation, i.e. the terms that contributing to the entropy production.

For our special application, we recall the special form of  $D\mathcal{E}$  and  $D\mathcal{S}$  given in (4.10) and construct an operator  $N_{\mathcal{E}}^* : \mathbb{R}^d \times \mathbb{R}^{d \times d} \times \mathbb{R}^3 \rightarrow \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^{d \times d} \times \mathbb{R}^3$  as follows:

$$N_{\mathcal{E}}(q)^* = \begin{pmatrix} \mathbf{D}(\square) & 0 & 0 & 0 & \frac{-\square}{E'_w} \mathbf{D} \\ -\frac{\varrho}{2}(\mathbf{v} \cdot \square) \mathbb{I} & \mathbf{F}_e^\top & 0 & 0 & \frac{-\square}{E'_w} \mathbf{F}_e^\top E'_{\mathbf{F}_e} \\ 0 & 0 & 1 & 0 & -E'_\alpha/E'_w \\ 0 & 0 & 0 & 1 & -E'_\beta/E'_w \\ 0 & 0 & 0 & 0 & 1/E'_w \end{pmatrix}.$$

For the later analysis, we introduce the vector of the reduced driving forces  $\boldsymbol{\eta} = N_{\mathcal{E}}(q)^* \boldsymbol{\zeta} \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^{d \times d} \times \mathbb{R}^3$  via

$$\boldsymbol{\eta} = \begin{pmatrix} \boldsymbol{\eta}^p \\ \boldsymbol{\eta}^{\mathbf{F}_e} \\ \eta^\alpha \\ \eta^\beta \\ \eta^w \end{pmatrix} = N_{\mathcal{E}}(q)^* \begin{pmatrix} \boldsymbol{\zeta}^p \\ \boldsymbol{\zeta}^{\mathbf{F}_e} \\ \zeta^\alpha \\ \zeta^\beta \\ \zeta^w \end{pmatrix} = \begin{pmatrix} \mathbf{D}(\boldsymbol{\zeta}^p) - (\zeta^w/E'_w) \mathbf{v} \\ \mathbf{F}_e^\top \boldsymbol{\zeta}^{\mathbf{F}_e} - \frac{\varrho}{2}(\mathbf{v} \cdot \boldsymbol{\zeta}^p) \mathbb{I} - (\zeta^w/E'_w) \mathbf{F}_e^\top E'_{\mathbf{F}_e} \\ \zeta^\alpha - \zeta^w E'_\alpha/E'_w \\ \zeta^\beta - \zeta^w E'_\beta/E'_w \\ \zeta^w/E'_w \end{pmatrix}.$$

Clearly, the first relation in (4.19) is satisfied, and using (4.10) again we have

$$N_{\mathcal{E}}(q)^* D\mathcal{S}(q) = \begin{pmatrix} -(1/\Theta) \mathbf{D} \\ -(1/\Theta) \mathbf{F}_e^\top (E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e}) \\ -(1/\Theta) (E'_\alpha - \Theta S'_\alpha) \\ -(1/\Theta) (E'_\beta - \Theta S'_\beta) \\ 1/\Theta \end{pmatrix}.$$

The third and fourth component are given in terms of the chemical potentials  $\mu^{\alpha,\beta}$  in the form  $\eta^\alpha = -\mu^\alpha/\Theta$  and  $\eta^\beta = -\mu^\beta/\Theta$ , because of (4.8b).

For the adjoint operator  $N_{\mathcal{E}} : \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^{d \times d} \times \mathbb{R}^3 \rightarrow \mathbb{R}^d \times \mathbb{R}^{d \times d} \times \mathbb{R}^3$  we obtain

$$N_{\mathcal{E}}(q) = \begin{pmatrix} \text{div}(\square) & -\frac{\varrho}{2} \text{tr}(\square) \mathbf{v} & 0 & 0 & 0 \\ 0 & \mathbf{F}_e & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \frac{-1}{E'_w} \mathbf{D} : \square & \frac{-1}{E'_w} (\mathbf{F}_e^\top E'_{\mathbf{F}_e}) : \square & -E'_\alpha/E'_w & -E'_\beta/E'_w & 1/E'_w \end{pmatrix}.$$

The non-diagonal entries in the last line will provide energy conservation as well as entropy production, see Section 4.6.

The full dual dissipation potential takes the form

$$\mathcal{R}^*(q, \zeta) = \mathcal{R}_{\text{simple}}^*(q, N_{\mathcal{E}}(q)^* \zeta),$$

and now assume that  $\mathcal{R}_{\text{simple}}^*$  has a block structure

$$\mathcal{R}_{\text{simple}}^*(q, \boldsymbol{\eta}) = \mathcal{R}_{\text{visc}}^*(q, \boldsymbol{\eta}^p) + \mathcal{R}_{\text{plast}}^*(q, \boldsymbol{\eta}^{\mathbf{F}_e}) + \mathcal{R}_\alpha^*(q, \eta^\alpha) + \mathcal{R}_\beta^*(q, \eta^\beta) + \mathcal{R}_{\text{heat}}^*(q, \eta^w).$$

Yet, hasten to say that this is a simplification that is not necessary at all and, actually (6.3) below would need a fully general structure. In fact, it is one of the big advantages of the GENERIC framework that it can easily handle coupling phenomena between different effects.

Even for the these five blocks we only write the simplest forms and leave the study of more general dissipation potentials to future work.

$$\mathcal{R}_{\text{visc}}^*(q, \boldsymbol{\eta}^p) = \int_{\Omega} \frac{\Theta}{2} \boldsymbol{\eta}^p : \mathbb{D}_{\text{visc}}(q) \boldsymbol{\eta}^p \, d\mathbf{x}, \quad \mathcal{R}_{\text{plast}}^*(q, \boldsymbol{\eta}^{\mathbf{F}_e}) = \int_{\Omega} R_{\text{plast}}^*(q, -\Theta \mathbb{M} \boldsymbol{\eta}^{\mathbf{F}_e}) \, d\mathbf{x}, \quad (4.20a)$$

$$\mathcal{R}_\alpha^*(q, \eta^\alpha) = \int_{\Omega} \frac{1}{2} \nabla \eta^\alpha \cdot \mathbb{A}_{\text{diff}}(q) \nabla \eta^\alpha + \frac{A_{\text{source}}(q)}{2} (\eta^\alpha)^2 \, d\mathbf{x}, \quad (4.20b)$$

$$\mathcal{R}_\beta^*(q, \eta^\beta) = \int_{\Omega} \frac{1}{2} \nabla \eta^\beta \cdot \mathbb{B}_{\text{diff}}(q) \nabla \eta^\beta \, d\mathbf{x}, \quad \mathcal{R}_{\text{heat}}^*(q, \eta^w) = \int_{\Omega} \frac{1}{2} \nabla \eta^w \cdot \mathbb{K}_{\text{heat}}(q) \nabla \eta^w \, d\mathbf{x}. \quad (4.20c)$$

With these choices we can write down the dissipative (irreversible) part of the evolution:

$$\mathbf{V}_{\text{irr}}(q) = \begin{pmatrix} \text{div}(\mathbb{D}_{\text{visc}}(q) \mathbf{D} + \frac{\varrho}{2} \text{tr}(\mathbf{L}_p) \mathbf{v}) \\ -\mathbf{F}_e \mathbf{L}_p \\ V_{\text{irr}}^\alpha(q) := \text{div} \left( \mathbb{A}_{\text{diff}} \nabla \frac{\mu^\alpha}{\Theta} \right) - A_{\text{source}} \frac{\mu^\alpha}{\Theta} \\ V_{\text{irr}}^\beta(q) := \text{div} \left( \mathbb{B}_{\text{diff}} \nabla \frac{\mu^\beta}{\Theta} \right) \\ \frac{1}{E'_w} \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} + \frac{1}{E'_w} E'_{\mathbf{F}_e} : (\mathbf{F}_e \mathbf{L}_p) - \frac{E'_\alpha}{E'_w} V_{\text{irr}}^\alpha - \frac{E'_\beta}{E'_w} V_{\text{irr}}^\beta - \frac{1}{E'_w} \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta} \right) \end{pmatrix},$$

where

$$\mathbf{L}_p = \theta \mathbb{M}^* \partial_{\boldsymbol{\eta}^{\mathbf{F}_e}} R_{\text{plast}}^*(q, \mathbb{M}(q) \underbrace{\mathbf{F}_e^\top (E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e})}_{=\text{Mandel-stress tensor (symmetric)}}).$$

## 4.5 The full GENERIC evolution equation

We can now assemble the whole GENERIC evolution equations

$$\dot{q} = \mathbf{V}_{\text{Ham}}(q) + \mathbf{V}_{\text{irr}}(q) = \mathbb{J}(q)\mathbb{D}\mathcal{E}(q) + \mathbb{K}(q)\mathbb{D}\mathcal{S}(q).$$

This leads to the following system for  $(\mathbf{v}, \mathbf{F}_e, \alpha, \beta, w)$ :

$$\frac{\partial}{\partial t}(\varrho\mathbf{v}) + \text{div}(\varrho\mathbf{v} \otimes \mathbf{v}) = \text{div}(\boldsymbol{\Sigma}_{\text{Cauchy}} - \beta(E'_\beta - \Theta S'_\beta)\mathbb{I} + \mathbb{D}_{\text{visc}}(q)\mathbf{D}) + \frac{\varrho}{2} \text{tr}(\mathbf{L}_p)\mathbf{v}, \quad (4.21a)$$

$$\frac{\partial \mathbf{F}_e}{\partial t} = -(\mathbf{v} \cdot \nabla)\mathbf{F}_e + (\nabla\mathbf{v})\mathbf{F}_e - \mathbf{F}_e \mathbf{L}_p, \quad (4.21b)$$

$$\frac{\partial \alpha}{\partial t} = -\mathbf{v} \cdot \nabla \alpha + \text{div}\left(\mathbb{A}_{\text{diff}} \nabla \frac{\mu^\alpha}{\Theta}\right) - A_{\text{source}} \frac{\mu^\alpha}{\Theta}, \quad (4.21c)$$

$$\frac{\partial \beta}{\partial t} = -\text{div}(\beta\mathbf{v}) + \text{div}\left(\mathbb{B}_{\text{diff}} \nabla \frac{\mu^\beta}{\Theta}\right), \quad (4.21d)$$

$$\frac{\partial w}{\partial t} = V_{\text{Ham}}^S + V_{\text{irr}}^E - \frac{1}{E'_w} \text{div}\left(\mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta}\right), \quad (4.21e)$$

where  $\varrho$  is from (4.3) and where we have

$$\boldsymbol{\Sigma}_{\text{Cauchy}} = (E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e})\mathbf{F}_e^\top + (E - \Theta S)\mathbb{I}, \quad (4.22a)$$

$$\mathbf{L}_p = \theta \mathbb{M}^* \partial_{\eta_{\mathbf{F}_e}} R_{\text{plast}}^*(q, \mathbb{M}(q)\boldsymbol{\Sigma}_{\text{Mandel}}) \quad \text{with } \boldsymbol{\Sigma}_{\text{Mandel}} = \mathbf{F}_e^\top (E'_{\mathbf{F}_e} - \Theta S'_{\mathbf{F}_e}), \quad (4.22b)$$

$$\mu^\alpha = E'_\alpha - \Theta S'_\alpha \quad \text{and} \quad \mu^\beta = E'_\beta - \Theta S'_\beta, \quad (4.22c)$$

$$V_{\text{Ham}}^S = \frac{1}{S'_w} \left( -\text{div}(S\mathbf{v}) - S'_{\mathbf{F}_e} : \frac{\partial \mathbf{F}_e}{\partial t} - S'_\alpha \frac{\partial \alpha}{\partial t} - S'_\beta \frac{\partial \beta}{\partial t} \right), \quad (4.22d)$$

$$V_{\text{irr}}^E = \frac{1}{E'_w} \left( -\text{div}(E\mathbf{v}) + \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} + E'_{\mathbf{F}_e} : (\mathbf{F}_e \mathbf{L}_p) - E'_\alpha \frac{\partial \alpha}{\partial t} - E'_\beta \frac{\partial \beta}{\partial t} \right). \quad (4.22e)$$

## 4.6 Energy conservation and entropy production

By construction, the solutions of a GENERIC system automatically satisfy the conservation of the total energy and the non-decay of the total entropy, namely

$$\frac{d}{dt} \mathcal{E}(q(t)) = 0 \quad \text{and} \quad \frac{d}{dt} \mathcal{S}(q(t)) = \langle \mathbb{D}\mathcal{S}(q(t)), \partial_\zeta \mathcal{R}^*(q(t), \mathbb{D}\mathcal{S}(q(t))) \rangle \geq 0.$$

However, in continuum mechanics it is also important to understand the local balance laws involving the mechanical power  $p_{\text{mech}}$ , the energy flux  $\mathbf{j}_{\text{ener}}$ , the entropy flux  $\mathbf{j}_{\text{entr}}$ , and the entropy production  $\sigma_{\text{prod}}$  in the form

$$\frac{\partial E}{\partial t} + \text{div}(E\mathbf{v}) = p_{\text{mech}} - \text{div}\mathbf{j}_{\text{ener}} \quad \text{and} \quad (4.23a)$$

$$\frac{\partial S}{\partial t} + \text{div}(S\mathbf{v}) = \sigma_{\text{prod}} - \text{div}\mathbf{j}_{\text{entr}} \quad \text{with } \sigma_{\text{prod}} \geq 0 \text{ in } \Omega. \quad (4.23b)$$

Here  $p_{\text{mech}}$  is due to the exchange of kinetic to the potential (=internal) energy. For deriving these local balance laws, we take advantage of the possibility of choosing an arbitrary thermal variable  $w$ . For deriving (4.23a) it is advantageous to choose  $w = e = E(\mathbf{F}_e, \alpha, \beta, e)$ , while for deriving (4.23b) it is advantageous to choose  $w = s = S(\mathbf{F}_e, \alpha, \beta, s)$ .

In particular, this subsection highlights the role of the specific form of the equation for  $w$  that involves the terms  $V_{\text{Ham}}^S$  and  $V_{\text{irr}}^E$ . These terms arise in a specific way by the construction of the GENERIC formulation.

The term  $V_{\text{irr}}^E$  stems from  $N_{\mathcal{E}}$  and can be seen as a providing the heat production through the dissipative processes. This is most elegantly seen by using our freedom to choose the thermal variable at our will: if we now make

$$\text{the specific choice } w = e, \quad \text{i.e. } E(\mathbf{F}_e, \alpha, \beta, e) = e,$$

we find  $E'_{\mathbf{F}_e} = \mathbf{0}$ ,  $E'_\alpha = 0 = E'_\beta$ ,  $E'_e = 1$  and  $S'_e = 1/\Theta$ . With this choice, the equation for the extensive variable  $w = e$  takes the form

$$\begin{aligned} \frac{\partial e}{\partial t} = \Theta & \left( -\text{div}(S\mathbf{v}) - S'_{\mathbf{F}_e} : ((\mathbf{v} \cdot \nabla) \mathbf{F}_e - (\nabla \mathbf{v}) \mathbf{F}_e + \mathbf{F}_e \mathbf{L}_p) + S'_\alpha \mathbf{v} \cdot \nabla \alpha + S'_\beta \text{div}(\beta \mathbf{v}) \right) \\ & + \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta} \right). \end{aligned}$$

With  $\Theta \text{div}(S\mathbf{v}) = \text{div}(e\mathbf{v}) - (e - \Theta S) \mathbb{I} : \mathbf{D} + \Theta (S'_{\mathbf{F}_e} : (\mathbf{v} \cdot \nabla) \mathbf{F}_e + S'_\alpha \mathbf{v} \cdot \nabla \alpha + S'_\beta \mathbf{v} \cdot \nabla \beta)$  we see several cancellations and arrive at

$$\begin{aligned} \frac{\partial e}{\partial t} + \text{div}(e\mathbf{v}) = \underbrace{\left( \Sigma_{\text{Cauchy}} - \beta (E'_\beta - \Theta S'_\beta) \mathbb{I} + \mathbb{D}_{\text{visc}} \mathbf{D} + \mathbf{F}_e \mathbf{L}_p \right) : \mathbf{D}}_{=: p_{\text{mech}} = \text{the mechanical power (in W/m}^3)} - \underbrace{\text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta} \right)}_{=: \mathbf{j}_{\text{ener}}}. \end{aligned} \quad (4.24)$$

Here we used that, because of the choice  $w = e$  and  $E'_{\mathbf{F}_e} = \mathbf{0}$ , the Cauchy stress tensor takes the form  $\Sigma_{\text{Cauchy}} = -\Theta S'_{\mathbf{F}_e} \mathbf{F}_e^\top - \Theta S \mathbb{I}$ , see (4.9). This establishes (4.23a) and shows that the internal variables  $\alpha$  and  $\beta$  do not contribute to the energy flux, because the assumed block structure of  $\mathcal{R}_{\text{simple}}^*$  did not allow for cross diffusion.

Finding the local balance law for the entropy density  $S$  is most easily done by making

$$\text{the specific choice } w = s, \quad \text{i.e. } S(\mathbf{F}_e, \alpha, \beta, s) = s.$$

Then, we find  $S'_{\mathbf{F}_e} = \mathbf{0}$ ,  $S'_\alpha = 0 = S'_\beta$ ,  $S'_s = 1$  and  $E'_s = \Theta$ . We also recall that  $V_{\text{Ham}}^S$  is such that for the purely Hamiltonian system the entropy density is simply transported as a extensive variable along the vector field  $\mathbf{v}$ , see (4.13). Thus, the term  $V_{\text{irr}}^w$  will produce the terms for entropy production  $\sigma_{\text{prod}}$  and for the entropy flux  $\mathbf{j}_{\text{entr}}$ .

Assembling the terms from the derivation in Sections 4.3 and 4.4, we find

$$\begin{aligned} \frac{\partial s}{\partial t} + \text{div}(s\mathbf{v}) &= \frac{1}{\Theta} \left( \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} + E'_{\mathbf{F}_e} : (\mathbf{F}_e \mathbf{L}_p) - E'_\alpha V_{\text{irr}}^\alpha - E'_\beta V_{\text{irr}}^\beta - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta} \right) \right) \\ &= \sigma_{\text{prod}} - \text{div}(\mathbf{j}_{\text{entr}}) \quad \text{with} \\ \sigma_{\text{prod}} &= \frac{1}{\Theta} \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} + \mathbb{M} \Sigma_{\text{Mandel}} : \partial_{\eta^{\mathbf{F}_e}} R_{\text{plast}}^* (\mathbb{M} \Sigma_{\text{Mandel}}) \\ &\quad + \nabla \frac{\mu^\alpha}{\Theta} \cdot \mathbb{A}_{\text{diff}} \nabla \frac{\mu^\alpha}{\Theta} + A_{\text{source}} \left( \frac{\mu^\alpha}{\Theta} \right)^2 + \nabla \frac{\mu^\beta}{\Theta} \cdot \mathbb{B}_{\text{diff}} \nabla \frac{\mu^\beta}{\Theta} + \nabla \frac{1}{\Theta} \cdot \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta}, \\ \mathbf{j}_{\text{entr}} &= \frac{\mu^\alpha}{\Theta} \mathbb{A}_{\text{diff}} \nabla \frac{\mu^\alpha}{\Theta} + \frac{\mu^\beta}{\Theta} \mathbb{B}_{\text{diff}} \nabla \frac{\mu^\beta}{\Theta} + \frac{1}{\Theta} \mathbb{K}_{\text{heat}} \nabla \frac{1}{\Theta}, \end{aligned} \quad (4.25)$$

where the chemical potentials take the form  $\mu^\alpha = E'_\alpha - \Theta \theta$  and  $\mu^\beta = E'_\beta - \Theta \theta$  because of the choice  $w = s = S$ . This establishes (4.23b).

## 5 How the system (3.2) arises from GENERIC

A basic ingredient of the model (3.2) is that the free energy is taken referential, whereas the actual free energy  $\psi = E - \Theta S$  is better fitted to directly fitted to the GENERIC approach in Sect. 4, but perhaps less standard in engineering or physics, see (4.2) for the relation. As in Section 4, we use the *actual entropy*  $s = -\psi'_\theta(\mathbf{F}_e, z, \theta)$ , the *actual chemical potential*  $\mu = \psi'_z(\mathbf{F}_e, z, \theta)$ , and the *actual internal energy* (Gibbs' relation)  $e = \psi + \theta s$ .

We will start from the system (4.21)–(4.22) with the choice  $w = e$  to see the energy balance in its standard form. However, we will then use the relation  $e = E(\mathbf{F}_e, z, \theta)$  for formulating the equations in terms of the temperature. Moreover, we will simplify the approach in Sect. 4 by assuming further

$$\text{tr} \mathbf{L}_p = 0, \quad \mathbb{M} = \text{dev} : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}_{\text{dev}}^{d \times d} : A \mapsto A - \frac{\text{tr} A}{d} \mathbb{I}, \quad \text{and} \quad A_{\text{source}} = 0. \quad (5.1a)$$

Taking  $R_{\text{plast}}$  whose convex conjugate  $R_{\text{plast}}^*$  occurs in (4.22b), we consider the dissipation potential  $r$  used in (3.2) as

$$r(z, \theta; \mathbf{D}, \mathbf{L}_p) = \frac{1}{2} \mathbf{D} : \mathbb{D}_{\text{visc}} \mathbf{D} + R_{\text{plast}} \left( z, \theta; \frac{\mathbf{L}_p}{\theta} \right) \quad \text{with} \quad \mathbb{D}_{\text{visc}} = \mathbb{D}_{\text{visc}}(z, \theta). \quad (5.1b)$$

It is to note that (5.1b) turns the kinetic equation (flow rule) (4.22b) into  $[R_{\text{plast}}]_{\mathbf{L}_p}'(z, \theta, \mathbf{L}_p / \theta) = \text{dev} \boldsymbol{\Sigma}_{\text{Mandel}}$  with the Mandel stress  $\boldsymbol{\Sigma}_{\text{Mandel}} = \mathbf{F}_e^\top \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)$ , where we used that  $(\mathbb{M}^*)^{-1}$  is the identity on  $\mathbb{R}_{\text{dev}}^{d \times d}$  where  $\mathbf{L}_p$  is valued. Again using (5.1b), we can write it as  $r'_{\mathbf{L}_p}(z, \theta; \mathbf{D}, \mathbf{L}_p) = \text{dev} \boldsymbol{\Sigma}_{\text{Mandel}}$ . When using (4.21)–(4.22), we realize that  $E - \Theta S = \psi$ . This altogether turns (4.21)–(4.22) into the system:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \mathbf{v}) + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) &= \rho \mathbf{g} + \text{div}(\boldsymbol{\Sigma}_{\text{Cauchy}} + \boldsymbol{\Sigma}_{\text{dissip}}) \quad \text{with} \quad \boldsymbol{\Sigma}_{\text{dissip}} = r'_{\mathbf{D}}(z, \theta; \mathbf{D}, \mathbf{L}_p) \\ \text{and} \quad \boldsymbol{\Sigma}_{\text{Cauchy}} &= \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) \mathbf{F}_e^\top + (\psi(\mathbf{F}_e, z, \theta) - \mathfrak{s}_{\text{EXT}} z \psi'_z(\mathbf{F}_e, z, \theta)) \mathbb{I}, \end{aligned} \quad (5.2a)$$

$$\dot{\mathbf{F}}_e = (\nabla \mathbf{v}) \mathbf{F}_e - \mathbf{F}_e \mathbf{L}_p, \quad (5.2b)$$

$$\dot{z} + \mathfrak{s}_{\text{EXT}} z \text{div} \mathbf{v} = \text{div} \left( \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} \right) \quad \text{with} \quad \mu = \psi'_z(\mathbf{F}_e, z, \theta), \quad (5.2c)$$

$$r'_{\mathbf{L}_p}(z, \theta; \mathbf{D}, \mathbf{L}_p) = \text{dev} \boldsymbol{\Sigma}_{\text{Mandel}} \quad \text{with} \quad \boldsymbol{\Sigma}_{\text{Mandel}} = \mathbf{F}_e^\top \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta), \quad (5.2d)$$

$$\begin{aligned} \frac{\partial e}{\partial t} + \text{div}(e \mathbf{v}) &= p_{\text{heat}} - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \right) + (\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) \mathbf{F}_e^\top + \psi(\mathbf{F}_e, z, \theta) \mathbb{I}) : \nabla \mathbf{v} \\ &\quad - \mathbf{F}_e^\top \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) : \mathbf{L}_p - \mathfrak{s}_{\text{EXT}} z \psi'_z(\mathbf{F}_e, z, \theta) \text{div} \mathbf{v} \\ \text{with the heat production rate} \quad p_{\text{heat}} &= \boldsymbol{\Sigma}_{\text{dissip}} : \mathbf{D} + r'_{\mathbf{L}_p}(z, \theta; \mathbf{D}, \mathbf{L}_p) : \mathbf{L}_p \\ \text{and the internal energy} \quad e &= \psi(\mathbf{F}_e, z, \theta) - \theta \psi'_\theta(\mathbf{F}_e, z, \theta), \end{aligned} \quad (5.2e)$$

with  $\mathfrak{s}_{\text{EXT}}$  from (3.1); note that we wrote (4.21c) and (4.21d) in a unified way so that  $z$  can be both  $\alpha$  or  $\beta$  and correspondingly  $\mathbb{K}_{\text{diff}}$  can be  $\mathbb{A}_{\text{diff}}$  or  $\mathbb{B}_{\text{diff}}$ .

To inspect the internal energy equation (4.24) and the entropy equation (4.25), let us realize that

$$p_{\text{mech}} = (\boldsymbol{\Sigma}_{\text{Cauchy}} - z(E'_z - \theta S'_z) \mathbb{I} + \boldsymbol{\Sigma}_{\text{dissip}}) : \mathbf{D}, \quad (5.3a)$$

$$\mathbf{j}_{\text{ener}} = \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta}, \quad (5.3b)$$

$$\sigma_{\text{prod}} = \frac{p_{\text{heat}}}{\theta} + \nabla \frac{\mu}{\theta} \cdot \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} + \nabla \frac{1}{\theta} \cdot \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta}$$

with  $p_{\text{heat}} = r'_{(\mathbf{D}, \mathbf{L}_p)}(z, \theta; \mathbf{D}, \mathbf{L}_p) : (\mathbf{D}, \mathbf{L}_p)$ ,

(5.3c)

$$\mathbf{j}_{\text{entr}} = \frac{\mu}{\theta} \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} + \frac{1}{\theta} \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta}.$$

(5.3d)

As articulated in Section 4, these general equations lead to the total energy balance and the total entropy balance, respectively. For this, we need to consider a fixed domain  $\Omega \subset \mathbb{R}^d$  and to prescribe some boundary conditions; for simplicity, we use impermeable boundary by prescribing

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \mathbf{j}_{\text{ener}} \cdot \mathbf{n} = 0, \quad \text{and} \quad \mathbf{j}_{\text{entr}} \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega$$

(5.4a)

with  $\mathbf{n}$  denoting the outward normal to the boundary  $\partial\Omega$  of the domain  $\Omega$ . Besides, we prescribe

$$(\boldsymbol{\Sigma}_{\text{Cauchy}} + \boldsymbol{\Sigma}_{\text{dissip}}) \mathbf{n} = \mathbf{0}, \quad \nabla \theta \cdot \mathbf{n} = 0, \quad \text{and} \quad \nabla \mu \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega.$$

(5.4b)

Actually, the last two conditions in (5.4b) allow the last condition (5.4a) to be omitted.

Integrating (4.24) over  $\Omega$  and using the specific form of  $p_{\text{mech}}$  and the momentum equation (3.2b) tested by  $\mathbf{v}$  together with the mass continuity equation (3.2a) above, we obtain *total energy balance*:

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} e \, d\mathbf{x} &= \int_{\Omega} p_{\text{mech}} \, d\mathbf{x} \stackrel{(4.24)}{=} \int_{\Omega} (\boldsymbol{\Sigma}_{\text{Cauchy}} + \boldsymbol{\Sigma}_{\text{dissip}}) : \mathbf{D} \, d\mathbf{x} \\ &= \int_{\Omega} \left( \rho \mathbf{g} - \frac{\partial}{\partial t} (\rho \mathbf{v}) - \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) \right) \cdot \mathbf{v} \, d\mathbf{x} \stackrel{(3.2a)}{=} \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{v} \, d\mathbf{x} - \frac{d}{dt} \int_{\Omega} \frac{\rho}{2} |\mathbf{v}|^2 \, d\mathbf{x}. \end{aligned}$$

(5.5)

It shows the conservation of the total energy  $\int_{\Omega} \frac{1}{2} \rho |\mathbf{v}|^2 + e \, d\mathbf{x}$  if the gravitation would be neglected, i.e. if  $\mathbf{g} = \mathbf{0}$ .

Integrating (4.25) over  $\Omega$  and using (5.3c), we obtain *total entropy balance*:

$$\frac{d}{dt} \int_{\Omega} s \, d\mathbf{x} = \int_{\Omega} \sigma_{\text{prod}} \, d\mathbf{x} = \int_{\Omega} \frac{p_{\text{heat}}}{\theta} + \nabla \frac{\mu}{\theta} \cdot \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} + \nabla \frac{1}{\theta} \cdot \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \, d\mathbf{x}.$$

(5.6)

Taking (4.25) multiplied by  $\theta$ , i.e.  $\theta \dot{s} = \theta \sigma_{\text{prod}} - \theta \text{div} \mathbf{j}_{\text{entr}} - \theta s \text{div} \mathbf{v}$ , and substituting  $s = -\psi'_{\theta}(\mathbf{F}_e, z, \theta)$ , we can see the heat equation in the “engineering form” in terms of temperature  $\theta$  as an intensive variable:

$$\begin{aligned} c(\mathbf{F}_e, z, \theta) \dot{\theta} &= \theta \sigma_{\text{prod}} - \theta \text{div} \mathbf{j}_{\text{entr}} + \theta \psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta) : \dot{\mathbf{F}}_e + \theta \psi''_{z\theta}(\mathbf{F}_e, z, \theta) \dot{z} + \theta \psi'_{\theta}(\mathbf{F}_e, z, \theta) \text{div} \mathbf{v} \\ &\stackrel{(5.3c,d)}{=} p_{\text{heat}} + \theta \nabla \frac{1}{\theta} \cdot \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} + \theta \nabla \frac{\mu}{\theta} \cdot \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} - \theta \text{div} \left( \frac{\mu}{\theta} \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} + \frac{1}{\theta} \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \right) \\ &\quad + \theta \psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta) : \dot{\mathbf{F}}_e + \theta \psi''_{z\theta}(\mathbf{F}_e, z, \theta) \dot{z} + \theta \psi'_{\theta}(\mathbf{F}_e, z, \theta) \text{div} \mathbf{v} \\ &\stackrel{(3.2d)}{=} p_{\text{heat}} - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \right) + \theta \psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta) : \dot{\mathbf{F}}_e \\ &\quad + (\theta \psi''_{z\theta}(\mathbf{F}_e, z, \theta) - \mu) \dot{z} + (\theta \psi'_{\theta}(\mathbf{F}_e, z, \theta) - \mathfrak{s}_{\text{EXT}} z \mu) \text{div} \mathbf{v} \\ &\stackrel{(2.6)}{=} p_{\text{heat}} - \text{div} \left( \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \right) + \theta (\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) \mathbf{F}_e^{\top} + \psi(\mathbf{F}_e, z, \theta) \mathbb{I})' : \nabla \mathbf{v} \\ &\quad - \theta \mathbf{F}_e^{\top} \psi''_{\mathbf{F}_e \theta}(\mathbf{F}_e, z, \theta) : \mathbf{L}_p - (\psi(\mathbf{F}_e, z, \theta) - \theta \psi'_{\theta}(\mathbf{F}_e, z, \theta))'_z \dot{z} - \mathfrak{s}_{\text{EXT}} z \psi'_z(\mathbf{F}_e, z, \theta) \text{div} \mathbf{v} \end{aligned}$$

$$\text{with the heat capacity } c(\mathbf{F}_e, z, \theta) = -\theta\psi''_{\theta\theta}(\mathbf{F}_e, z, \theta). \quad (5.7)$$

Then we use the kinematic equation (2.6) with the algebra  $A:(BC) = (B^\top A):C = (AC^\top):B$  so that, using also  $e = \psi - \theta\psi'_\theta$  and realizing that  $e'_\theta(\mathbf{F}_e, z, \theta) = \psi'_\theta - (\theta\psi'_\theta)'_\theta = -\theta\psi''_{\theta\theta}$  is the heat capacity  $c$ , we can evaluate the left-hand side of (4.24) as

$$\begin{aligned} & \frac{\partial e}{\partial t} + \operatorname{div}(e\mathbf{v}) = \dot{e} + e\operatorname{div}\mathbf{v} \\ & = e'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta):\dot{\mathbf{F}}_e + e'_z(\mathbf{F}_e, z, \theta)\dot{z} + e'_\theta(\mathbf{F}_e, z, \theta)\dot{\theta} + e(\mathbf{F}_e, z, \theta)\operatorname{div}\mathbf{v} \\ & = c(\mathbf{F}_e, z, \theta)\dot{\theta} + (\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) - \theta\psi''_{\mathbf{F}_e\theta}(\mathbf{F}_e, z, \theta)):\dot{\mathbf{F}}_e \\ & \quad + (\psi'_z(\mathbf{F}_e, z, \theta) - \theta\psi''_{z\theta}(\mathbf{F}_e, z, \theta))\dot{z} + (\psi(\mathbf{F}_e, z, \theta) - \theta\psi'_\theta(\mathbf{F}_e, z, \theta))\operatorname{div}\mathbf{v}, \\ & \stackrel{(2.6)}{=} c(\mathbf{F}_e, z, \theta)\dot{\theta} \\ & \quad + (\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)\mathbf{F}_e^\top + \psi(\mathbf{F}_e, z, \theta)\mathbb{I}):\nabla\mathbf{v} - \theta(\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)\mathbf{F}_e^\top + \psi(\mathbf{F}_e, z, \theta)\mathbb{I})'_\theta:\nabla\mathbf{v} \\ & \quad - \mathbf{F}_e^\top(\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) - \theta\psi''_{\mathbf{F}_e\theta}(\mathbf{F}_e, z, \theta)):\mathbf{L}_p + (\psi'_z(\mathbf{F}_e, z, \theta) - \theta\psi''_{z\theta}(\mathbf{F}_e, z, \theta))\dot{z}. \end{aligned}$$

Thus, substituting for  $c(\mathbf{F}_e, z, \theta)\dot{\theta}$  from (5.7), we obtain just (5.2e).

In terms of the referential free energy  $\psi$  instead of the actual free energy  $\psi$  used for GENERIC, the system (5.2a-d) with (5.2e) written in the form (5.7) and completed with the mass continuity equation transforms into the original system (3.2). Indeed, recalling (4.2), it is to be noted that the Cauchy stress rewrites as

$$\begin{aligned} \Sigma_{\text{Cauchy}} &= \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)\mathbf{F}_e^\top + (\psi(\mathbf{F}_e, z, \theta) - \mathfrak{s}_{\text{EXT}}z\psi'_z(\mathbf{F}_e, z, \theta))\mathbb{I} \\ &= \frac{\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)\mathbf{F}_e^\top - \mathfrak{s}_{\text{EXT}}z\psi'_z(\mathbf{F}_e, z, \theta)\mathbb{I}}{\det\mathbf{F}_e}, \end{aligned} \quad (5.8)$$

which reveals the conservative part of the Cauchy stress in (3.2b). Here we used the algebra  $F^{-1} = \operatorname{Cof}^\top F / \det F$  and the calculus  $\det'(F) = \operatorname{Cof} F$  for

$$\begin{aligned} \frac{\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e}\mathbf{F}_e^\top &= \frac{\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta) - \psi(\mathbf{F}_e, z, \theta)\mathbf{F}_e^{-\top}}{\det\mathbf{F}_e}\mathbf{F}_e^\top + \frac{\psi(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e}\mathbb{I} \\ &= \left( \frac{\psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e} - \frac{\psi(\mathbf{F}_e, z, \theta)\operatorname{Cof}\mathbf{F}_e}{(\det\mathbf{F}_e)^2} \right)\mathbf{F}_e^\top + \frac{\psi(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e}\mathbb{I} \\ &= \left[ \frac{\psi(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e} \right]'_{\mathbf{F}_e}\mathbf{F}_e^\top + \frac{\psi(\mathbf{F}_e, z, \theta)}{\det\mathbf{F}_e}\mathbb{I} \stackrel{(4.2)}{=} \psi'_{\mathbf{F}_e}(\mathbf{F}_e, z, \theta)\mathbf{F}_e^\top + \psi(\mathbf{F}_e, z, \theta)\mathbb{I}. \end{aligned} \quad (5.9)$$

This calculation is to be used also for (5.7), which then gives the temperature equation (3.2f). The diffusion equation (3.2d) arises directly from (5.2c) when considering (4.2), while (5.2d) relies on  $\operatorname{tr}\mathbf{L}_p = 0$ .

**Remark 5.1 (Energy in J/kg.)** Another variant of the referential free energy  $\psi$  often used in literature is to express it in terms of J/kg instead of J/m<sup>3</sup>, i.e. Joule per a referential volume. This is actually the original Einstein idea of expressing elastic moduli in such physical units, i.e. in fact in (m/s)<sup>2</sup>, which is compatible with his famous formula “ $e/m=c^2$ ”. Then the actual free energy is, instead of (4.2), given by  $\psi(\mathbf{F}_e, z, \theta) = \varrho\psi(\mathbf{F}_e, z, \theta)$ . The corresponding variant of the system (3.2) arises by replacing the factor  $1/\det\mathbf{F}_e$  by  $\varrho$  everywhere in (3.2b,d–f).

## 6 Examples of application

The general model (3.2) has many applications in finitely-strained continuum thermo-mechanics. Let us illustrate it on two examples only, both involving interesting phenomena studied in continuum mechanics, namely various *phase transitions*. They can be primarily *volumetric* or *deviatoric* (isochoric), the former one being induced by high pressure [6].

Another highly developed part of continuum mechanics is *poromechanics* in a broader sense, cf. [12, 13, 15]. Effects as advection and diffusion are typically accompanied or coupled with mechanical swelling or squeezing, i.e. volumetric changes. In this way, the coupling with the mentioned volumetric phase transitions can occur. Substantial volumetric changes are especially during various solid-solid phase transitions with applications in geo-engineering (e.g. thawing of permafrost), petrology, materials science (hydrogels or metal plasticity and hydrogenation metal-hydride transition during hydrogen diffusion in metals), and geophysics (mantle dynamics and dewatering/dehydration of rocks).

We will briefly illustrate this rich variety of applications with two examples, one with the volumetric phase transitions and the other with the deviatoric phase transitions. There is a hierarchy of various kinds of models. Here we confine ourselves to a rather phenomenological Biot-type model.

### 6.1 Earth's mantle dynamics, phase transitions and (de)hydration

The first example concerns with the volumetric phase transitions in Earth's mantle associated with mass density jumps at specific depths, combined also with "water" diffusion. In contrast to the general model devised in [61] which uses additive decomposition and a linearized convective model as most frequently used in geophysics, here we used a fully nonlinear model with a multiplicative decomposition and a thermodynamically consistently formulated diffusion, as in the system (3.2).

In fact, the water in the mantle is chemically bonded rather than real liquid water in pores. Actually, there are many hydrous minerals [52]. Altogether, most of the water on the planet Earth is not in the oceans but in its mantle, the rough estimation being mostly from 1 to 10 times the ocean mass. A particularly large amount of water (about 1–2 wt%) is located in the mantle transition zone between 410 km and 660 km below Earth's surface. On these interfaces (and also some others), phase transitions are volumetric. We confine ourselves on unhysteretic situations governed by a model with a convex energy.

A prominent modelling activity in geophysical mantle dynamics is the applications of descending slabs undergoing dehydration. More in detail, it originates when oceanic plates subduct continental plates. Being relatively cold and dense, they are descending deep into the Earth's mantle. They are originally hydrated by water from oceans, with water content being typically more than 1%. On their route into Earth's interior, they are subjected by ever increasing pressure and undergo a series of phase transitions. The most important and sharp transitions are under pressures about 14 GPa and 24 GPa which are at the mentioned depth about 410 km and 660 km below Earth's surface, where transitions from olivine to wadsleyite and ringwoodite to bridgmanite/magnesiowustite are undergoing, respectively. Both these phase transitions are accompanied by quite sharp increase of mass density.

Descending slabs can either stagnate on the 660 km-discontinuity or continue their journey into

the lower mantle up to the core-mantle boundary deep in 2.900 km. While undergoing their phase transition reaching 24 GPa pressure at 660 km depth, they tend to dehydrate while hydrating the surrounding mantle, cf. [25, 52]. In this way, the mantle transition zone 410–660 km is hydrated so that it now represents the by-far largest reservoir of (chemically bound) water on the planet Earth.

Understanding deep slab processes in the mantle and modelling fluid transport in subduction zones was articulated as one of major directions in geophysical modelling [20]. For pure slab descent (without dehydration), incompressibility is usually adopted while taking into account temperature effects as in [8, 9, 11, 59, 72] or the dehydration and phase transitions are incorporated very phenomenologically or rather indirectly [59, 67, 71], which is the main difference from our isothermal approach. In particular, “slab dehydration also seems to be a possible mechanism to switch from stagnation to penetration” [2] in addition to the viscosity increase in regions where seismic tomography has imaged slab stagnation [66].

The conservative part of the model can use a neo-Hookean Biot-type free energy

$$\psi(\mathbf{F}_e, z, \theta) = \mathbf{K}(J, \theta) + G(J^{-2/d} \text{tr}(\mathbf{F}_e \mathbf{F}_e^\top) - d) + \theta \frac{B}{2} |z + b(J - J_\tau)|^2 + c\theta(1 - \ln \theta) + \delta_{[0,1]}(z), \quad (6.1)$$

where  $J = \det \mathbf{F}_e$  and  $\delta_{[0,1]}$  denotes the indicator function of the interval  $[0, 1]$ ; therefore  $z$  is understood as an intensive variable valued in  $[0, 1]$ . Note that (6.1) is consistent with the ansatz (3.3). Another important ingredient is a proper viscosity. Although there are quantitatively not much precise ideas about the radial viscosity profile in Earth mantle, there seems a general agreement that there is a substantial increase of viscosity at the 660 km-interface, cf. [30] for comparison of various profiles in literature. The Maxwellian-type viscosity potential  $\nu_2(z, \theta; \cdot)$  in (4.20) can be quadratic in terms of  $L_p$  (then it models so-called *diffusion creep* in the mantle) or polynomial with the exponent  $p \neq 2$ . For  $p \sim 1.3$ , it is used to model so-called *dislocation creep*. Such power-law fluids with  $p < 2$  models are known in mathematical fluid theory under the name of *shear-thickening non-Newtonian* viscous, or here viscoelastic (in the Jeffreys rheology) *fluids*. Such shear-thickening rheology is an important modelling aspect leading to certain “lubrication” effects that facilitate an easy descent of cold slabs in the surrounding warmer Earth mantle, cf. [8, 10, 68].

Physically, there are various simplifications when having in mind the geophysical applications mentioned above. In particular, we do not distinguish between bound water and free water, assuming that it can be roughly modelled by varying water mobility suitably, while for a “multi-water” variant we refer to [75]. Anyhow, our thermo-hydro-mechanical model we have devised seems well competitive with the usual geophysical models for rock dehydration in subducting slabs like [48, 75, 76] which typically involve many simplifications as the mentioned incompressibility or ignoring temperature variations etc.

**Remark 6.1 (State equation and phase transitions.)** Considering  $B = 0$  in (6.1) for a moment, the actual bulk stored energy  $\mathcal{K}(J, \theta) = \mathbf{K}(J, \theta)/J$  with  $\mathbf{K}$  from (6.1) yields the (actual) pressure  $p = -\mathcal{K}'_J(J, \theta)$ . This determines the state equation  $p = \pi(\varrho, \theta) := -\mathcal{K}'_J(\varrho_r/\varrho, \theta)$ . Then  $\varrho$  is a function of pressure and temperature  $\varrho = \rho(p, \theta)$ , namely  $\varrho = \varrho_r/J = \varrho_r/[\mathcal{K}'_J(\cdot, \theta)]^{-1}(-p) = \varrho_r/[\mathcal{K}^*(\cdot, \theta)\mathbf{K}'_p(-p)] =: \rho(p, \theta)$  where  $\mathcal{K}^*(\cdot, \theta)$  denotes the convex conjugate to  $\mathcal{K}(\cdot, \theta)$  acting on  $-p$ . The mentioned mass-density discontinuities and the corresponding volumetric phase transitions

can be modelled by a convex smooth function  $\mathcal{K}(\cdot, \theta)$  which has two linear segments. Thus the dependence of the pressure  $p = -\mathcal{K}'_J(\cdot, \theta)$  on  $J$  has two horizontal plateaus (here taking the values 14 GPa and 24 GPa); cf. Figure 1. Then  $\rho(\cdot, \theta)$  is discontinuous with two jumps at 14 GPa and 24 GPa. We should then speak rather about a set-valued function and write the state equation as  $\varrho \in \rho(p, \theta)$ . In general, the mentioned phase transitions at specific pressures thus depend also on temperature. The thermic character of these phase transitions is related to the so-called *Clapeyron slope*  $\partial p / \partial \theta = \pi'_\theta(\varrho, \theta) = -[\mathcal{K}]''_{J\theta}(\varrho_R / \varrho, \theta)$ . For positive (resp. negative)  $\partial p / \partial \theta$ , the corresponding *phase transition* is *exothermic* (resp. *endothermic*). Adiabatic effects due to volume changes still contribute slightly to this thermic character but, in fact, this contribution is rather minor in the phase transitions in Earth's mantle. Specifically, the transition from lower-density ringwoodite (above 660 km) to higher-density perovskite (below 660 km) is endothermic with the Clapeyron slope  $-2.5$  MPa/K, while the transition from olivine (above 410 km) to wadsleyite (below 410 km) is opposite with the Clapeyron slope  $1.6$  MPa/K. This temperature dependence is not depicted in Figure 1, however.

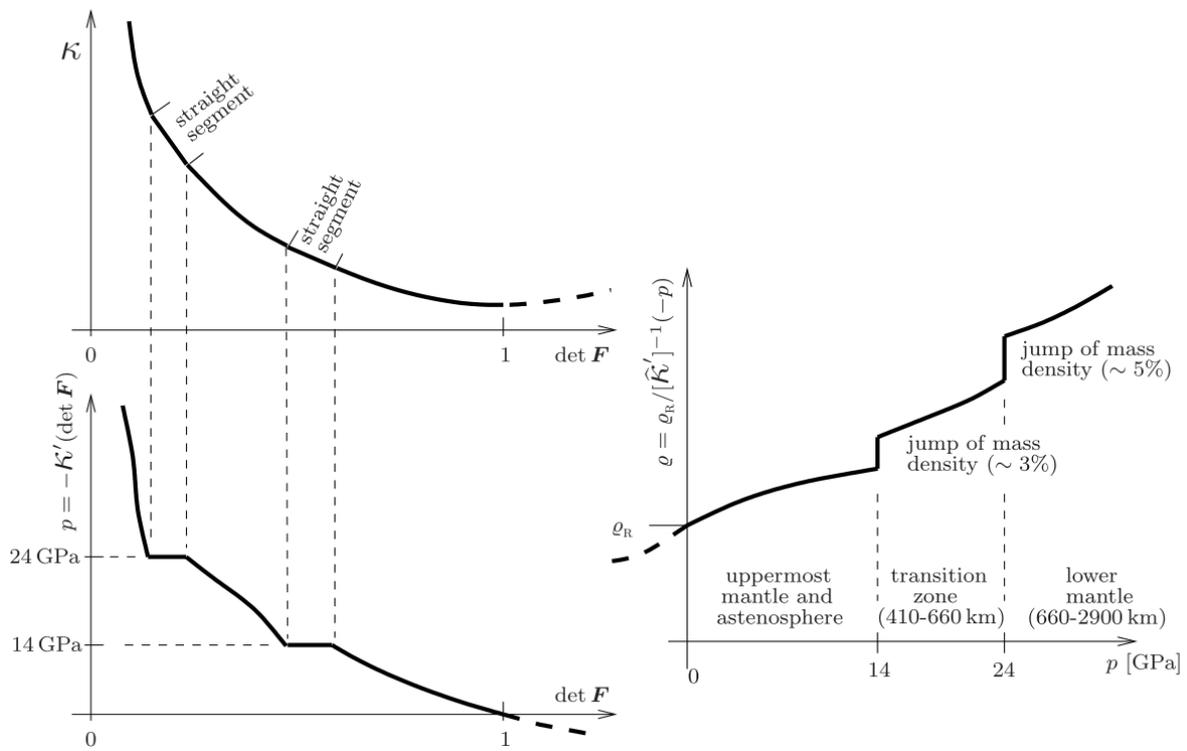


Figure 1: A schematic illustration of an isothermal phase transition (rock compaction) occurring at two specific pressures 14 GPa (at  $\sim 410$  km depth) and 24 GPa (at  $\sim 660$  km depth) in Earth's mantle modelled by a convex function  $\mathcal{K}(\cdot, \theta)$ .

## 6.2 Martensitic phase transition with plasticity and diffusion

Our second example is the martensitic phase transformation in so-called shape-memory alloys, extensively studied for decades in hundreds of articles and also in monographs such as [1, 7, 57]. At the single-crystal level, it is modelled by a nonconvex multi-well free energies with  $1 + n$  wells as orbits of the types  $SO(d)\mathbf{F}_i$  with  $\mathbf{F}_0 = \mathbb{I}$  for the cubic austenite and  $\mathbf{F}_i$  with  $i = 1, \dots, n$

for  $n$  lower symmetrical variants of martensite; in the 3-dimensional case,  $n = 3$  for tetragonal,  $n = 6$  for orthorhombic, or  $n = 12$  for monoclinic martensite. The transition between particular martensitic phases (variants), i.e. re-orientation of martensite, is isochoric (i.e. volume preserving) and the transition between cubic austenite and a particular martensitic variant is (almost) isochoric, too. For this,  $\det \mathbf{F}_i = 1$  is assumed and the potential  $\psi(\cdot, \theta)$  is multi-well in its deviatoric part only. A certain (slightly academical) example can be

$$\psi(\mathbf{F}_e, \theta) = \mathbf{K}(\det \mathbf{F}_e, \theta) + \min_{i=0, \dots, n} \left( G_i \left( \frac{\text{tr}(\mathbf{F}_e \mathbf{F}_e^\top \mathbf{F}_i^{-\top} \mathbf{F}_i^{-1})}{(\det \mathbf{F}_e)^{2/d}} - d \right) - c_i \theta \ln \frac{\theta}{\theta_\tau} \right) \quad (6.2)$$

with the transition temperature  $\theta_\tau$  at which austenite is energetically equilibrated with martensite and  $c_i$  the heat capacities of particular phases; typically  $c_0 > c_1 = \dots = c_n$ , which ensures that austenite is energetically dominant for  $\theta > \theta_\tau$  and vice versa.

This isochoric phase transition can be accompanied by another isochoric process, *plasticity*. Plasticity in shape-memory alloys is a studied phenomenon in materials science, see e.g. [24, 70]; for a model in a Lagrangian isothermal quasistatic situation see [33].

The transitions between these  $1 + n$  phases as well as the plasticity are activated processes and, in order to evolve, they need (and dissipate) some specific activation energy. As in [32], the former one can be modelled by a 1-homogeneous contribution to the dissipation potential involving a nonlinear “phase indicator” function  $\lambda : \mathbb{R}^{d \times d} \rightarrow \Delta \subset \mathbb{R}^{1+n}$  where  $\Delta = \{(\lambda_0, \dots, \lambda_n); \lambda_i \geq 0, \sum_{i=0}^n \lambda_i = 1\}$  denotes the so-called Gibbs simplex. For  $\mathbf{F}_e$  in the mentioned wells,  $\lambda(\mathbf{F}_e)$  takes values in on of the vertex of  $\Delta$ . The corresponding term in the dissipation potential is then  $|\dot{\lambda}(\mathbf{F}_e)|$ , as devised in [60] in the Lagrangian setting. Another contribution  $\sigma |\mathbf{L}_p|$  models the plasticity with  $\sigma = \sigma(\theta) > 0$  playing the role of a yield stress needed to activate the plastification. To put this contribution into the form  $r(\mathbf{F}_e, z, \theta; \nabla \mathbf{v}, \mathbf{L}_p)$  acting on the rates  $\nabla \mathbf{v}$  and  $\mathbf{L}_p$  as in (4.20), we use (2.6) and the calculus  $|\dot{\lambda}(\mathbf{F}_e)| = |\lambda'(\mathbf{F}_e) \dot{\mathbf{F}}_e| = |\lambda'(\mathbf{F}_e)((\nabla \mathbf{v}) \mathbf{F}_e - \mathbf{L}_p \mathbf{F}_e)|$ . Overall, the nonsmooth dissipation potential  $r(\mathbf{F}_e, \theta; \cdot, \cdot)$  reads as

$$r(\mathbf{F}_e, \theta; \mathbf{L}, \mathbf{L}_p) = |\lambda'(\mathbf{F}_e)(\mathbf{L} \mathbf{F}_e - \mathbf{L}_p \mathbf{F}_e)| + \sigma(\theta) |\mathbf{L}_p| \quad \text{with } \mathbf{L} \text{ a placeholder for } \nabla \mathbf{v}. \quad (6.3)$$

Of course, the partial derivative occurring in (3.2b) and (5.2d) should then be the convex subdifferentials. Yet, the potential depending on  $\mathbf{D}$  is now to be generalized for the full velocity gradient  $\mathbf{L} = \nabla \mathbf{v}$  and, moreover, the general coupling between  $\mathbf{L}$  and  $\mathbf{L}_p$  in (6.3) does not comply with the (slightly simplified) analysis in Sect. 4.3 which then should be enhanced by allowing more cross-effects.

**Remark 6.2 (Metal-hydride phase transition.)** The deviatoric martensitic phase transition and plasticity can even be combined with the diffusion, particularly of hydrogen, and the associated volumetric transition, known as the *metal-hydride phase transition*. For experimental evidence and small-strain models we refer e.g. to [28, 69] and [34, 39, 40, 74], respectively.

## 7 Notes to analysis

There is a certain agreement that models of solids at large strains analytically require usage of some higher-gradient theories, unless some very weak (e.g. of measure-valued-type) solution concepts are

used. It is used in the conservative part for the Lagrangian setting while rather in the dissipative part for the Eulerian setting. The latter case, which can be used here, is referred as *multipolar continua*, devised by Mindlin [44] and Toupin [73] and later used e.g. by [19, 49–51]. Such multipolar modification (regularization), which expands the dissipative stress by a term like  $-\operatorname{div}(\nu|\nabla^2\mathbf{v}|^{p-2}\nabla^2\mathbf{v})$  with  $p > d$  and  $\nu = \nu(\theta) > 0$ , has been used in isothermal situations with inelastic deformation without diffusion and without inertia in [62] and with diffusion but without inelastic deformation in [64], while an anisothermal model without diffusion and without inelastic deformation in [63] and with inelastic deformation in [65]. In addition, another dissipative gradient term can be used for  $\mathbf{L}_p$ , which expands the kinetic equation (3.2d) by a Laplace-type term.

The a-priori estimation strategy (to be applied for a suitable Galerkin semi-discretization such as in [62–65]) is to use first the total-energy balance (5.5), which gives a uniform-in-time  $L^1(\Omega)$ -estimate of  $\int_{\Omega} \frac{1}{2}\varrho|\mathbf{v}|^2 + e \, d\mathbf{x}$ .

Then, one should estimate the dissipative terms. Actually, if it were no diffusion, one can use the dissipation-energy balance arising from the sole mechanical part of the system, i.e. from (3.2a-c,e) tested successively by  $\frac{1}{2}|\mathbf{v}|^2$ ,  $\mathbf{v}$  (while using also (5.2b)), and  $\mathbf{L}_p$ , which would give an  $L^1$ -estimate for the dissipation rate which would be then use in the  $L^1$ -theory for the heat equation to obtain an estimate for  $\nabla\theta$ . Yet, with diffusion, it must to be more tricky. To this aim, one should use the entropy balance (5.6) which, on the other hand, can yield directly an estimate on  $\nabla\theta$  under suitable assumption. The last point, developed in the context of viscoelastic fluids in [18, Sect. 2.2.3], seems an advantageous technique even if diffusion would not be involved. More specifically, we integrate (5.6) in time with using (5.1b) to obtain

$$\begin{aligned} \int_0^T \int_{\Omega} \frac{\mathbb{D}_{\text{visc}}\mathbf{e}(\mathbf{v}) : \mathbf{e}(\mathbf{v})}{\theta} + \frac{[R_{\text{plast}}]_{\mathbf{L}_p}'(z, \theta; \mathbf{L}_p/\theta) : \mathbf{L}_p}{\theta} + \nabla \frac{\mu}{\theta} \cdot \mathbb{K}_{\text{diff}} \nabla \frac{\mu}{\theta} + \nabla \frac{1}{\theta} \cdot \mathbb{K}_{\text{heat}} \nabla \frac{1}{\theta} \, d\mathbf{x} dt \\ = \int_{\Omega} \psi'_{\theta}(\mathbf{F}_e(0), z(0), \theta(0)) - \psi'_{\theta}(\mathbf{F}_e(T), z(T), \theta(T)) \, d\mathbf{x} < +\infty. \end{aligned}$$

Under appropriate assumptions (in particular, assuming a polynomial-type growth of the heat capacity rather than a constant heat capacity), the right-hand side can be shown bounded by using the already proved a-priori estimates. Then, assuming suitable growth of  $\mathbb{D}_{\text{visc}} = \mathbb{D}_{\text{visc}}(\theta)$ ,  $\mathbb{K}_{\text{diff}} = \mathbb{K}_{\text{diff}}(\theta)$ , and  $\mathbb{K}_{\text{heat}} = \mathbb{K}_{\text{heat}}(\theta)$ , we can obtain a-priori estimates of  $\mathbf{e}(\mathbf{v})$ ,  $\nabla\mu$ , and  $\nabla\theta$ . Analogously, also  $\mathbf{L}_p$  can be estimated under suitable assumption on  $R_{\text{plast}}$ . The mentioned multipolar modification can yields an estimate on  $\nabla^2\mathbf{v}$ .

The last mentioned estimate would imply that the velocity field  $\mathbf{v}$  is Lipschitz continuous in space, which in turn guarantees a certain regularity of  $\mathbf{F}_e$  and  $\varrho$ , including bounds on  $\nabla\mathbf{F}_e$  and positivity of  $\det \mathbf{F}_e$  and  $\varrho$ . Assuming uniform convexity of  $\psi(\mathbf{F}_e, \cdot, \theta)$ , from  $\nabla\mu$  and  $\nabla\mathbf{F}_e$  and also  $\nabla\theta$  we can estimate  $\nabla z$ ; realize that  $\mu = \psi'_z(\mathbf{F}_e, z, \theta)$  so that

$$\nabla z = \frac{\nabla\mu - \psi''_{\mathbf{F}_e z}(\mathbf{F}_e, z, \theta)\nabla\mathbf{F}_e - \psi''_{z\theta}(\mathbf{F}_e, z, \theta)\nabla\theta}{\psi''_{zz}(\mathbf{F}_e, z, \theta)}.$$

The details concerning the above estimated and relevant assumption on the data are rather technical and we avoid specifying them.

All these kinds of estimates would allow for a limit passage in a suitable (semi) discretization constructed similarly as in [62–65]. In such a way, one could prove the existence of suitably defined weak solutions of an initial-boundary-value problem on a finite time interval  $[0, T]$ .

## A Appendix: Jacobi's identity for Poisson operators with block structure

In many applications, the Poisson operator  $\mathbb{J}$  has a block structure on the product space  $X = X_1 \times \cdots \times X_N$ , namely for  $q = (q_1, q_2, \dots, q_N)$  we have

$$\mathbb{J}(q) = \begin{pmatrix} \mathbb{J}_{11}(q_1) & \mathbb{J}_{12}(q_2) & \cdots & \mathbb{J}_{1N}(q_N) \\ \mathbb{J}_{21}(q_2) & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{J}_{N1}(q_N) & 0 & \cdots & 0 \end{pmatrix} \quad \text{with } \mathbb{J}_{n1}(q_n)^* = -\mathbb{J}_{1n}(q_n). \quad (\text{A.1})$$

Note that the operators  $\mathbb{J}_{n1}$  and  $\mathbb{J}_{1n}$  are allowed only to depend on the component  $q_n$ . The following result provides necessary and sufficient conditions for such  $\mathbb{J}$  to satisfy Jacobi's identity

$$\langle \zeta_1, D\mathbb{J}(q)[\mathbb{J}(q)\zeta_2]\zeta_3 \rangle + \text{cycl.perm} \equiv 0 \quad \text{for all } q \in X \text{ and all } \zeta_1, \zeta_2, \zeta_3 \in X^*. \quad (\text{A.2})$$

**Proposition A.1 (Jacobi's identity)** *Assume that  $X$  has the block structure  $X = X_1 \times \cdots \times X_N$  for some  $N \geq 2$  and assume that  $\mathbb{J}$  satisfies (A.1). Then,  $\mathbb{J}$  satisfies Jacobi's identity (A.2) if and only if the following conditions hold:*

$$\mathbb{J}_{11} \text{ satisfies Jacobi's identity on } X_1; \quad (\text{A.3a})$$

$$D\mathbb{J}_{11}(q_1) = D\mathbb{J}_{11}(0) =: \mathbb{A} : X_1 \rightarrow \text{Lin}_{\text{skw}}(X_1^*, X_1), \text{ i.e. } \mathbb{J}_{11}(q_1) = \mathbb{J}_{11}(0) + \mathbb{A}q_1; \quad (\text{A.3b})$$

for  $n \in \{2, \dots, N\}$  and all  $\zeta \in X_n^*$ ,  $v, w \in X_1^*$ ,  $q_n \in X_n$  we have the identity

$$\langle v, (\mathbb{A}\mathbb{J}_{1n}(q_n)\zeta)w \rangle_{X_1} = \langle \zeta, D\mathbb{J}_{n1}(q_n)[\mathbb{J}_{n1}(q_n)v]w \rangle_{X_n} - \langle \zeta, D\mathbb{J}_{n1}(q_n)[\mathbb{J}_{n1}(q_n)w]v \rangle_{X_n}. \quad (\text{A.3c})$$

*Proof.* Writing  $\zeta^a = (\zeta_1^a, \dots, \zeta_N^a) \in X_1^* \times \cdots \times X_N^*$  and using the special form of  $\mathbb{J}$  in (A.1) gives

$$\begin{aligned} \langle \zeta^1, D\mathbb{J}(q)[\mathbb{J}(q)\zeta^2]\zeta^3 \rangle &= \langle \zeta_1^1, D\mathbb{J}_{11}(q_1)[\mathbb{J}_{11}(q_1)\zeta_1^2]\zeta_1^3 \rangle + \sum_{n=2}^N \left( \langle \zeta_1^1, D\mathbb{J}_{11}(q_1)[\mathbb{J}_{1n}(q_n)\zeta_n^2]\zeta_1^3 \rangle \right. \\ &\quad \left. + \langle \zeta_1^1, D\mathbb{J}_{1n}(q_n)[\mathbb{J}_{n1}(q_n)\zeta_1^2]\zeta_n^3 \rangle + \langle \zeta_n^1, D\mathbb{J}_{n1}(q_n)[\mathbb{J}_{n1}(q_n)\zeta_1^2]\zeta_1^3 \rangle \right). \end{aligned}$$

Adding cyclic permutations and considering first  $\zeta_n^a = 0$  for  $n \geq 2$ , we see that it is necessary that  $\mathbb{J}_{11}$  satisfies Jacobi's identity on  $X_1$ , which is the assumption (A.3a).

The remaining terms are linear in  $(\zeta_n^a)_{a=1,2,3, n \geq 2}$  and bilinear in  $\zeta_1^a$ . Fixing one  $n \in \{2, \dots, N\}$  and setting  $\zeta_m^a = 0$  for  $m \notin \{1, n\}$ , we obtain a linear expression in  $\zeta_n^a$  for each  $a \in \{1, 2, 3\}$ . Considering all cyclic permutations this leads to the three terms that have to sum up to 0. Choosing one  $a$  and denoting by  $b$  and  $c$  the other two indices, the condition reads

$$0 = \langle \zeta_1^b, D\mathbb{J}_{11}(q_1)[\mathbb{J}_{1n}(q_n)\zeta_n^a]\zeta_1^c \rangle + \langle \zeta_1^c, D\mathbb{J}_{1n}(q_n)[\mathbb{J}_{n1}(q_n)\zeta_1^b]\zeta_n^a \rangle + \langle \zeta_n^a, D\mathbb{J}_{n1}(q_n)[\mathbb{J}_{n1}(q_n)\zeta_1^c]\zeta_1^b \rangle.$$

Since the first term depends on  $q_1$  but not the other two, this relation can only hold if  $D\mathbb{J}_{11}$  is independent of  $q_1$ , which provides the condition (A.3b).

Moreover, using  $\mathbb{J}_{1n} = -\mathbb{J}_{n1}^*$  we see that the last condition is the same as (A.3c). Hence, the necessity of (A.3) is established. However, by construction the sufficiency is clear.  $\square$

## References

- [1] R. Abeyaratne and J.K. Knowles. *Evolution of Phase Transition*. Cambridge Univ. Press, Cambridge, 2006.
- [2] R. Agrusta, S. Goes, and J. van Hunen. Subducting-slab transition-zone interaction: Stagnation, penetration and mode switches. *Earth and Planetary Science Letters*, 464:10–23, 2017.
- [3] J.F. Besseling and E. van der Giessen. *Mathematical Modelling of Inelastic Deformation*. Chapman & Hall/Springer, 1994.
- [4] P. Betsch and M. Schiebl. Energy-momentum-entropy consistent numerical methods for large-strain thermoelasticity relying on the GENERIC formalism. *Int. J. Numer. Meth. Eng.*, 119(12):1216–1244, 2019.
- [5] P. Betsch and M. Schiebl. Structure-preserving space-time discretization of large-strain thermo-viscoelasticity in the framework of GENERIC. *Num. Meth. Engrg.*, 122:3448–3488, 2021.
- [6] P. Bhardwaj and S. Singh. Pressure induced structural phase transitions – a review. *Cent. Eur. J. Chem.*, 10:1391–1422, 2012.
- [7] K. Bhattacharya. *Microstructure of martensite: why it forms and how it gives rise to the shape-memory effect*. Oxford Univ. Press, 2003.
- [8] M.I. Billen. Modeling the dynamics of subducting slabs. *Annu. Rev. Earth Planet. Sci.*, 36:325–356, 2008.
- [9] M. Běhounková and H. Čížková. Long-wavelength character of subducted slabs in the lower mantle. *Earth & Planetary Sci. Letters*, 275:43–53, 2008.
- [10] H. Čížková, A.P. van den Berg, W. Spakman, and C. Matyska. The viscosity of Earth’s lower mantle inferred from sinking speed of subducted lithosphere. *Phys. Earth & Planetary Interiors*, 200–201:56–62, 2012.
- [11] H. Čížková, J. van Hunen, and A. van den Berg. Stress distribution within subducting slabs and their deformation in the transition zone. *Phys. Earth & Planetary Interiors*, 161:202–214, 2007.
- [12] O. Coussy. *Poromechanics*. J.Wiley, Chichester, 2004.
- [13] J.H. Cushman. *The Physics of Fluids in Hierarchical Porous Media: Angstroms to Miles*. Springer, Dordrecht, 1997.
- [14] Y.F. Dafalias. The plastic spin concept and a simple illustration of its role in finite plastic transformations. *Mech. Mater.*, 3:223–233, 1984.
- [15] S. de Boer. *Trends in Continuum Mechanics of Porous Media*. Springer 2005.
- [16] M. H. Duong, M. A. Peletier, and J. Zimmer. GENERIC formalism of a Vlasov-Fokker-Planck equation and connection to large-deviation principles. *Nonlinearity*, 26(11):2951–2971, 2013.
- [17] B.J. Edwards. An analysis of single and double generator thermodynamics formalisms for the macroscopic description of complex fluids. *J. Non-Equilib. Thermodyn.*, 23(4):301–333, 1998.
- [18] E. Feireisl and A. Novotný. *Singular Limits in Thermodynamics of Viscous Fluids*. Birkhäuser, Basel, 2009.
- [19] E. Fried and M.E. Gurtin. Traction, balance, and boundary conditions for nonsimple materials with application to liquid flow at small-length scales. *Arch. Ration. Mech. Anal.*, 182:513–554, 2006.
- [20] T. Gerya. Future directions in subduction modeling. *J. Geodynamics*, 52:344–378, 2011.
- [21] M. Grmela and H.C. Öttinger. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. II. Illustrations of a general formalism. *Phys. Rev. E (3)*, 56(6):6620–6655, 1997.

- [22] M.E. Gurtin and L. Anand. The decomposition  $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$ , material symmetry, and plastic irrotationality for solids that are isotropic-viscoplastic or amorphous. *Intl. J. Plasticity*, 21:1686–1719, 2005.
- [23] M.E. Gurtin, E. Fried, and L. Anand. *The Mechanics and Thermodynamics of Continua*. Cambridge Univ. Press, New York, 2010.
- [24] L. Heller et al. On the plastic deformation accompanying cyclic martensitic transformation in thermomechanically loaded NiTi. *Intl. J. Plasticity*, 111:53–71, 2018.
- [25] M.M. Hirschmann. Water, melting, and the deep Earth H<sub>2</sub>O cycle. *Annu. Rev. Earth Planet. Sci.*, 34:629–653, 2006.
- [26] M. Hütter and B. Svendsen. Thermodynamic model formulation for viscoplastic solids as general equations for non-equilibrium reversible-irreversible coupling. *Contin. Mech. Thermodyn.*, 24(3):211–227, 2012.
- [27] M. Hütter and T.A. Tervoort. Finite anisotropic elasticity and material frame indifference from a nonequilibrium thermodynamics perspective. *J. Non-Newton. Fluid Mech.*, 152:45–52, 2008.
- [28] H.M. Jiang et al. Effect of hydrogen on super-elastic behavior of NiTi shape memory alloy wires: Experimental observation and diffusional-mechanically coupled constitutive model. *J. Mech. Behavior Biomedical Mater.*, 2022.
- [29] M. Jirásek and Z.P. Bažant. *Inelastic Analysis of Structures*. J.Wiley, Chichester, 2002.
- [30] G. Kaufmann and K. Lambeck. Mantle dynamics, postglacial rebound and the radial viscosity profile. *Phys. Earth & Planetary Interiors*, 121:301–324, 2000.
- [31] E. Kröner. Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen. *Arch. Ration. Mech. Anal.*, 4:273–334, 1960.
- [32] M. Kružík, A. Mielke, and T. Roubíček. Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in CuAlNi. *Meccanica*, 40:389–418, 2005.
- [33] M. Kružík and J. Zimmer. A model of shape memory alloys taking into account plasticity. *IMA J. Appl. Math.*, 76:193–216, 2011.
- [34] A. Lachiguer et al. Modeling of hydrogen effect on the superelastic behavior of Ni-Ti shape memory alloy wires. *Smart Mater. Struct.*, 25:Art.no.115047, 2016.
- [35] R. Lasarzik. Analysis of a thermodynamically consistent Navier-Stokes-Cahn-Hilliard model. *Nonl. Analysis*, 213:112526/1–33, 2021.
- [36] G. Lebon, D. Jou, and J. Casas-Vázquez. *Understanding Non-equilibrium Thermodynamics*. Springer-Verlag, 2008.
- [37] E. Lee and D. Liu. Finite-strain elastic-plastic theory with application to plain-wave analysis. *J. Applied Phys.*, 38:19–27, 1967.
- [38] E.H. Lee. Elastic-plastic deformation at finite strains. *J. Appl. Mech.*, 36:1–6, 1969.
- [39] W.E. Letaief, T. Hassine, and F. Gamaoun. A coupled model between hydrogen diffusion and mechanical behavior of superelastic NiTi alloys. *Smart Mater. Struct.*, 26:Art.no.075001, 2017.
- [40] W.E. Letaief et al. Coupled diffusion-mechanical model of NiTi alloys accounting for hydrogen diffusion and ageing. *Intl. J. Appl. Mech.*, 12:Art.no.2050039, 2020.
- [41] J.E. Marsden and T.S. Ratiu. *Introduction to Mechanics and Symmetry*, volume 17 of *Texts in Applied Mathematics*. Springer-Verlag, New York, second edition, 1999.
- [42] A. Mielke. Formulation of thermoelastic dissipative material behavior using GENERIC. *Contin. Mech. Thermodyn.*, 23(3):233–256, 2011.
- [43] A. Mielke, M. A. Peletier, and J. Zimmer. Deriving a GENERIC system from a hamiltonian system. *Submitted*, 2024.
- [44] R.D. Mindlin. Micro-structure in linear elasticity. *Archive Ration. Mech. Anal.*, 16:51–78, 1964.

- [45] P.J. Morrison. Bracket formulation for irreversible classical fields. *Phys. Lett. A*, 100(8):423–427, 1984.
- [46] P.J. Morrison. A paradigm for joined Hamiltonian and dissipative systems. *Phys. D*, 18(1-3):410–419, 1986.
- [47] P.J. Morrison. Thoughts on brackets and dissipation: old and new. *J. Physics: Conf. Series*, 169:012006, 12, 2009.
- [48] A. Nakao, H. Iwamori, and T. Nakakuki. Effects of water transportation on subduction dynamics: Roles of viscosity and density reduction. *Earth & Planetary Sci. Letters*, 454:178–191, 2016.
- [49] J. Nečas. Theory of multipolar fluids. In L. Jentsch and F. Tröltzsch, editors, *Problems and Methods in Mathematical Physics*, pages 111–119, Wiesbaden, 1994. Vieweg+Teubner.
- [50] J. Nečas, A. Novotný, and M. Šilhavý. Global solution to the ideal compressible heat conductive multipolar fluid. *Comment. Math. Univ. Carolinae*, 30:551–564, 1989.
- [51] J. Nečas and M. Ružička. Global solution to the incompressible viscous-multipolar material problem. *J. Elasticity*, 29:175–202, 1992.
- [52] E. Ohtani. Hydration and dehydration in Earth’s interior. *Annu. Rev. Earth Planet. Sci.*, 49:253–278, 2021.
- [53] H.C. Öttinger. *Beyond Equilibrium Thermodynamics*. John Wiley, New Jersey, 2005.
- [54] M. Pavelka, V. Klika, and M. Grmela. *Multiscale Thermo-Dynamics. Introduction to GENERIC*. De Gruyter, 2018.
- [55] M. Pavelka, I. Peshkov, and V. Klika. On Hamiltonian continuum mechanics. *Physica D*, 408:Art.no.132510, 2020.
- [56] P. Pelech, K. Tuma, M. Pavelka, M. Šípka, and M. Sýkora. On compatibility of the natural configuration framework with general equation for non-equilibrium reversible-irreversible coupling (GENERIC): derivation of anisotropic rate-type models. *J. Non-Newtonian Fluid Mech.*, 305:Art.no.104808, 2022,.
- [57] M. Pitteri and G. Zanzotto. *Continuum Models for Phase Transitions and Twinning in Crystals*. Chapman & Hall/CRC, Boca Raton, 2003.
- [58] K.R. Rajagopal and A.R. Srinivasa. On the thermomechanics of materials that have multiple natural configurations. Part I: Viscoelasticity and classical plasticity. *Zeits. angew. Math. Phys.*, 55:861–893, 2004.
- [59] G. Richard, M. Monnereau, and M. Rabinowicz. Slab dehydration and fluid migration at the base of the upper mantle: implications for deep earthquake mechanisms. *Geophys. J. Int.*, 168:1291–1304, 2007.
- [60] T. Roubíček. Models of microstructure evolution in shape memory alloys. In B. Gambin P. Ponte Castañeda, J.J. Telega, editor, *Nonlinear Homogenization and its Applications to Composites, Polycrystals and Smart Materials*. Springer, 2004.
- [61] T. Roubíček. Thermodynamically consistent model for poroelastic rocks towards tectonic and volcanic processes and earthquakes. *Geophysical J. Intl.*, 227:1893–1904, 2021.
- [62] T. Roubíček. Quasistatic hypoplasticity at large strains Eulerian. *J. Nonlin. Sci.*, 32:Art.no.45., 2022.
- [63] T. Roubíček. Thermodynamics of viscoelastic solids, its Eulerian formulation, and existence of weak solutions. *Zeitschrift f. angew. Math. Phys.*, 75:Art.no.51., 2024.
- [64] T. Roubíček and U. Stefanelli. Viscoelastodynamics of swelling porous solids at large strains by an Eulerian approach. *SIAM J. Math. Anal.*, 55:2475–2876, 2023.
- [65] T. Roubíček and G. Tomassetti. Inhomogeneous finitely-strained thermoplasticity with hardening by an Eulerian approach. *Disc. Cont. Dynam. Systems - S*, 17:181–220, 2023.

- [66] M.L. Rudolph, V. Lekić, and C. Lithgow-Bertelloni. Viscosity jump in Earth's mid-mantle. *Science*, 350:1349–1352, 2015.
- [67] L.H. Rüpke, J.P. Morgan, M. Hort, and J.A.D. Connolly. Serpentine and the subduction zone water cycle. *Earth & Planetary Sci. Letters*, 223:17–34, 2004.
- [68] C.G. Sammis, J.C. Smith, G. Schubert, and D.A. Yuen. Viscosity-depth profile of the Earth's mantle: Effects of polymorphic phase transitions. *J. Geophys. Res.*, 82:3747–3761, 1977.
- [69] R. Schmidt, M. Schlereth, H. Wipf, W. Assmus, and Mullner. Hydrogen solubility and diffusion in the shape-memory alloy NiTi. *J. Phys. Condensed Matter*, 1:2473–2482, 1989.
- [70] P. Šittner et al. On the coupling between martensitic transformation and plasticity in NiTi: experiments and continuum based modelling. *Progress in Materials Science*, 98:249–298, 2018.
- [71] N. Suenaga, Y. Ji, S. Yoshioka, and D. Feng. Subduction thermal regime, slab dehydration, and seismicity distribution beneath Hikurangi based on 3-D simulations. *J. Geophys. Res. Solid Earth*, 123:3080–3097, 2018).
- [72] P.J. Tackley, D. Stevenson, G. Glatzmaier, and G. Schubert. Effects of an endothermic phase transition at 670 km depth in a spherical model of convection in the Earth's mantle. *Nature*, 361:699–704, 1993.
- [73] R.A. Toupin. Elastic materials with couple stresses. *Arch. Ration. Mech. Anal.*, 11:385–414, 1962.
- [74] N. Ulf et al. Modeling of hydrogen effects on the thermomechanical behavior of NiTi-based shape memory alloys. *Shape Memory & Superelasticity*, 5:206–217, 2019.
- [75] A. Zafferi, K. Huber, D. Peschka, J. Vrijmoed, T. John, and M. Thomas. A porous-media model for reactive fluid-rock interaction in a dehydrating rock. *J. Math. Phys.*, 64:Art.no.091504, 2023.
- [76] A. Zafferi, D. Peschka, and M. Thomas. GENERIC framework for reactive fluid flows. *Z. angew. Math. Mech.*, 103:e202100254, 2023.