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Formulation of thermo-elastic dissipative material behavior using GENERIC

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Abstract

We show that the coupled balance equations for a large class of dissipative materials can be cast in the form of GENERIC (General Equations for Non-Equilibrium Reversible Irreversible Coupling). In dissipative solids, also called generalized standard materials, the state of a material point is decribed by dissipative internal variables in addition to the elastic deformation and the temperature. The framework GENERIC allows for an efficient derivation of thermodynamically consistent coupled field equations, while revealing additional underlying physical structures, like the role of the free energy as the driving potential for reversible effects and the role of the free entropy (Massieu potential) as the driving potential for dissipative effects.

Applications to large and small-strain thermoplasticity is given. Moreover, for the quasistatic case, where the deformation can be statically eliminated, we derive a generalized gradient structure for the internal variable and the temperature with a reduced entropy as driving functional.

1 Introduction

The aim of this work is to present thermomechanical models of *dissipative materials*, which are also called *generalized standard materials*, in the unifying framework of GENERIC, namely *General Equations for Non-Equilibrium Reversible Irreversible Coupling*. This framework provides a unification of (i) reversible dynamics obtained like Hamiltonian effects via a Poisson structure L and an energy functional $\mathscr{E}$ and (ii) dissipative dynamics like gradient flows obtained from a dissipative geometric structure K (the inverse of a sub-Riemannian structure) and an entropy functional $\mathscr{S}$. If X denotes the state of the system in the state space $\mathscr{X}$, then the evolution equation for a the GENERIC system $(\mathscr{X},\mathscr{E},\mathscr{S},L,K)$ reads

$$\dot{X} = L(X)\mathrm{D}\mathscr{E}(X) + K(X)\mathrm{D}\mathscr{S}(X). \tag{1.1}$$

The central additional property of the GENERIC framework is the noninteraction condition

$$L(x)\mathrm{D}\mathscr{S}(X) \equiv 0 \quad \text{and} \quad \mathrm{K}(X)\mathrm{D}\mathscr{E}(X). \tag{1.2}$$

We refer to the original papers [GrÖ97, ÖtG97] and to further developments in [MG*00, Ött06, HüT08a, HüT08b] with many application in different physical systems. We highlight in particular the book [Ött05], which shows that the framework of GENERIC is a very versatile tool for coarse graining a microscopic system $(\mathscr{X}_0, L_0, K_0, \mathscr{E}_0, \mathscr{S}_0)$ to obtain a macroscopic system $(\mathscr{X}_1, L_1, K_1, \mathscr{E}_1, \mathscr{S}_1)$.

In this work we want to show that many equations considered in elastic temperature-dependent solids with internal variables can be formulations in GENERIC, namely those for closed systems where the energy $\mathscr{E}$ is preserved and the entropy $\mathscr{S}$ increases. We will discuss these basic properties of GENERIC in Section 2.

We want to emphasize that using the framework of GENERIC is very advantageous for modeling purposes. First, the derivation of a complete system of consistent partial differential equations for all desirable quantities is easier, if one can focus the attention to the quintuple $(\mathscr{X},\mathscr{E},\mathscr{S},L,K)$ rather than to the balance laws and the constitutive equations. Second, the separation of reversible effects via $L\mathrm{D}\mathscr{E}$ from irreversible effects via $K\mathrm{D}\mathscr{S}$ is helpful in the interpretation of effects. Third, we will see that thermodynamic transformations between temperature θ, internal energy u, and entropy s can be made more efficiently in this framework. Moreover, the framework helps to understand several physical concepts, because of its clear emphasis on structures and functionals.

As one major consequence, we will see that the fundamental driving forces for a reversible variable ϕ and an irreversible variable z different, namely

$$f_{\mathrm{rev}} = \mathrm{D}_\phi\mathscr{E} - \theta{*}\mathrm{D}_\phi\mathscr{S} \quad \text{and} \quad f_{\mathrm{irr}} = \mathrm{D}_z\mathscr{S} - (1/\theta){*}\mathrm{D}_z\mathscr{E},$$

see Section 4.1 for the definition of the "$\alpha*$". While it is well-established from the isothermal theory that f_{rev} is the variational derivative $\delta_w\overline{\psi}$ of the *free energy* $\psi = \overline{\psi}(w,\theta)$, it is much less known that f_{irr} is given as variational derivative $\delta_w\overline{\eta}$ of the *free entropy* $\eta = \overline{\eta}(w,\theta) = -\overline{\psi}(w,\theta)/\theta$, also called *Massieu potential* [1869]. For temperature-dependent systems with $\overline{\psi}$ depending on ∇w as well, we have to be aware that multiplication with $\frac{1}{\theta}$ does not commute with variational derivates:

$$\delta_w\overline{\eta} = -\frac{1}{\theta}\partial_w\overline{\psi} + \mathrm{div}\,\big(\frac{1}{\theta}\partial_\nabla\overline{\psi}\big) \quad \neq \quad -\frac{1}{\theta}\delta_w\overline{\psi} = -\frac{1}{\theta}\partial_w\overline{\psi} + \frac{1}{\theta}\,\mathrm{div}\,\big(\partial_\nabla\overline{\psi}\big). \tag{1.3}$$

However, to satisfy the first and second law of thermodynamics locally in a solid, this distinction is crucial, see the discussion in Section 4.2.

In fact, we will show that dissipative solids can be described by special formulations within GENERIC, where the geometric structures L and K are of the form

$$L(X) = M_\mathscr{S} L_0 M_\mathscr{S}^* \quad \text{and} \quad K(X) = N_\mathscr{E} L_0 N_\mathscr{E}^*,$$

where the Poisson structure L_0 and the dissipation structure K_0 are relatively simple and the operators $M_\mathscr{S}$ and $N_\mathscr{E}$ are obtained from $\mathscr{S}$ and $\mathscr{E}$ in a rather canonical way, see Section 2.4. If X has the form $X = (w,\theta)$, then we define

$$M_\mathscr{S} = \begin{pmatrix} I & 0 \\ \mathrm{D}_w\mathscr{S} & \mathrm{D}_\theta\mathscr{S} \end{pmatrix}^{-1} \quad \text{giving} \quad M_\mathscr{S}^* = \begin{pmatrix} I & -\frac{\square}{\mathrm{D}_\theta\mathscr{S}}{*}\mathrm{D}_w\mathscr{S} \\ 0 & \frac{1}{\mathrm{D}_\theta\mathscr{S}} \end{pmatrix}.$$

From this we find the noninteraction condition (1.2) as well as the reversible driving force f_{rev} in $M_\mathscr{S}\mathrm{D}\mathscr{E}$.

In Section 2.3 we show that it is illuminating to express the internal energy $u = U(w,\tau)$ and the entropy $s = S(w,\tau)$ in terms of an arbitrary thermodynamical variable τ, which can be for instance θ, u, or s. Here w stand for all other variables (and their gradients). We always have the condition $\theta = \Theta(w,\tau) = \partial_\tau U(w,\tau)/\partial_\tau S(w,\tau)$. This arbitrariness gives more flexibility in modeling and highlight the contributions of energy and entropy more clearly. For instance, for all τ we have the reversible driving force

$$\partial_w U(w,\tau) - \Theta(w,\tau)\partial_w S(w,\tau) = \partial_w \overline{\psi}(w,\Theta(w,\tau))$$

and the irreversible driving force

$$\partial_w S(w,\tau) - \frac{1}{\Theta(w,\tau)}\partial_w U(w,\tau) = \partial_w \overline{\eta}(w,\Theta(w,\tau)).$$

In Section 2.5 we generalize the formulation of GENERIC by replacing the linear dissipation operator K by the subdifferential of a general dual entropy-production potential $\mathscr{K}(X;\cdot) : \mathrm{T}^*_X\mathscr{X} \to [0,\infty]$, i.e. $K(X)\mathrm{D}\mathscr{S}(X)$ is replaced by $\partial_\xi \mathscr{K}(X,\mathrm{D}\mathscr{S}(X))$. In particular, we have for the total entropy $\mathscr{S}$ the relation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(X) = \langle \partial_\xi \mathscr{K}(X;\mathrm{D}\mathscr{S}(X)), \mathrm{D}\mathscr{S}(X)\rangle \geq 0.$$

In Section 2.6 we discuss how one can derive the dissipative Hamiltonian system

$$\dot{X} = (L - \frac{1}{\theta_*}K)\mathrm{D}\mathscr{F}_* \quad \text{with} \quad \mathscr{F}_* = (\mathscr{E} - \theta_*\mathscr{S})\big|_{\theta=\theta_*}$$

from (1.1), if a suitable coupling to a heat bath at temperature θ_* is added.

Section 3 is devoted to finite-dimensional examples, which are intended to serve as introduction to the formulation via GENERIC. Moreover, these examples explain the different thermodynamics concepts, namely the modeling via the arbitrary thermodynamic variable τ and the the occurrence of the reversible and irreversible driving forces. The first example explains how classical linear damping in a Hamiltonian system can be formulated via $K\mathrm{D}\mathscr{S}$. The second example is a rheological model where internal friction elements are models.

The modeling of dissipative solids is developed in Section 4. After giving proper definitions of the differentials $\delta_z E$,$\Delta_z E$, and $\alpha{*}\delta_z E$, we discuss the purely dissipative Penrose-Fife phase-field model, which couples the order parameter $z : \Omega \to \mathbb{R}$ to the heat equation. In Section 4.3 we start with the modeling of thermoviscoelasticity in terms of the deformation $\varphi : \Omega \to \mathbb{R}^d$ and the thermodynamic variable τ. Entropy production occurs via viscous dissipation induced by $\dot{\boldsymbol{F}} = \nabla\dot{\varphi} = \nabla \mathrm{D}_p\mathscr{E}$ and by heat conduction induced by $\nabla(1/\theta)$. We show that the classical equations of thermoviscoelasticity are obtained from GENERIC in a straightforward manner.

In Section 4.4 we study general dissipative solids (also called generalized standard materials) with an internal variable z, which may describe quite different physical properties like magnetization, polarization, phase fractions or densities of species, order parameters, effective transformation strains, or plastic variables. For the isothermal case, there is a large theory for deriving the associated balance equations, see e.g. [ZiW87, Hac97, Alb98, Mie06], while we propose a general approach for the nonisothermal case. We refer to [Mie10] for a similar approach to thermal couplings to reaction diffusion systems. Our motivation and applications will be mainly in plasticity, that is why we consider general dual entropy-production potentials $\mathscr{K}$ as introduced in Section 2.5. In particular, we emphasize that we allow for functionals $\mathscr{E}$ and $\mathscr{S}$ where the densities U and S depend also on ∇z, which leads to the non-commutativity explained in (1.3). Finally, we show how the system simplifies in a standard situation with small strains.

Section 5 is devoted to quasistatic models, where the kinetic energy is neglected, i.e. in the balance of linear momentum the acceleration term is dropped. Under the additional assumption that there are no viscoelastic effects, the first equation is a static balance, from which the elastic deformation can be calculated as a function the other variables, viz. $\boldsymbol{\phi} = Q(z,\tau)$. We show that under certain conditions the remaining equations for (z,τ) can be written as a generalized gradient system $(\mathscr{X}^{\mathrm{red}}, \mathscr{S}^{\mathsf{qs}}, \mathscr{K}^{\mathsf{qs}})$ on the reduced state space $\mathscr{X}^{\mathrm{red}}$ for (z,τ) with the natural restrictions of $\mathscr{S}^{\mathsf{qs}}$ and $\mathscr{K}^{\mathsf{qs}}$ of the original structures $\mathscr{S}$ and $\mathscr{K}$, respectively.

Throughout Sections 4 and 5, we ignore all boundary terms when doing integration by parts. This is a realistic procedure for closed systems, where we assume that it is thermally isolated (insulation condition $\nabla\theta\cdot\nu = 0$ on $\partial\Omega$), stress free on the boundary, and that the internal variables z satisfy natural boundary conditions $\nabla z\cdot\nu = 0$.

2 The GENERIC framework

The framework of GENERIC was introduced by Öttinger and Grmela in [GrÖ97, ÖtG97]. It is based on a quintuple $(\mathscr{X}, \mathscr{E}, \mathscr{S}, L, K)$, where the smooth functionals $\mathscr{E}$ and $\mathscr{S}$ on a smooth manifold $\mathscr{X}$, where $\mathscr{E}$ denotes the total energy and the $\mathscr{S}$ the total entropy. Moreover, on $\mathscr{X}$ we have given a Poisson structure L and a dissipative structure K, i.e., for each $X\in\mathscr{X}$ the operators $L(X)$ and $K(X)$ map the cotangent space $\mathrm{T}^*_x\mathscr{X}$ into the tangent space $\mathrm{T}_x\mathscr{X}$. The evolution of the system is given by the differential equation

$$\dot{X} = L(X)\mathrm{D}\mathscr{E}(X) + K(X)\mathrm{D}\mathscr{S}(X), \tag{2.1}$$

where $\mathrm{D}\mathscr{E}$ and $\mathrm{D}\mathscr{S}$ are the differentials taking values in the cotangent space.

2.1 The structure of GENERIC

The crucial conditions on the structure L and K are the symmetries

$$L(X) = -L(X)^* \text{ and } K(X) = K(X)^* \tag{2.2}$$

and the structural properties

$$\begin{aligned}&L \text{ satisfies Jacobi's identity,}\\ &K(X) \text{ is positive semi-definite, i.e., } \langle\xi, K(X)\xi\rangle \geq 0.\end{aligned} \tag{2.3}$$

Jacobi's identity for L means that $\{\{\mathscr{F}_1,\mathscr{F}_2\}_L,\mathscr{F}_3\}_L + \{\{\mathscr{F}_2,\mathscr{F}_3\}_L,\mathscr{F}_1\}_L + \{\{\mathscr{F}_3,\mathscr{F}_1\}_L,\mathscr{F}_2\}_L \equiv 0$ for all functions $\mathscr{F}_j : \mathscr{X}\to\mathbb{R}$, where the Poisson bracket is defined via

$$\{\mathscr{F},\mathscr{G}\}_L(X) := \langle \mathrm{D}\mathscr{F}(X), L(X)\mathrm{D}\mathscr{G}(X)\rangle.$$

Finally, the central condition states that the energy functional does not contribute to dissipative mechanisms and that the entropy functional does not contribute to reversible dynamics, which is the following *noninteraction condition*:

$$\forall X \in \mathscr{X}: \quad L(X)\mathrm{D}\mathscr{S}(X) = 0 \quad \text{and} \quad K(X)\mathrm{D}\mathscr{E}(X) = 0. \tag{2.4}$$

Of course, the structure of GENERIC is geometric in the sense that it is invariant under coordinate transformations. Introducing new coordinates $X = x(Y)$ we define the transformed functionals $\overline{\mathscr{E}}$ and $\overline{\mathscr{S}}$ in the usual way, namely

$$\overline{\mathscr{E}}(Y) = \mathscr{E}(x(Y)) \text{ and } \overline{\mathscr{S}}(Y) = \mathscr{S}(x(Y)).$$

Moreover, the transformed geometric structures $\overline{L}$ and $\overline{K}$ are obtained via

$$\overline{L}(Y) = \mathrm{D}x(Y)^{-1}L(x(Y))\mathrm{D}x(Y)^{-*} \text{ and } \overline{K}(Y) = \mathrm{D}x(Y)^{-1}K(x(Y))\mathrm{D}x(Y)^{-*}, \tag{2.5}$$

where $\mathrm{D}x(Y)^{-*} : \mathrm{T}^*_Y\mathscr{Y} \to \mathrm{T}^*_{x(Y)}\mathscr{X}$ denotes the adjoint of the inverse of $\mathrm{D}x(Y) : \mathrm{T}_Y\mathscr{Y} \to \mathrm{T}_{x(Y)}\mathscr{X}$. Clearly, the transformed system $\dot{Y} = \overline{L}(Y)\mathrm{D}\overline{\mathscr{E}}(Y) + \overline{K}(Y)\mathrm{D}\overline{\mathscr{S}}(Y)$ is equivalent to the original system (2.1).

2.2 Basic properties of the GENERIC formulation

The first observation is that (2.3) and (2.4) imply energy conservation and entropy increase:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}(X(t)) = \langle \mathrm{D}\mathscr{E}(X), \dot{X}\rangle = \langle \mathrm{D}\mathscr{E}(X), L\mathrm{D}\mathscr{E} + K\mathrm{D}\mathscr{S}\rangle = 0 + 0 = 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(X(t)) = \langle \mathrm{D}\mathscr{S}(X), \dot{X}\rangle = \langle \mathrm{D}\mathscr{S}(X), L\mathrm{D}\mathscr{E} + K\mathrm{D}\mathscr{S}\rangle = 0 + \langle \mathrm{D}\mathscr{S}, K\mathrm{D}\mathscr{S}\rangle \geq 0.$$

Note that we would need much less than the two conditions (2.3) and (2.4) to guarantee these two properties. However, the next property needs (2.4) in its full strength.

Next, we show that equilibria can be obtained by the *maximum entropy principle*. If x_* maximizes $\mathscr{S}$ under the constraint $\mathscr{E}(X) = E_0$, then we obtain a Lagrange multiplier $\lambda_* \in \mathbb{R}$ such that $\mathrm{D}\mathscr{S}(X_*) = \lambda_*\mathrm{D}\mathscr{E}(X_*)$. Assuming that $\lambda_* \neq 0$ we immediately find that x_* is an equilibrium of (2.1). Indeed,

$$L(X_*)\mathrm{D}\mathscr{E}(X_*) = \tfrac{1}{\lambda_*}L(X_*)\mathrm{D}\mathscr{S}(X_*) = 0 \text{ and } K(X_*)\mathrm{D}\mathscr{S}(X_*) = \lambda_* K(X_*)\mathrm{D}\mathscr{E}(X_*) = 0,$$

where we have used (2.4).

Remark 2.1 (Metriplectic systems) *The framework of GENERIC has its origins in the metriplectic formulations from [Kau84, Mor86]. There, equations of the form*

$$\dot{X} = (L(X) - D(X))\mathrm{D}\mathscr{F}(X),$$

are considered, where L is a Poisson structure and D is symmetric and positive semidefinite dissipation structure. However, there is only one functional $\mathscr{F}$ that is a Liapunov functional. Clearly, GENERIC is more general as we obtain the metriplectic form simply by taking $\mathscr{F} = \mathscr{E} - \theta_*\mathscr{S}$ and $D = -\frac{1}{\theta_*}K$.

2.3 Thermodynamic transformations and driving forces

Since modeling of temperature-dependent systems fundamentally relies on the thermodynamically formalism involving the energies, entropies and the temperature, we give some elementary transformation rules between different representations. For the subsequent developments, it will be crucial to be able to choose either one of the three quantities *internal energy* u, *entropy* s, or *temperature* θ as the independent variable and express the others in terms of the first. In principle, all formulations will be equivalent, but at certain stages one of the three formulations will more advantageous. Moreover, using an arbitrary thermodynamic variable τ will highlight certain structures more clearly. Certainly, for modeling a given material it is most common to use the temperature in the constitutive function, but for deriving suitable geometric structures internal energy and entropy are better (cf. also [Mie10]).

Subsequently, we denote all other state variables by w, which may include the strain $\boldsymbol{F}$ and the internal variables z. We start with the formulation using the temperature, because it is most common in solid mechanics.

Temperature θ:
We consider a general free energy $\psi = \overline{\psi}(w,\theta)$ and the associated internal energy and entropy

$$u = \overline{u}(w,\theta) = \overline{\psi}(w,\theta) - \theta\partial_\theta\overline{\psi}(w,\theta) = \overline{\psi} + \theta\overline{s}, \quad s = \overline{s}(w,\theta) = -\partial_\theta\psi(w,\theta). \tag{2.6}$$

In general we assume that the specific heat $\partial_\theta\overline{u}$ is strictly positive. We have the relations

$$\partial_\theta\overline{u} = \theta\partial_\theta\overline{s} \quad \text{and} \quad \partial_w\overline{\psi} = \partial_w\overline{u} - \theta\partial_w\overline{s}. \tag{2.7}$$

Entropy s:
We may solve $s = \overline{s}(w,\theta)$ in terms of $\theta = \widetilde{\Theta}(w,s)$. We express the internal energy in terms of (w,s), namely $u = \widetilde{u}(w,s) = \overline{u}(w,\widetilde{\Theta}(w,s))$. We then have

$$\theta = \partial_s\widetilde{u}(w,s) = \widetilde{\Theta}(w,s), \quad \partial_w\widetilde{u}(w,s) = \partial_w\overline{u} - \theta\partial_w\overline{s} = \partial_w\overline{\psi}(w,\widetilde{\Theta}(w,s)). \tag{2.8}$$

To prove the latter relation, we use $\widetilde{u}(w,s) = \overline{u}(w,\partial_s\widetilde{u}(w,s))$ and find after differentiation (a) $\partial_w\widetilde{u}(w,s) = \partial_w\overline{u} + \partial_\theta\overline{u}\,\partial_s\partial_w\widetilde{u}$. Moreover, differentiating the relation $\theta = \partial_s\widetilde{u}(w,\overline{s}(w,\theta))$ with respect to θ and w gives (b) $1 = \partial_s^2\widetilde{u}\,\partial_\theta\overline{s}$ and (c) $0 = \partial_s\partial_w\widetilde{u} + \partial_s^2\widetilde{u}\,\partial_w\overline{s}$. From (b) and the first relation in (2.7) we have $\partial_\theta\overline{u} = \theta\partial_\theta\overline{s} = \theta/\partial_s^2\widetilde{u}$. Inserting this into (a) and using (c) gives the second relation in (2.8).

Internal energy u:
We use (w,u) as variables and write $s = \widehat{s}(w,e)$ by solving $u = \widetilde{u}(w,s)$. We have

$$\partial_e\widehat{s}(w,e) = \frac{1}{\theta}, \quad \partial_w\widehat{s} = -\frac{1}{\theta}\partial_w\widetilde{u} = \partial_w\overline{s} - \frac{1}{\theta}\partial_w\overline{u} = -\frac{1}{\theta}\partial_w\overline{\psi}. \tag{2.9}$$

Example 2.2 *We finally give a standard example of a free energy $\overline{\psi}$, where the functions $\overline{u}, \overline{s}, \widetilde{u},$ and $\widehat{s}$ can be given explicitly. We consider*

$$\overline{\psi}(w,\theta) = -\psi_0(\theta) + \psi_1(w) + \theta\psi_2(w), \quad \textit{where } \psi_0(\theta) = c\theta(\log\theta - 1). \tag{2.10}$$

This leads to the following expressions:

$$\overline{u}(w,\theta)=c\theta+\psi_1(w),\qquad \overline{s}(w,\theta)=c\log\theta-\psi_2(w),\qquad \overline{\theta}(w,\theta)=\theta,$$
$$\widetilde{u}(w,s)=c\mathrm{e}^{(s+\psi_2(w))/c}+\psi_1(w),\quad \widetilde{s}(w,s)=s,\qquad \widetilde{\theta}(w,s)=\mathrm{e}^{(s+\psi_2(w))/c},$$
$$\widehat{u}(w,u)=u,\qquad \widehat{s}(w,u)=c\log\tfrac{u-\psi_1(w)}{c}-\psi_2(w),\quad \widehat{\theta}(w,u)=(u-\psi_1(w))/c.$$

In particular, we see that convexity of ψ_1 and ψ_2 implies that $\widetilde{u}$ is convex and that $\widehat{s}$ is concave in w.

In the sequel, we will often use the variable τ to denote any of the three choices $\tau\in\{\theta,u,s\}$. Even other choices such as $\tau=\varphi(\theta)$ are possible. We then write $u=U(w,\tau)$ and $s=S(w,\tau)$. In all these cases we have

$$\theta=\Theta(w,\tau)=\frac{\partial_\tau U(w,\tau)}{\partial_\tau S(w,\tau)},\tag{2.11}$$

which relates to the classical definition of temperature, usually written via differential forms as $\theta\mathrm{d}S=\mathrm{d}E$. To prove this relation we start from a general function $\tau=T(w,\theta)$ and its inverse $\theta=\Theta(w,\tau)$. Applying the chain rule to $U(w,\tau)=\overline{u}(w,\Theta(w,\tau))$, we obtain $\partial_\tau E=\partial_\theta\overline{u}\,\partial_\tau\Theta$. Using the analogous relation for S we arrive at $\frac{\partial_\tau E}{\partial_\tau S}=\frac{\partial_\theta\overline{u}\,\partial_\tau\Theta}{\partial_\theta\overline{s}\,\partial_\tau\Theta}=\frac{\partial_\theta\overline{u}}{\partial_\theta\overline{s}}=\theta$.

Thermodynamic driving forces for the variable w should be given by an expression in terms of U and S as functions of (w,τ) that do not depend on the particular choice of τ. Introducing the Helmholtz *free entropy* (also called Massieu [1869] potential or Massieu-Planck potential) $\eta=-\psi/\theta=s-u/\theta$, we have the following relations

$$\begin{aligned}&\partial_wU(w,\tau)-\Theta(w,\tau)\partial_wS(w,\tau)=\partial_w\overline{\psi}(w,\Theta(w,\tau)),\\&\partial_wS(w,\tau)-\frac{1}{\Theta(w,\tau)}\partial_wU(w,\tau)=\partial_w\overline{\eta}(w,\Theta(w,\tau)).\end{aligned}\tag{2.12}$$

These relations can also be proved using the chain rule giving

$$\begin{aligned}\partial_wU(w,\tau)&=\partial_w\overline{u}(w,\Theta(w,\tau))+\partial_\theta\overline{u}(w,\Theta(w,\tau))\partial_w\Theta(w,\tau),\\\partial_wS(w,\tau)&=\partial_w\overline{s}(w,\Theta(w,\tau))+\partial_\theta\overline{s}(w,\Theta(w,\tau))\partial_w\Theta(w,\tau).\end{aligned}$$

Taking the two linear combinations given in (2.12) the relation $\partial_\theta\overline{u}=\theta\partial_\theta\overline{s}$ shows that the term involving $\partial_w\Theta$ cancels.

We will see below that the first expression gives the reversible thermodynamical driving forces while the second expression gives the irreversible thermodynamical driving forces. Thus, the derivative of the Helmholtz free energy $\overline{\psi}$ gives the reversible driving forces, while the derivatives of the free entropy $\overline{\eta}$ (also called Massieu potential) gives the irreversible driving forces. This observation will be fundamental throughout this work.

As written in (2.12) the two different forces only differ by a factor $-\Theta$. However, we will see later that for systems where the variable w also appears via its gradient ∇w the partial derivative ∂_w needs to be replaced by the variational derivative δ_w, see Section 4.1. Then, it will be essential to distinguish whether the factor appears inside or outside the divergence operator, cf. (1.3).

2.4 Special form of GENERIC

In this subsection we provide a special form of GENERIC, which immediately displays the noninteraction conditions (2.4). It will turn out that all applications studied in this paper can be written in a slight variant of this specialized form. However, we don't know how general this structure can be applied in other applications.

We consider a system with states $X = (w, \tau)$, where $\tau \in \mathbb{R}$ is the thermodynamic variable in the sense of Section 2.3. For a functional $\mathscr{H}$ we define the matrix

$$M_{\mathscr{H}}(w,\tau) = \begin{pmatrix} I & 0 \\ \mathrm{D}_w\mathscr{H}(w,\tau)^* & \mathrm{D}_\tau\mathscr{H}(w,\tau) \end{pmatrix}^{-1},$$

which leads to the formulas

$$M_{\mathscr{H}} = \begin{pmatrix} I & 0 \\ -\frac{1}{\mathrm{D}_\tau\mathscr{H}}\mathrm{D}_w\mathscr{H}^* & \frac{1}{\mathrm{D}_\tau\mathscr{H}} \end{pmatrix} \quad \text{and} \quad M_{\mathscr{H}}^* = \begin{pmatrix} I & -\frac{1}{\mathrm{D}_\tau\mathscr{H}}*\mathrm{D}_w\mathscr{H} \\ 0 & \frac{1}{\mathrm{D}_\tau\mathscr{H}} \end{pmatrix},$$

where the operation "$\alpha*\mathrm{D}_w$" is explained in (4.1).

Our special GENERIC system for functionals $\mathscr{E}$ and $\mathscr{S}$ have the form

$$\begin{pmatrix} \dot{w} \\ \dot{\tau} \end{pmatrix} = M_{\mathscr{S}}L_0M_{\mathscr{S}}^*\mathrm{D}\mathscr{E} + M_{\mathscr{E}}K_0M_{\mathscr{E}}^*\mathrm{D}\mathscr{S}, \tag{2.13}$$

where L_0 and K_0 are a Poisson and a dissipative structure, respectively. Note that $L = M_{\mathscr{S}}L_0M_{\mathscr{S}}^*$ and $K = M_{\mathscr{E}}K_0M_{\mathscr{E}}^*$ automatically define a Poisson and a dissipative structure, respectively. For K this is elementary, while for L the skew symmetry is elementary as well and the Jacobi identity follows from its invariance under coordinate transformations, see e.g. [Mie91, Sect. 4.2] for a direct proof. For the latter assertion we note that $L(w,\tau) = M_{\mathscr{S}}L_0M_{\mathscr{S}}^*$ is simply the transformation in the sense of (2.5) associated with the mapping $X = (w,s) = (w, S(w,\tau)) = x(Y)$, where $Y = (w,\tau)$.

We only need to impose the additional condition $L_0(w,\tau)\binom{0}{1} \equiv 0 \equiv K_0(w,\tau)\binom{0}{1}$, then the noninteraction conditions (2.4) are satisfied due to the obvious identities

$$M_{\mathscr{E}}^*\mathrm{D}\mathscr{E} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad M_{\mathscr{S}}^*\mathrm{D}\mathscr{S} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The special form (2.13) also reveals the role of the reversible and irreversible driving forces via

$$M_{\mathscr{S}}^*\mathrm{D}\mathscr{E} = \begin{pmatrix} \mathrm{D}_w\mathscr{E} - \theta*\mathrm{D}_w\mathscr{S} \\ \theta \end{pmatrix} \quad \text{and} \quad M_{\mathscr{E}}^*\mathrm{D}\mathscr{S} = \begin{pmatrix} \mathrm{D}_w\mathscr{S} - \frac{1}{\theta}*\mathrm{D}_w\mathscr{E} \\ 1/\theta \end{pmatrix},$$

where the upper components are to be compared with (2.12).

While the construction of $L = M_{\mathscr{S}}L_0M_{\mathscr{S}}^*$ depends strongly on the specific form of $M_{\mathscr{S}}$ (which is the inverse of the derivative of the mapping $(w,\tau) \mapsto (w, S(w,\tau))$), there is much more freedom to replace the operator $M_{\mathscr{E}}$ by any operator $N_{\mathscr{E}} : \mathscr{V}^* \to \mathscr{X}$ satisfying the relation $N_{\mathscr{E}}\mathrm{D}\mathscr{E} \equiv \binom{0}{1}$. Note that $\mathscr{V}$ can be an arbitrary linear space, such that $K_0(w,\tau) : \mathscr{V} \to \mathscr{V}^*$ is linear and positive semidefinite (or subdifferential of a positive convex functional, see the next subsection). Then, the new dissipative structure $K = N_{\mathscr{E}}K_0N_{\mathscr{E}}^* : \mathscr{X}^* \to \mathscr{X}$ is dissipative again.

2.5 Generalized GENERIC

In this subsection we give a generalization of the GENERIC framework to the case where the dissipative forces do not depend linearly on $\mathrm{D}\mathscr{S}$. This is essential for our applications in plasticity, where the stress-strain relation cannot be linear, because plastic effects are not seen unless the positive yield stress is reached.

For this, we note that K generates an entropy-production potential

$$\mathscr{K}(X;\xi) = \frac{1}{2}\langle \xi, K(X)\xi\rangle,$$

which means that $\mathrm{D}_\xi \mathscr{K}(X;\mathrm{D}\mathscr{S}(X)) = K(X)\mathrm{D}\mathscr{S}(X)$ gives the dissipative forces. Obviously, $\mathscr{K}(X;\cdot)$ is a nonnegative, quadratic functional.

We now allow for general entropy-production potentials $\mathscr{K}$ such that for all X the function $\mathscr{K}(X;\cdot)$ is convex, nonnegative, and satisfies $\mathscr{K}(X;0)=0$. We do not assume differentiability of $\mathscr{K}(X;\cdot)$, but use the convex subdifferential

$$\partial_\xi \mathscr{K}(X;\xi) = \{\, V \mid \mathscr{K}(X;\widetilde{\xi}) \geq \mathscr{K}(X;\xi) + \langle \widetilde{\xi}-\xi, V\rangle \text{ for all } \widetilde{\xi}\,\},$$

to denote the set of all possible rates V that are compatible with the force ξ.

Now, the generalized GENERIC is given as the differential inclusion

$$\dot{X} \in L(X)\mathrm{D}\mathscr{E}(X) + \partial_\xi \mathscr{K}(X;\mathrm{D}\mathscr{S}(X)),$$

and the orthogonality relation (2.4) is replaced by

$$\forall X \in \mathscr{X},\ \xi \in \mathscr{X}^*,\ \lambda \in \mathbb{R}: \quad L(X)\mathrm{D}\mathscr{S}(X) = 0 \text{ and } \mathscr{K}(X;\xi+\lambda \mathrm{D}\mathscr{E}(X)) = \mathscr{K}(X;\xi). \quad (2.14)$$

Indeed, the latter condition leads to the relation $\langle \mathrm{D}\mathscr{E}(X), V\rangle = 0$ for all $V \in \partial_\xi \mathscr{K}(X;\xi)$, which is what we really need.

It is also interesting to introduce the primal entropy-production potential $\mathscr{G}(X;\cdot) : \mathrm{T}_X\mathscr{X} \to [0,\infty]$ using the Legendre-Fenchel transformation

$$\mathscr{G}(X;V) \overset{\text{def}}{=} \sup\{\, \langle \xi, V\rangle - \mathscr{K}(X;\xi) \mid \xi \in \mathrm{T}^*_X\mathscr{X}\,\}.$$

We also write $\mathscr{G}(X;\cdot) = \mathscr{K}^*(X;\cdot)$ and $\mathscr{K}(X;\cdot) = \mathscr{G}^*(X;\cdot)$. The relation (2.14) implies $\mathscr{G}(X;V) = \infty$ for all V satisfying $\langle \mathrm{D}\mathscr{E}(X), V\rangle \neq 0$. Hence, energy conservation is already encoded into the definition of $\mathscr{G}$.

The classical equivalences for subdifferentials of Legendre-Fenchel transforms give

$$\xi \in \partial_V \mathscr{G}(X;V) \ \Leftrightarrow\ V \in \partial_\xi \mathscr{K}(X;\xi) \ \Leftrightarrow\ \mathscr{K}(X;\xi) + \mathscr{G}(X;V) = \langle \xi, V\rangle.$$

Thus, for the rate of the total entropy we find the relation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(X) \ &= \ \langle \mathrm{D}\mathscr{S}(X), \partial_\xi \mathscr{K}(X;\mathrm{D}\mathscr{S}(X))\rangle \ = \ \langle \partial_V \mathscr{G}(X;\dot{X}), \dot{X}\rangle \\ &= \ \mathscr{K}(X;\mathrm{D}\mathscr{S}(X)) + \mathscr{G}(X;\dot{X}) \geq 0.\end{aligned}$$

Remark 2.3 *It seems possible to generalize the dissipative terms even further. The subdifferential may be replaced by a general multi-valued operator that is monotone. In fact, as was observed in [Alb98], the second law of thermodynamics follows even from premonotonicity.*

2.6 Dissipative Hamiltonian systems as isothermal limits

Often temperature effects can be neglected and the model can be approximated by an isothermal model. We show here how this can be deduced consistently from the GENERIC form if we add some coupling to an external heat bath fixed to a given temperature $\theta_* > 0$. In particular, we will replace the two functionals $\mathscr{E}$ and $\mathscr{S}$ by one, namely the free energy $\mathscr{F}_*$ at the given temperature θ_*.

We start from a general system for the variable $X = (Y, \theta)$ in the form

$$\begin{pmatrix} \dot{Y} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} L & \alpha \\ -\alpha^{\mathsf{T}} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{D}_Y \overline{\mathscr{E}} \\ \mathrm{D}_\theta \overline{\mathscr{E}} \end{pmatrix} + \begin{pmatrix} K & \beta \\ \beta^{\mathsf{T}} & \Lambda \end{pmatrix} \begin{pmatrix} \mathrm{D}_Y \overline{\mathscr{S}} \\ \mathrm{D}_\theta \overline{\mathscr{S}} \end{pmatrix} - \begin{pmatrix} 0 \\ A(\theta - \theta_*) \end{pmatrix}, \tag{2.15}$$

where the coupling operator A is assumed to be positive definite.

We define the functional $\mathscr{F}^\circ(Y, \theta) = \overline{\mathscr{E}}(Y, \theta) - \theta_* \overline{\mathscr{S}}(Y, \theta)$. Using the relations $\mathrm{D}_\theta \overline{\mathscr{E}}(Y, \theta) = \partial_\theta \overline{u} = \theta \partial_\theta \overline{s} = \theta \mathrm{D}_\theta \mathscr{S}(Y, \theta)$ (see (2.7)), we find the crucial relation

$$\mathrm{D}_\theta \mathscr{F}^\circ(Y, \theta_*) = 0 \quad \text{for all } Y. \tag{2.16}$$

Moreover, the GENERIC structure (2.15) can be rewritten as

$$\begin{pmatrix} \dot{Y} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} L - \frac{1}{\theta_*} K & \alpha - \frac{1}{\theta_*} \beta \\ -\alpha^{\mathsf{T}} - \frac{1}{\theta_*} \beta^{\mathsf{T}} & -\frac{1}{\theta_*} \Lambda \end{pmatrix} \begin{pmatrix} \mathrm{D}_Y \mathscr{F}^\circ \\ \mathrm{D}_\theta \mathscr{F}^\circ \end{pmatrix} - \begin{pmatrix} 0 \\ A(\theta - \theta_*) \end{pmatrix},$$

The equation for $\dot{Y}$ takes the form

$$\dot{Y} = \big(L - \tfrac{1}{\theta_*} K\big) \mathrm{D} \mathscr{F}^\circ + \underbrace{\big(\alpha - \tfrac{1}{\theta_*} \beta\big) \mathrm{D}_\theta \mathscr{F}^\circ}_{= O(\|\theta - \theta_*\|)},$$

where we used (2.16) to estimate the last term. Defining the isothermal free energy $\mathscr{F}_*(Y) = \mathscr{F}^\circ(Y, \theta_*)$ and neglecting all terms of order $\theta - \theta_*$ we arrive at the isothermal damped Hamiltonian system

$$\dot{Y} = \big(L(Y, \theta_*) - \frac{1}{\theta_*} K(Y, \theta_*)\big) \mathrm{D} \mathscr{F}_*(Y). \tag{2.17}$$

Note that L still defines a Poisson structure and that K is positive semi-definite. Hence, $\mathscr{F}_*$ is a Liapunov function for (2.17).

The error term $\theta - \theta_*$ can only be neglected, if the temperature equation keeps this term small. The heat equation reads

$$\dot{\theta} = \underbrace{-\alpha^{\mathsf{T}} \mathrm{D}_Y \mathscr{F}^\circ(Y, \theta)}_{\text{latent heat prod.}} \underbrace{- \frac{1}{\theta_*} \beta^{\mathsf{T}} \mathrm{D}_Y \mathscr{F}^\circ(Y, \theta)}_{\text{diss. heat prod.}} \underbrace{- \frac{1}{\theta_*} \Lambda \mathrm{D}_\theta \mathscr{F}^\circ(Y, \theta)}_{\text{heat conduction}} \underbrace{- A(\theta - \theta_*)}_{\text{heat exchange}} .$$

Clearly, (2.16) implies that the heat conduction term involving $\mathrm{D}_\theta \mathscr{F}^\circ(Y, \theta)$ is small. However, $\mathrm{D}_Y \mathscr{F}^\circ(Y, \theta) = \mathrm{D} \mathscr{F}_*(Y) + O(\|\theta - \theta_*\|)$ will not be small in general. Hence, the assumption $\theta \approx \theta_*$ will only be reasonable, if the latent heating coefficient α and the heat production via dissipation are relatively small compared to the strength of the operator A, which connects the system to the heat bath with the constant temperature θ_*. (We will see in the examples in Section 3 that both, α and β have a prefactor $\frac{1}{\partial_\theta \overline{s}(Y, \theta))} = \frac{\theta}{\partial_\theta \overline{u}(Y, \theta))}$ which is certainly small if the specific heat $\partial_\theta \overline{u}$ is large.)

3 Finite-dimensional examples

3.1 A damped mechanical system

The first example treats a finite-dimensional mechanical system with configuration $q \in \mathbb{R}^m$.The kinetic energy is given by a positive definite mass matrix $M \in \mathbb{R}^{m\times m}$, and the free energy $\overline{\psi} : \mathbb{R}^m \times (0,\infty)$ depends on q and the temperature θ, which is assumed to be the same for the whole mechanical system. The full state space is $\mathscr{X} = \mathrm{T}^*\mathbb{R}^m \times (0,\infty)$ with points $X = (q, p, \theta)$ where $p = M\dot{q}$ is the momentum.

The total energy is $\mathscr{E}(q, p, \theta) = \frac{1}{2}\langle p, M(q)^{-1}p\rangle + \overline{u}(q, \theta)$ with the free energy $\overline{u}(q, \theta) = \overline{\psi}(q, \theta) - \theta\partial_\theta\overline{\psi}(q, \theta)$ and the entropy is $\mathscr{S}(q, p, \theta) = \overline{s}(q, \theta) = -\partial_\theta\overline{\psi}(q, \theta)$. Throughout we assume that the specific heat $\partial_\theta\overline{u}(q, \theta)$ is positive in the region of interest. We now want to construct L and K such that the following mechanical system is obtained. Allowing for a linear mechanical dissipation $D(q, \theta) \in \mathbb{R}^{m\times m}_{>0}$ the momentum balance reads

$$M\ddot{q} + D(q, \theta)\dot{q} + \partial_q\overline{\psi}(q, \theta) = 0. \tag{3.1}$$

The total energy $\mathscr{E}$ must be conserved, which gives, after employing the momentum balance, the relation

$$\dot{\theta}\partial_\theta\overline{u}(q, \theta) = \langle D(q, \theta)\dot{q} + \theta\partial_\theta\partial_q\overline{\psi}(q, \theta), \dot{q}\rangle = \langle D(q, \theta)M^{-1}p - \theta\partial_q s(q, \theta), M^{-1}p\rangle. \tag{3.2}$$

We construct suitable structures $\overline{L}$ and $\overline{K}$ in the form

$$\overline{L}(X) = \begin{pmatrix} 0 & I & 0 \\ -I & 0 & \overline{A}(q, \theta) \\ 0 & -\overline{A}(q, \theta)^\mathsf{T} & 0 \end{pmatrix} \text{ and } \overline{K}(X) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \overline{K}_{pp}(X) & \overline{K}_{p\theta}(X) \\ 0 & \overline{K}_{p\theta}(X)^\mathsf{T} & \overline{K}_{\theta\theta}(X) \end{pmatrix}, \tag{3.3}$$

where

$$\begin{aligned} \overline{A}(q, \theta) &= \frac{1}{\partial_\theta\overline{s}(q, \theta)}\partial_q\overline{s}(q, \theta), \quad \overline{K}_{\theta\theta}(X) = \tfrac{\langle M^{-1}p, D(q,\theta)M^{-1}p\rangle}{\partial_\theta\overline{s}(q,\theta)\partial_\theta\overline{u}(q,\theta)}, \\ \overline{K}_{p\theta}(X) &= \tfrac{-1}{\partial_\theta\overline{s}(q,\theta)}D(q, \theta)M^{-1}p, \quad \overline{K}_{pp}(X) = \tfrac{\partial_\theta\overline{u}(q,\theta)}{\partial_\theta\overline{s}(q,\theta)}D(q, \theta). \end{aligned}$$

Note that the vector $\overline{A}(q, \theta)$ is needed for the exchange of latent heat, which is a reversible effect. Clearly, $\overline{L}\mathrm{D}\overline{\mathscr{S}} \equiv 0$, $\overline{K}\mathrm{D}\overline{\mathscr{E}} \equiv 0$, and $\overline{\mathscr{K}} = \frac{1}{2}\langle\overline{K}\cdot, \cdot\rangle$ satisfies

$$\overline{\mathscr{K}}(X, \xi_q, \xi_p, \xi_\theta) = \tfrac{\partial_\theta\overline{u}(q,\theta)}{2\partial_\theta\overline{s}(q,\theta)}\langle\xi_p - \tfrac{\xi_\theta}{\partial_\theta\overline{u}(q,\theta)}M^{-1}p, D(q, \theta)[\xi_p - \tfrac{\xi_\theta}{\partial_\theta\overline{u}(q,\theta)}M^{-1}p]\rangle \;\geq\; 0.$$

The derivation of this form and the proof that L satisfies the Jacobi identity follows most easily by deriving the general form (2.13). Using the general thermodynamic variable $\tau = T(q, \theta)$ and $Y = (q, p, \tau)$ we have the special GENERIC form

$$\dot{Y} = M_{\mathscr{S}}(Y)L_0(Y)M^*_{\mathscr{S}}(Y)\mathrm{D}\mathscr{E}(Y) + M_{\mathscr{E}}(Y)K_0(Y)M^*_{\mathscr{E}}(Y)\mathrm{D}\mathscr{S}(Y), \tag{3.4}$$

where $\mathscr{E}(q,p,\tau) = \frac{1}{2}\langle q, M(q)^{-1}p\rangle + U(q,\tau)$ and $\mathscr{S}(q,p,\tau) = S(q,\tau)$. The linear operators have the form

$$L_0 = \begin{pmatrix} 0 & I & 0 \\ -I & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad M_{\mathscr{S}} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -\frac{1}{\partial_\tau S}\partial_q \mathscr{S}^\mathsf{T} & 0 & \frac{1}{\partial_\tau S} \end{pmatrix},$$

$$K_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Theta(Y)D(Y) & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_{\mathscr{E}} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -\frac{1}{\partial_\tau U}\partial_q \mathscr{U}^\mathsf{T} & -\frac{1}{\partial_\tau U}(M^{-1}p)^\mathsf{T} & \frac{1}{\partial_\tau U} \end{pmatrix}.$$

We obtain the reversible and irreversible driving forces

$$M^*_{\mathscr{S}}\mathrm{D}\mathscr{E} = \begin{pmatrix} \partial_q U - \frac{\partial_\tau U}{\partial_\tau S}\partial_q S \\ M^{-1}p \\ \frac{\partial_\tau U}{\partial_\tau S} \end{pmatrix} = \begin{pmatrix} \partial_q \overline{\Psi}(q, \Theta(q,\tau)) \\ \dot q \\ \Theta(q,\tau) \end{pmatrix} \text{ and } M^*_{\mathscr{E}}\mathrm{D}\mathscr{S} = \begin{pmatrix} \partial_q S - \frac{1}{\theta}\partial_q U \\ -\frac{1}{\theta}\dot q \\ -1/\theta \end{pmatrix},$$

respectively. Multiplying from the right by $M_{\mathscr{S}}L_0$ and $M_{\mathscr{E}}K_0$ we obtain the equation

$$\dot Y = \begin{pmatrix} \dot q \\ \dot p \\ \dot \tau \end{pmatrix} = \begin{pmatrix} M^{-1}p \\ -\partial_q \overline{\Psi}(q, \Theta(q,\tau)) - D(Y)\dot q \\ -\frac{1}{\partial_\tau S}\langle \partial_q S, \dot q\rangle + \frac{1}{\partial_\tau U}\langle \dot q, D(Y)\dot q\rangle \end{pmatrix},$$

where we have substituted $M^{-1}p$ by $\dot q$ in the third component of the right-hand side. This component contains first a term for the transfer of latent heat and second a term for the heating by viscous damping.

With the given settings it is now easy to check that (3.4) is exactly the same as the system (3.1) and (3.2). Choosing $\tau = u$ we find $\dot u = -\theta \partial_q \widehat{s}(q,u)\cdot \dot q + \dot q \cdot D \cdot \dot q = (\partial_q \overline{\Psi} + D\dot q)\cdot \dot q$, where the right-hand side is the rate of the mechanical work. For $\tau = s$ we find the entropy production $\dot s = \frac{1}{\theta}\dot q \cdot D \cdot \dot q$. Finally, choosing $\tau = \theta$, we recover $\overline{L} = M_{\overline{\mathscr{S}}}L_0 M^*_{\overline{\mathscr{S}}}$ and $\overline{K} = M_{\overline{\mathscr{E}}}K_0 M^*_{\overline{\mathscr{E}}}$ as given above.

3.2 A rheological example

Next we treat a linear elastic element with $q \in \mathbb{R}^m$ and an internal state $z \in \mathbb{R}^n$, which can be generated by combining Kelvin-Voigt elements. All the dissipation is now in the internal variable z. We start with a formulation based on the entropy. The mechanical system of linear differential equations is given in the form

$$M\ddot q + B_{qq}(s)q + B_{qz}(s)z + b_q(s) = 0, \quad V\dot z + B_{qz}(s)^\mathsf{T} q + B_{zz}(s)z + b_z(s) = 0, \tag{3.5}$$

where s is the entropy. This is combined with the total energy

$$\begin{aligned} \widetilde{\mathscr{E}}(q,p,z,s) &= \frac{1}{2}\langle p, M^{-1}p\rangle + \widetilde{u}(q,z,s) \\ \text{with } \widetilde{u}(q,z,s) &= \frac{1}{2}\langle B(s)\tbinom{q}{z}, \tbinom{q}{z}\rangle + \langle b(s), \tbinom{q}{z}\rangle + c(s), \end{aligned} \tag{3.6}$$

which is assumed to be conserved. Here $b = \binom{b_q}{b_z}$ and B is the block matrix $\begin{pmatrix} B_{qq} & B_{qz} \\ B_{qz}^\top & B_{zz} \end{pmatrix}$, which is assumed to be positive definite. Moreover, we assume $\theta = \partial_s \widetilde{u}(q,z,s) > 0$. Inserting (3.5) energy conservation leads to

$$\theta \dot{s} = \dot{s}\, \partial_s \widetilde{u}(q,z,s) = \langle \partial_z \widetilde{u}(q,z,s), V^{-1} \partial_z \widetilde{u}(q,z,s) \rangle = \langle \dot{z}, V\dot{z} \rangle \geq 0. \tag{3.7}$$

Obviously (3.5) contains the driving forces $\partial_q \widetilde{u}(q,z,s)$ and $\partial_z \widetilde{u}(q,z,s)$ in the first and the second equation, respectively. By (2.8) we have $\partial_q \widetilde{u}(q,z,s) = \partial_q \overline{\Psi}(q,z,\Theta(q,z,s))$, which is the correct driving force for reversible variables. However, as we have emphasized above (and will do again below, see Section 4.2) the latter driving force for the irreversible variable z should be better expressed in derivatives of the free entropy $\overline{\eta}$, namely the form $\partial_q \overline{\eta}(q,z,\Theta(q,z,s)) = -\frac{1}{\Theta(q,z,s)} \partial_q \widetilde{u}(q,z,s)$ by (2.12). However, in the present special case the difference is just a factor θ, which can be compensated for in V.

We write the above system in the special GENERIC form of Section 2.4 with $X = (q,p,z,\tau) \in \mathscr{X} = \mathrm{T}\mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}$, where τ is an arbitrary thermodynamic variable and

$$L_0 = \begin{pmatrix} 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad K_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \theta V^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.8}$$

with $\theta = \Theta(q,z,\tau)$. Using $\mathscr{E}(q,p,z,\tau) = \frac{1}{2}\langle p, M^{-1}p \rangle + U(q,z,\tau)$ and $\mathscr{S}(q,p,z,\tau) = S(q,z,\tau)$ and the definitions of $M_{\mathscr{E}}$ and $M_{\mathscr{S}}$ we find the driving forces

$$M_{\mathscr{S}}^*(X)\mathrm{D}\mathscr{E}(X) = \begin{pmatrix} \partial_q U - \theta \partial_q S \\ M^{-1}p \\ \partial_z U - \theta \partial_z S \\ \theta \end{pmatrix} \quad \text{and} \quad M_{\mathscr{E}}^*(X)\mathrm{D}\mathscr{S}(X) = \begin{pmatrix} \partial_q S - \frac{1}{\theta}\partial_q U \\ -\frac{1}{\theta} M^{-1} p \\ \partial_z S - \frac{1}{\theta}\partial_z U \\ 1/\theta \end{pmatrix}$$

and arrive at the evolutionary system

$$\begin{pmatrix} \dot{q} \\ \dot{p} \\ \dot{z} \\ \dot{\tau} \end{pmatrix} = \begin{pmatrix} M^{-1}p \\ \partial_q U - \theta \partial_q S \\ \theta V^{-1}(\partial_z S - \frac{1}{\theta}\partial_z U) \\ -\frac{1}{\partial_\tau S}\langle \partial_q S, \dot{q} \rangle - \frac{1}{\partial_\tau U}\langle \partial_z U, \theta V^{-1}(\partial_z S - \frac{1}{\theta}\partial_z U) \rangle \end{pmatrix}.$$

Clearly, the first three equations are correct. To see that the fourth equation is also the right one, it suffices to choose $\tau = s$. Then $\partial_q S \equiv 0 \equiv \partial_z S$ and $U = \widetilde{u}$, and we arrive at $\dot{s} = \frac{1}{\theta}\langle \partial_z \widetilde{u}, V^{-1} \partial_z \widetilde{u} \rangle$ as in (3.7), which shows that the second law of thermodynamics holds. In fact, the advantage of the general form is that we may also choose $\tau = u$ to obtain (because of $\partial_z U \equiv 0$)

$$\dot{u} = -\theta \langle \partial_q \widehat{s}(q,z,u), \dot{q} \rangle = \langle \partial_q \overline{\Psi}(q,z,\Theta(q,z,u)), \dot{q} \rangle,$$

which shows that the first law of thermodynamics holds (i.e. the internal energy is only changed by changes of the mechanical work, but not by changes of z).

Another important point of the GENERIC structure is that it allows us to introduce more general dissipation mechanisms. Clearly, we could add damping in the form $D(q,z,s)\dot{q}$ to the first equation of (3.5) by simply adding $K_{22} = \theta D$ as second diagonal block for K_0 in (3.8). Yet if we want to have cross-damping in (3.5), then K_0 needs to have off-diagonal blocks in the form

$$K_0 = \theta \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & K_{22} & K_{23} & 0 \\ 0 & K_{23}^\top & K_{33} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Using $\tau = s$ as in (3.5) leads to the nontrivially coupled system

$$M\ddot{q} + \partial_q\widetilde{u}(q,z,s) + K_{22}\dot{q} + K_{23}\partial_z\widetilde{u}(q,z,s) = 0, \quad \dot{z} + K_{23}^\top\dot{q} + K_{33}\partial_z\widetilde{u}(q,z,s) = 0.$$

Without the GENERIC form, it would be much more difficult to find the correct way K_{23} has to occur in both equations. Moreover, it is now easy to derive the equation for $\dot{s}$, $\dot{u}$, and $\dot{\theta}$.

4 GENERIC from for generalized standard materials

We consider a body Ω which is described by the deformation $\boldsymbol{\phi} : \Omega \to \mathbb{R}^d$, the internal state $z : \Omega \to \mathbb{R}^m$, and the temperature $\theta : \Omega \to]0,\infty[$. The reference density $\rho : \Omega \to [0,\infty[$ is assumed to be fixed.

We will consider several thermodynamic densities like the free energy, internal energy, or the entropy defined at every point x in the body. We consider them as functions of x and $(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}, z, \nabla z)$ as well as a generic thermodynamic variable τ like temperature θ, internal energy u, or entropy s.

Before starting the derivation of the balance equations from GENERIC we provide a consistent notation for various differentials and give the definition of $\alpha{*}\delta_w$. After discussing the purely dissipative Penrose-Fife model in Section 4.2, we consider the simple system of thermoviscoelasticity in Section 4.3. The addition of internal variables like plasticity will then be discussed in Section 4.4. We conclude this section by looking at a simplified model with small strains.

To simplify the presentation, we will consistently drop all surface integrals. Whenever we use the divergence theorem we assume that the corresponding surface fluxes vanish by the choice of the boundary conditions. This is consistent with closed systems which are thermally insulated, i.e. they satisfy $\nabla\theta \cdot \nu = 0$ on $\partial\Omega$. Similarly, we assume that $\nabla z \cdot \nu = 0$ for internal variables z. For the deformation $\boldsymbol{\phi}$ we may either assume that $\boldsymbol{\phi} = 0$ on $\Gamma_{\mathrm{Dir}} \subset \partial\Omega$ or that the stresses are 0 on $\Gamma_{\mathrm{Neu}} = \partial\Omega \backslash \Gamma_{\mathrm{Dir}}$.

4.1 Notations of differentials

We will use the following notations for different types of derivatives of densities h and functionals $\mathscr{H}$ given in the form

$$h = H(w, \nabla w, \tau) \quad \text{and} \quad \mathscr{H}(w,\tau) = \int_\Omega H(w(x), \nabla w(x), \tau(x))\,\mathrm{d}x,$$

where w stands for $\boldsymbol{\phi}$, z, or both. The functional derivative $\mathrm{D}_w\mathscr{H}$ is the same as the variational derivative $\delta_w h$, namely

$$\begin{aligned} &\delta_w H \overset{\text{def}}{=} \partial_w H - \mathrm{div}\big(\partial_{\nabla w} H\big), && \delta_\tau H = \partial_\tau H, \\ &\mathrm{D}_w\mathscr{H} = \delta_w H, && \mathrm{D}_\tau\mathscr{H} = \partial_\tau H. \end{aligned}$$

We also need a directional derivative, where the integration by part is not used. For this we write

$$\Delta_w H(w,\nabla w,\tau)[v] \overset{\text{def}}{=} \partial_w H(w,\nabla w,\tau)\cdot v + \partial_{\nabla w} H(w,\nabla w,\tau):\nabla v$$

While the above notions are standard, we now introduce a new notation for variational derivatives. For a scalar function $\alpha : \Omega \to \mathbb{R}$ and h and $\mathscr{H}$ as above we write

$$\alpha*\mathrm{D}_w\mathscr{H}(w,\tau) \overset{\text{def}}{=} \alpha*\delta_w H(w,\nabla w,\tau) \overset{\text{def}}{=} \alpha\partial_w H(w,\nabla w,\tau) - \mathrm{div}\big(\alpha\partial_{\nabla w} H(w,\nabla w,\tau)\big). \tag{4.1}$$

Here the operation "$\alpha*\delta_w$" should be seen as one operator acting on the density H not as a composition of two operations. Clearly we have linearity in α. If H does not depend on ∇w, it is the simple multiplication, but otherwise we have

$$\alpha*\delta_w H = \alpha\,\delta_w H - \nabla\alpha\cdot\partial_{\nabla w} H. \tag{4.2}$$

The last term is only 0 if α is constant of if H does not depend on ∇w. which is not 0 for nonconstant α. In the applications below α will be either θ or $1/\theta$ and we are certainly interested in nonconstant temperature.

The importance of this notion is seen when we consider the relation of $\mathrm{D}_w\mathscr{H} = \delta_w h$ and $\Delta_w h$. The following identities will be useful below:

$$\alpha*\delta_w H\cdot v = \alpha\Delta_w H[v] - \mathrm{div}\big(\alpha v\cdot\partial_{\nabla w} H\big), \tag{4.3a}$$

$$\Longrightarrow \quad \langle \alpha*\mathrm{D}_w\mathscr{H}(w,\tau), v\rangle = \int_\Omega \alpha*\delta_w H\cdot v\,\mathrm{d}x = \int_\Omega \Delta_w H[v]\,\alpha\,\mathrm{d}x. \tag{4.3b}$$

4.2 The phase-field model of Penrose and Fife

The problem of appearing gradients of internal variables was realized first in phase-field models, where $z : \Omega \to \mathbb{R}$ is a phase indicator. A first correct temperature-dependent model was introduced in [PeF90], see also [PeF93] for further discussion of the thermodynamic correctness and [SpZ93] for an analysis giving existence and uniqueness results.

Most often, the Penrose-Fife model is given in the form

$$\dot z = m(z,\theta)\big(k\Delta z - \psi_1'(z) - \frac{\psi_0'(z)}{\theta}\big), \quad c\dot\theta + \psi_0'(z)\dot z \;=\; \mathrm{div}\big(\frac{\kappa(z,\theta)}{\theta^2}\nabla\theta\big), \tag{4.4}$$

which associates with the energy and entropy functionals in the form

$$\begin{aligned} &\mathscr{E}(z,\theta) = \int_\Omega U(z(x),\theta(x))\,\mathrm{d}x && \text{with } U(z,\theta) = c\theta + \psi_0(z), \\ &\mathscr{S}(z,\theta) = \int_\Omega S(z,\nabla z,\tau)\,\mathrm{d}x && \text{with } S(z,\nabla z,\tau) = c\log\theta - \psi_1(z) - \frac{k}{2}|\nabla z|^2. \end{aligned}$$

Since this model does not contain reversible processes, we expect a GENERIC structure in the purely dissipative form $\binom{\dot z}{\dot\theta} = M_{\mathscr{E}} K_0 M_{\mathscr{E}}^* \mathrm{D}\mathscr{S}$. Obviously we find

$$M_{\mathscr{E}} = \begin{pmatrix} 1 & 0 \\ -\frac{\partial_z E}{\partial_\theta E} & \frac{1}{\partial_\theta E} \end{pmatrix} \quad \text{and} \quad K_0(z,\theta) = \begin{pmatrix} m(z,\theta) & 0 \\ 0 & -\operatorname{div}\big(\kappa(z,\theta)\nabla\Box\big) \end{pmatrix},$$

where $\Box$ indicates the position into which the argument has to be inserted. Note that the driving force $M_{\mathscr{E}}^*\mathrm{D}\mathscr{S}$ takes the form

$$M_{\mathscr{E}}^*\mathrm{D}\mathscr{S} = \begin{pmatrix} 1 & -\frac{\partial_z U}{\partial_\theta U} \\ 0 & \frac{1}{\partial_\theta U} \end{pmatrix} \begin{pmatrix} \delta_z S \\ \partial_\theta S \end{pmatrix} = \begin{pmatrix} \delta_z S - \frac{1}{\theta}\partial_z U \\ \frac{1}{\theta} \end{pmatrix},$$

where we used the relation $\partial_\theta S/\partial_\theta U = 1/\theta$.

While the above Penrose-Fife model (4.4) is for the special free energy $\psi = \overline{\psi}(z,\nabla z,\theta) = -c\theta(\log\theta - 1) + \psi_0(z) + \theta\,(\psi_1(z) + \frac{k}{2}|\nabla z|^2)$, we now emphasize that even in the case of a general $\overline{\psi}$ the thermodynamically consistent form is

$$\dot z = m(z,\theta)\delta_z\big(\frac{-\overline{\psi}}{\theta}\big), \quad \dot u + \operatorname{div}\big(\kappa\nabla(1/\theta)\big) = 0.$$

Thus, the driving force of z is given in terms of the *free entropy* $\overline{\eta} = -\overline{\psi}/\theta$, namely $\delta_z\overline{\eta} = \delta_z S - (1/\theta)*\delta_z U$.

Remark 4.1 (Free-energy differentials is not a dissipative driving force)
We emphasize the last point above, since in some works the driving force for z is taken to be $\delta_z\overline{\psi} = \delta_z U - \theta*\delta_z S$. Here we show that this leads to thermodynamic inconsistencies. Hence, we start from

$$\dot z = -\frac{m}{\theta}\delta_z\overline{\psi} = -\frac{m}{\theta}\partial_z\overline{\psi} + \frac{m}{\theta}\operatorname{div}\big(\partial_{\nabla z}\overline{\psi}\big) \neq -\frac{m}{\theta}\partial_z\overline{\psi} + m\operatorname{div}\big(\frac{1}{\theta}\partial_{\nabla z}\overline{\psi}\big). \tag{4.5}$$

If we add the correct first law of thermodynamics, namely

$$\dot u + \operatorname{div}\big(\kappa\nabla(1/\theta)\big) = 0, \tag{4.6}$$

then we can calculate the entropy-balance equation as follows. From $u = \overline{\psi} + \theta s$ we find

$$\dot s = \frac{1}{\theta}\big(\dot u - \Delta_z\overline{\psi}[\dot z]\big) = \frac{1}{\theta}\big(\dot u - \partial_z\overline{\psi}\cdot\dot z - \partial_{\nabla z}\overline{\psi}\cdot\nabla\dot z\big).$$

Eliminating $\partial_z\overline{\psi}$ via (4.5) *we arrive at*

$$\dot s = \operatorname{div}\big(\tfrac{1}{\theta}\kappa\nabla\tfrac{1}{\theta}\big) + \kappa|\nabla\tfrac{1}{\theta}|^2 + \tfrac{\dot z^2}{m} - \tfrac{1}{\theta}\big[\operatorname{div}\big(\partial_{\nabla z}\overline{\psi}\big) + \partial_{\nabla z}\overline{\psi}\cdot\nabla\dot z\big]$$

To check that the second law of thermodynamics holds we need to show that the last term $\frac{1}{\theta}[\ldots]$ can be decomposed into a positive entropy production term and a divergence of an entropy flux. However, this is not possible here. Thus, we cannot even guarantee the integrated version of the second law, viz. $\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S} \geq 0$ along solutions. In the correct equation

(4.4) *the factor* $\frac{1}{\theta}$ *is inside the divergence and the last expression is a divergence (where we used* (4.3a) *with* $\alpha = 1/\theta$*).*

Alternatively the phase-field equation (4.5) *could be complemented by a correct entropy equation, namely*

$$\dot{s} + \tfrac{1}{\theta}\operatorname{div}\big(\kappa\nabla\tfrac{1}{\theta}\kappa\big) = \tfrac{\dot{z}^2}{m} \quad\Longleftrightarrow\quad \dot{s} + \operatorname{div}\big(\tfrac{\kappa}{\theta}\nabla\tfrac{1}{\theta}\big) = \kappa|\nabla\tfrac{1}{\theta}|^2 + \nabla\tfrac{\dot{z}^2}{m} \geq 0.$$

We refer to [Rou10] for the occurrence of such an approach. To check the first law of thermodynamics we calculate

$$\dot{u} = \theta\dot{s} + \Delta_z\overline{\psi}[\dot{z}] = -\operatorname{div}\big(\kappa\nabla\tfrac{1}{\theta}\big) + \operatorname{div}\big(\dot{z}\cdot\partial_{\nabla z}\overline{\psi}\big).$$

Again we find a disturbing term displaying changes of the internal energy induced by changes of the internal variable. However, the term is a divergence and, hence, has the nice feature that the global energy $\mathscr{E}$ *is preserved along solutions.*

4.3 Thermoviscoelasticity in GENERIC form

We first postulate a GENERIC system describing an elastic body with temperature dependence by using the direct modeling of GENERIC systems as described above. We then show that the obtained equations are exactly the classical balance equations for linear momentum and energy. We will stay close to the special GENERIC form in Section 2.4, but we need to change slightly the dissipation structure to obtain viscoelasticity. We refer to Remark 4.2 for more general dissipation mechanisms.

The energy functional $\mathscr{E}$ and the entropy functional $\mathscr{S}$ are given as follows:

$$\begin{aligned}
&\mathscr{E}(\boldsymbol{\phi},\boldsymbol{p},\tau) = \int_\Omega E(x,\boldsymbol{\phi}(x),\nabla\boldsymbol{\phi}(x),\boldsymbol{p}(x),\tau(x))\,\mathrm{d}x\\
&\text{with } E(x,\boldsymbol{\phi},\boldsymbol{F},\boldsymbol{p},\tau) = \frac{1}{2\rho(x)}|\boldsymbol{p}|^2 + U(x,\boldsymbol{F},\tau) - \boldsymbol{f}_{\mathsf{vol}}(x)\cdot\boldsymbol{\phi},\\
&\mathscr{S}(\boldsymbol{\phi},\boldsymbol{p},\tau) = \int_\Omega S(x,\nabla\boldsymbol{\phi}(x),\tau(x))\,\mathrm{d}x,
\end{aligned}$$

where ρ is the fixed density in the reference configuration and $\boldsymbol{f}_{\mathsf{vol}}$ is a volume force. For notational simplicity we will not write the explicit dependence on $x \in \Omega$ in the sequel. In principle, we may have more complicated dependence of E on $\boldsymbol{\phi}$ (like for centrifugal forces), but then S may also depend on $\boldsymbol{\phi}$.

We use a variant of the special GENERIC form (2.13) for $X = (\boldsymbol{\phi},\boldsymbol{p},\tau)$, namely

$$\dot{X} = M_{\mathscr{S}}L_0M_{\mathscr{S}}^*\mathrm{D}\mathscr{E} + N_{\mathscr{E}}K_0N_{\mathscr{E}}^*\mathrm{D}\mathscr{S}, \tag{4.7}$$

where we use the following simple structures:

$$L_0 = \begin{pmatrix} 0 & I & 0\\ -I & 0 & 0\\ 0 & 0 & 0\end{pmatrix}, \quad K_0 = \operatorname{diag}(0, K_{\mathsf{visco}}, K_{\mathsf{heat}}). \tag{4.8}$$

Here K_{visco} contains the viscoelastic terms, and K_{heat} gives the heat conduction with $K_{\mathsf{heat}}1 \equiv 0$. We will specify these operators below.

We recall the definition of $M_{\mathscr{S}}$, and its adjoints from Section 2.4 to obtain

$$M_{\mathscr{S}} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -\frac{1}{\partial_\tau S}\Delta_{\boldsymbol{\phi}} S[\square] & 0 & \frac{1}{\partial_\tau S} \end{pmatrix} \text{ and } M^*_{\mathscr{S}} = \begin{pmatrix} I & 0 & -(\frac{\square}{\partial_\tau S}) * \delta_{\boldsymbol{\phi}} S \\ 0 & I & 0 \\ 0 & 0 & \frac{1}{\partial_\tau S} \end{pmatrix}, \qquad (4.9)$$

where "$\square$" indicates where the argument should be inserted. For $N_{\mathscr{E}}$ we use

$$N_{\mathscr{E}} = \begin{pmatrix} I & 0 & 0 \\ 0 & -\operatorname{div} & 0 \\ -\frac{1}{\partial_\tau U}\Delta_{\boldsymbol{\phi}} \boldsymbol{E}[\square] & -\frac{1}{\partial_\tau U}\nabla \partial_{\boldsymbol{p}} E{:}\square & \frac{1}{\partial_\tau U} \end{pmatrix} \text{ and } N^*_{\mathscr{E}} = \begin{pmatrix} I & 0 & -(\frac{\square}{\partial_\tau U}) * \delta_{\boldsymbol{\phi}} E \\ 0 & \nabla & -\frac{\square}{\partial_\tau U}\dot{\boldsymbol{F}} \\ 0 & 0 & \frac{1}{\partial_\tau U} \end{pmatrix}.$$

It is important here to note that $N_{\mathscr{E}}$ maps $\mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R}$ into $\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$, i.e. the second column needs a matrix in $\mathbb{R}^{d\times d}$ as an argument, whereas the second row produces a vector in $\mathbb{R}^d$. Similarly, $N^*_{\mathscr{E}}$ converts a vector into a matrix. Moreover, as was already done in $N^*_{\mathscr{E}}$, we will continue to use $\dot{\boldsymbol{F}}$ as the shorthand for $\nabla \partial_{\boldsymbol{p}} E = \nabla(\frac{1}{\rho}\boldsymbol{p}) = \nabla \dot{\boldsymbol{\phi}}$.

As in Section 2.4 we obtain the orthogonality relations from

$$M^*_{\mathscr{S}}(X)\mathrm{D}\mathscr{S}(X) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \text{ and } N^*_{\mathscr{E}}(X)\mathrm{D}\mathscr{E}(X) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \in \mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R}.$$

More importantly, the driving forces are given by

$$M^*_{\mathscr{S}}\mathrm{D}\mathscr{E} = \begin{pmatrix} \delta_{\boldsymbol{\phi}} E - \theta * \delta_{\boldsymbol{\phi}} S \\ \frac{1}{\rho}\boldsymbol{p} \\ \theta \end{pmatrix} \quad \text{and} \quad N^*_{\mathscr{E}}\mathrm{D}\mathscr{S} = \begin{pmatrix} \delta_{\boldsymbol{\phi}} S - (1/\theta) * \delta_{\boldsymbol{\phi}} U \\ -\frac{1}{\theta}\dot{\boldsymbol{F}} \\ 1/\theta \end{pmatrix}.$$

Inserting this together with (4.8) and the definitions of $M_{\mathscr{S}}$ and $N_{\mathscr{E}}$ into (4.7) we find

$$\begin{pmatrix} \dot{\boldsymbol{\phi}} \\ \dot{\boldsymbol{p}} \\ \dot{\tau} \end{pmatrix} = \begin{pmatrix} \frac{1}{\rho}\boldsymbol{p} \\ -\big(\delta_{\boldsymbol{\phi}} U - \theta * \delta_{\boldsymbol{\phi}} S\big) - \operatorname{div}\Big(K_{\mathsf{visco}}\big(\frac{-1}{\theta}\dot{\boldsymbol{F}}\big)\Big) \\ \frac{-1}{\partial_\tau S}\Delta_{\boldsymbol{\phi}} S[\frac{1}{\rho}\boldsymbol{p}] - \frac{1}{\partial_\tau U}\dot{\boldsymbol{F}}{:}K_{\mathsf{visco}}\big(\frac{-1}{\theta}\dot{\boldsymbol{F}}\big) + \frac{1}{\partial_\tau U}K_{\mathsf{heat}}\big(\frac{1}{\theta}\big) \end{pmatrix} \qquad (4.10)$$

Using $\partial_{\boldsymbol{\phi}} S \equiv 0$ the first term in the third component is $\frac{-1}{\partial_\tau S}\Delta_{\boldsymbol{\phi}} S[\frac{1}{\rho}\boldsymbol{p}] = \frac{-1}{\partial_\tau S}\partial_{\boldsymbol{F}} S{:}\dot{\boldsymbol{F}}$.

We now show that (4.10) really provides the classical equations of thermoviscoelasticity, if we choose K_{visco} and K_{heat} as follows

$$K_{\mathsf{visco}}\boldsymbol{A} = \theta \boldsymbol{\Lambda}\boldsymbol{A} \quad \text{and} \quad K_{\mathsf{heat}}\alpha = -\operatorname{div}\big(\widetilde{\kappa}\nabla\alpha\big),$$

where $\boldsymbol{\Lambda}$ is a positive (semi) definite viscosity operator of fourth order (which may depend on $\boldsymbol{F} = \nabla\boldsymbol{\phi}$ and θ) and $\widetilde{\kappa}$ is a positive definite heat conduction matrix (which may also depend on $\boldsymbol{F}$ and θ). Eliminating $\boldsymbol{p}$ from the first component in (4.10) yields

$$\begin{aligned} \rho\ddot{\boldsymbol{\phi}} &= -\boldsymbol{f}_{\mathsf{vol}} + \operatorname{div}\big(\partial_{\boldsymbol{F}} U - \theta\partial_{\boldsymbol{F}} S + \boldsymbol{\Lambda}\dot{\boldsymbol{F}}\big), \\ \partial_\tau U\,\dot{\tau} &= \big(-\theta\partial_{\boldsymbol{F}} S + \boldsymbol{\Lambda}\dot{\boldsymbol{F}}\big){:}\dot{\boldsymbol{F}} + \operatorname{div}\big(\tfrac{\widetilde{\kappa}}{\theta^2}\nabla\theta\big). \end{aligned}$$

To find the classical form we choose $\tau = \theta$, which gives $U = \overline{u} = \overline{\psi} - \theta\partial_\theta\overline{\psi}$, $S = \overline{s} = -\partial_\theta\overline{\psi}$. We are lead to the classical system for thermoviscoelasticity, viz.

$$\rho\ddot{\boldsymbol{\phi}} = -\boldsymbol{f}_{\mathrm{vol}} + \mathrm{div}\,\big(\partial_{\boldsymbol{F}}\overline{\psi} + \boldsymbol{\Lambda}\dot{\boldsymbol{F}}\big), \quad \theta\dot{s} = \dot{\boldsymbol{F}}{:}\boldsymbol{\Lambda}\dot{\boldsymbol{F}} + \mathrm{div}\,\big(\tfrac{\widetilde{\kappa}}{\theta^2}\nabla\theta\big), \tag{4.11}$$

where we used $s = -\partial_\theta\overline{\psi}(\boldsymbol{F},\theta)$ giving $\dot{s} = -\partial_\theta^2\overline{\psi}(\boldsymbol{F},\theta)\dot{\theta} - \partial_\theta\partial_{\boldsymbol{F}}\overline{\psi}(\boldsymbol{F},\theta){:}\dot{\boldsymbol{F}}$. More discussion on the thermodynamic correctness (first and second law of thermodynamics) is given in the following subsection, where plasticity is included as well.

Remark 4.2 (Different viscous dampings) *One may wonder why it is necessary to use the operator $N_{\mathscr{E}}$ instead of $M_{\mathscr{E}}$ for the dissipation structure. Here we shortly give the differences obtained from using $M_{\mathscr{E}}$. The damping will be different, but still consistent with thermodynamics. We now define $K(X) = M_{\mathscr{E}}\widetilde{K}_0 M_{\mathscr{E}}^*$ with*

$$M_{\mathscr{E}} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -\frac{1}{\partial_\tau U}\Delta_{\boldsymbol{\phi}}\boldsymbol{E}[\Box] & -\frac{1}{\partial_\tau U}\partial_{\boldsymbol{p}}E^{\mathsf{T}} & \frac{1}{\partial_\tau U} \end{pmatrix} \text{ and } M_{\mathscr{E}}^* = \begin{pmatrix} I & 0 & -(\frac{\Box}{\partial_\tau U})*\delta_{\boldsymbol{\phi}}E \\ 0 & I & -\frac{\Box}{\partial_\tau U}\dot{\boldsymbol{\phi}} \\ 0 & 0 & \frac{1}{\partial_\tau U} \end{pmatrix},$$

where we continue to use $\dot{\boldsymbol{\phi}}$ in place of $\partial_{\boldsymbol{p}}E = \frac{1}{\rho}\boldsymbol{p}$. Note that $M_{\mathscr{E}}$ and $M_{\mathscr{E}}^*$ take a vector in $\mathbb{R}^d$ as the argument for the second column. For $\widetilde{K}_0$ we use the block-diagonal operator

$$\widetilde{K}_0 = \mathrm{diag}(0, \widetilde{K}_{\mathit{visco}}, K_{\mathit{heat}}) \;\; \text{with } \widetilde{K}_{\mathit{visco}}\boldsymbol{v} = \frac{\theta}{2}\boldsymbol{v}{\cdot}\boldsymbol{\Lambda}_0{\cdot}\boldsymbol{v} + \frac{\theta}{2}\nabla\boldsymbol{v}{:}\boldsymbol{\Lambda}_1{:}\nabla\boldsymbol{v}.$$

With this choice the first equation of the classical system (4.11) *turns into*

$$\rho\ddot{\boldsymbol{\phi}} = -\boldsymbol{f}_{\mathit{vol}} + \mathrm{div}\,\big(\partial_{\boldsymbol{F}}\overline{\psi}\big) - \boldsymbol{\Lambda}_0\dot{\boldsymbol{\phi}} + \mathrm{div}\,\big(\theta\boldsymbol{\Lambda}_1\nabla(\tfrac{1}{\theta}\dot{\boldsymbol{\phi}})\big).$$

While the term with $\boldsymbol{\Lambda}_0$ gives classical linear damping, the term involving $\boldsymbol{\Lambda}_1$ expands into $\mathrm{div}\,\big(\boldsymbol{\Lambda}_1(\dot{\boldsymbol{F}} + \frac{1}{\theta}\nabla\theta\otimes\dot{\boldsymbol{\phi}})\big)$, where the last term seems to be quite unusual in the modeling of viscous solids.

4.4 GENERIC formulation for Generalized Standard Materials

We proceed as in the previous section but now we allow for an additional internal variable z, which occurs in the internal energy and the entropy together with its gradient ∇z. Thus, this section generalizes the isothermal theory for a large class of dissipative solids (also called generalized standard materials), see e.g. [ZiW87, Hac97, Mie06]. A general nonisothermal treatment doesn't seem to be available.

We consider functionals of the form

$$\mathscr{E}(\boldsymbol{\phi},\boldsymbol{p},z,\tau) = \int_\Omega E(x,\boldsymbol{\phi}(x),\nabla\boldsymbol{\phi}(x),\boldsymbol{p}(x),z(x),\nabla z(x),\tau(x))\,\mathrm{d}x$$

$$\text{with } E(x,\boldsymbol{\phi},\boldsymbol{F},\boldsymbol{p},z,A\tau) = \frac{1}{2\rho(x)}|\boldsymbol{p}|^2 + U(x,\boldsymbol{F},z,A,\tau) - \boldsymbol{f}_{\mathrm{vol}}(x){\cdot}\boldsymbol{\phi},$$

$$\mathscr{S}(\boldsymbol{\phi},\boldsymbol{p},z,\tau) = \int_\Omega S(x,\nabla\boldsymbol{\phi}(x),z(x),\nabla z(x),\tau(x))\,\mathrm{d}x,$$

To include viscoelasticity, we use the same slight variant of the special GENERIC form (2.13) as in the previous subsection. For $X = (\boldsymbol{\phi}, \boldsymbol{p}, z, \tau)$ we consider

$$\dot{X} = M_{\mathscr{S}}(X)L_0 M^*_{\mathscr{S}}(X)\mathrm{D}\mathscr{E}(X) + N_{\mathscr{E}}\partial_\xi \mathscr{K}_0(X; N^*_{\mathscr{E}}(X)\mathrm{D}\mathscr{S}(X)), \tag{4.12}$$

where now $\partial_\xi \mathscr{K}_0$ is the subdifferential of a general entropy-production potential $\mathscr{K}_0$ replacing the linear operator K_0. To handle viscoelastic, thermoplastic materials we choose $\mathscr{K}_0$ to contain viscoelastic effects, plastic dissipation, and heat conduction in the form

$$\mathscr{K}_0(X; \zeta_{\boldsymbol{\phi}}, \zeta_{\boldsymbol{p}}, \zeta_z, \zeta_\tau) = \mathscr{K}_{\mathsf{visc}}(X; \zeta_{\boldsymbol{p}}) + \mathscr{K}_{\mathsf{plast}}(X; \zeta_z) + \mathscr{K}_{\mathsf{heat}}(X; \zeta_\tau), \tag{4.13a}$$

where the viscous and the heat part are as above, namely

$$\mathscr{K}_{\mathsf{visc}}(X; \zeta_{\boldsymbol{p}}) = \int_\Omega \theta \zeta_{\boldsymbol{p}} \mathbin{:} \boldsymbol{\Lambda} \zeta_{\boldsymbol{p}} \,\mathrm{d}x \quad \text{and} \quad \mathscr{K}_{\mathsf{heat}}(X; \zeta_\tau) = \int_\Omega \nabla \zeta_\tau \cdot \widetilde{\kappa} \nabla \zeta_\tau \,\mathrm{d}x,$$

where we recall that $\zeta_{\boldsymbol{p}} \in \mathbb{R}^{d\times d}$ is a matrix, which associates with $\dot{\boldsymbol{F}}$.

The new part is the plastic entropy production, which is not a quadratic functional. The primal plastic entropy-production potential is assumed to have the form

$$\mathscr{G}_{\mathsf{plast}}(X, \dot{z}) = \int_\Omega G_{\mathsf{plast}}(x, \boldsymbol{F}(x), z(x), \tau(x); \dot{z}(x)) \,\mathrm{d}x,$$

where $G_{\mathsf{plast}}(\ldots; \dot{z})$ is typically of the form

$$G_{\mathsf{plast}}(\ldots; \dot{z}) = G_1(\ldots; \dot{z}) + \frac{1}{2}\dot{z} \mathbin{:} \mathbb{G}(\ldots) \mathbin{:} \dot{z}.$$

Here the symmetric and positive definite tensor $\mathbb{G}$ models viscoplastic effects, whereas $G_1(\ldots, \cdot)$ models the rate-independent plasticity, because it is positively homogeneous of degree 1, i.e. $G_1(\ldots; \gamma\dot{z}) = \gamma G_1(\ldots; \dot{z})$ for all $\gamma > 0$. The simplest form is $G_1(\ldots; \dot{z}) = \frac{1}{\theta}\sigma_{\mathsf{yield}}(\ldots)|\dot{z}|$, where the yield stress σ_{yield} may depend on $(\boldsymbol{F}, z, \theta)$. The dual entropy-production potential $\mathscr{K}_{\mathsf{plast}}$ is obtained by Legendre-Fenchel transform, which can be done independently for each $x \in \Omega$. With $K_{\mathsf{plast}}(\ldots; \cdot) = G^*_{\mathsf{plast}}(\ldots; \cdot)$ we obtain

$$\mathscr{K}_{\mathsf{plast}}(X; \xi_z) = \int_\Omega K_{\mathsf{plast}}(x, \boldsymbol{F}(x), z(x), \tau(x); \xi_z(x)) \,\mathrm{d}x.$$

We now build the GENERIC system in the form (4.12) with $\mathscr{K}_0$ from above,

$$L_0 = \begin{pmatrix} 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad M_{\mathscr{S}} = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ -\frac{1}{\partial_\tau S}\Delta_{\boldsymbol{\phi}} S[\Box] & 0 & -\frac{1}{\partial_\tau S}\Delta_z S[\Box] & \frac{1}{\partial_\tau S} \end{pmatrix}, \tag{4.13b}$$

and the modified operator $N_{\mathscr{E}}$ defined as

$$N_{\mathscr{E}} = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & -\operatorname{div} & 0 & 0 \\ 0 & 0 & I & 0 \\ -\frac{1}{\partial_\tau U}\Delta_{\boldsymbol{\phi}} \boldsymbol{E}[\Box] & -\frac{1}{\partial_\tau U}\nabla \partial_{\boldsymbol{p}} E \mathbin{:} \Box & -\frac{1}{\partial_\tau U}\Delta_z \boldsymbol{E}[\Box] & \frac{1}{\partial_\tau U} \end{pmatrix}. \tag{4.13c}$$

By construction we have $M^*_{\mathscr{S}}\mathrm{D}\mathscr{S} = (0,0,0,1)^\mathsf{T}$ and $N^*_{\mathscr{E}}\mathrm{D}\mathscr{E} = (0,0,0,1)^\mathsf{T}$ and the noninteraction conditions (2.4) hold. Moreover, we find the driving forces

$$M^*_{\mathscr{S}}\mathrm{D}\mathscr{E} = \begin{pmatrix} \delta_{\boldsymbol{\phi}} U - \theta * \delta_{\boldsymbol{\phi}} S \\ \frac{1}{\rho}\boldsymbol{p} \\ \delta_z U - \theta * \delta_z S \\ \theta \end{pmatrix} \quad \text{and} \quad N^*_{\mathscr{E}}\mathrm{D}\mathscr{S} = \begin{pmatrix} \delta_{\boldsymbol{\phi}} S - \frac{1}{\theta} * \delta_{\boldsymbol{\phi}} U \\ -\frac{1}{\theta}\dot{\boldsymbol{F}} \\ \delta_z S - \frac{1}{\theta} * \delta_z U \\ 1/\theta \end{pmatrix},$$

where again $\dot{\boldsymbol{F}}$ was used as abbreviation for $\nabla \partial_{\boldsymbol{p}} E$. Inserting this together with (4.13) into (4.12) we arrive at

$$\begin{pmatrix} \dot{\boldsymbol{\phi}} \\ \dot{\boldsymbol{p}} \\ \dot{z} \\ \dot{\tau} \end{pmatrix} = \begin{pmatrix} \frac{1}{\rho}\boldsymbol{p} \\ -\big(\delta_{\boldsymbol{\phi}} U - \theta * \delta_{\boldsymbol{\phi}} S\big) + \partial_{\zeta_{\boldsymbol{p}}} \mathscr{K}_{\mathsf{visc}}(\ldots; -\frac{1}{\theta}\dot{\boldsymbol{F}}) \\ \partial_\zeta \mathscr{K}_{\mathsf{plast}}\big(\ldots; \delta_z S - \frac{1}{\theta} * \delta_z U\big) \\ \frac{-\Delta_{\boldsymbol{\phi}} S[\frac{1}{\rho}\boldsymbol{p}]}{\partial_\tau S} + \frac{\dot{\boldsymbol{F}}:\boldsymbol{\Lambda}:\dot{\boldsymbol{F}}}{\partial_\tau U} - \frac{1}{\partial_\tau U}\Delta_z U\big[\partial_\zeta K_{\mathsf{plast}}\big(\ldots; \delta_z S - \frac{1}{\theta} * \delta_z U\big)\big] + \frac{1}{\partial_\tau U}\partial_{\zeta_\tau} \mathscr{K}_{\mathsf{heat}}\big(\frac{1}{\theta}\big) \end{pmatrix}.$$

This model provides a thermodynamically consistent system for thermoviscoelastic viscoplasticity, or more generally for general dissipative solids.

We now discuss the form of the latter system in more detail. The first two components can be written as the usual balance of linear momentum in the form

$$\rho \ddot{\boldsymbol{\phi}} = \mathrm{div}\, \boldsymbol{\Sigma}_{\mathsf{elast}} - \boldsymbol{f}_{\mathsf{vol}} \quad \text{with } \boldsymbol{\Sigma}_{\mathsf{elast}} = \partial_{\boldsymbol{F}} U - \theta \partial_{\boldsymbol{F}} S + \Lambda \dot{\boldsymbol{F}}. \tag{4.14}$$

The third component gives the plastic flow law, which can be rewritten using the primal entropy-production potential G_{plast} in the two equivalent forms

$$\dot{z} = \partial_\zeta K_{\mathsf{plast}}\big(\ldots; \delta_z S - \frac{1}{\theta} * \delta_z U\big) \quad \Longleftrightarrow \quad 0 \in \partial_{\dot{z}} G_{\mathsf{plast}}(\ldots; \dot{z}) + \frac{1}{\theta} * \delta_z U - \delta_z S. \tag{4.15}$$

Finally, the last component gives the energy-entropy balance. To check the first and second law, we choose $\tau = u$ and $\tau = s$, respectively.

First law of thermodynamics. For the case $\tau = u$ we use that $S(w,u) = \widehat{s}(w,u)$ gives $\partial_u \widehat{s} = 1/\theta$ and $\theta \partial_w \widehat{s}(w,u) = -\partial_w \overline{\psi}(w, \widehat{\theta}(w,u))$. Thus we have

$$\dot{u} = \big(\partial_{\boldsymbol{F}} \overline{\psi} + \dot{\boldsymbol{F}}:\boldsymbol{\Lambda}\big):\dot{\boldsymbol{F}} - \mathrm{div}\,\big(\widetilde{\kappa}\nabla(1/\theta)\big).$$

The first term on the right-hand side is $\boldsymbol{\Sigma}_{\mathsf{elast}}:\dot{\boldsymbol{F}}$ and represents the rate of the mechanical work, while the second term is the divergence of the heat flux. Thus, the first law of thermodynamics holds in its local form, as the internal energy is not influenced by changes of the internal variable z. Moreover, we easily obtain the conservation of the total energy $\mathscr{E}$ by using (4.14) and the divergence theorem.

Second law of thermodynamics. For the case $\tau = s$ we have the relation $u = \widetilde{u}(w,s)$, which provides $\theta = \partial_s\widetilde{u}$ and $\partial_w\widetilde{u}(w,s) = \partial_w\overline{\psi}(w,\widetilde{\theta}(w,s))$. Thus we find the relation

$$\dot{s} = \frac{1}{\theta}\dot{\boldsymbol{F}}{:}\boldsymbol{\Lambda}{:}\dot{\boldsymbol{F}} - \frac{1}{\theta}\Delta_z\widetilde{u}[\dot{z}] - \frac{1}{\theta}\operatorname{div}\big(\widetilde{\kappa}\nabla(1/\theta)\big).$$

The last term on the right-hand side is reformulated routinely as

$$-\tfrac{1}{\theta}\operatorname{div}\big(\widetilde{\kappa}\nabla\tfrac{1}{\theta})\big) = \nabla\tfrac{1}{\theta}\cdot\widetilde{\kappa}\cdot\nabla\tfrac{1}{\theta} - \operatorname{div}\big(\tfrac{1}{\theta}\widetilde{\kappa}\nabla\tfrac{1}{\theta}\big),$$

which gives a positive entropy-production term plus a divergence term. The second term on the right-hand side can be reformulated similarly, because multiplying (4.15) by $\dot{z}$ yields

$$\dot{z}\cdot\partial_{\dot{z}}G_{\mathsf{plast}}(\dots,\dot{z}) = -\frac{1}{\theta}{*}\delta_z\widetilde{u}\cdot\dot{z} = -\Delta_z\widetilde{u}[\dot{z}] + \operatorname{div}(\frac{1}{\theta}\dot{z}\cdot\partial_{\nabla z}\widetilde{u}),$$

where we used the identity (4.3a) with $\alpha = 1/\theta$. We find

$$-\frac{1}{\theta}\Delta_z\widetilde{u}[\dot{z}] = \dot{z}\cdot\partial_{\dot{z}}G_{\mathsf{plast}}(\dots,\dot{z}) - \operatorname{div}(\frac{1}{\theta}\dot{z}\cdot\partial_{\nabla z}\widetilde{u}).$$

Thus, defining the entropy flux $\boldsymbol{h}_{\mathsf{entr}} = \frac{1}{\theta}\dot{z}\cdot\partial_{\nabla z}\widetilde{u} + \frac{1}{\theta}\widetilde{\kappa}\nabla\frac{1}{\theta}$ yields

$$\dot{s} - \operatorname{div}\boldsymbol{h}_{\mathsf{entr}} = \sigma_{\mathsf{prod}}^{\mathsf{entr}} \geq 0 \quad \text{with } \sigma_{\mathsf{prod}}^{\mathsf{entr}} = \tfrac{1}{\theta}\big(\dot{\boldsymbol{F}}{:}\boldsymbol{\Lambda}{:}\dot{\boldsymbol{F}} + \dot{z}\cdot\partial_{\dot{z}}G_{\mathsf{plast}}(\dots,\dot{z})\big) + \nabla\tfrac{1}{\theta}\cdot\widetilde{\kappa}\cdot\nabla\tfrac{1}{\theta},$$

where $\sigma_{\mathsf{prod}}^{\mathsf{entr}}$ is the entropy-production rate.

Summarizing we find the increase of the total entropy in the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(X(t)) = \int_\Omega \sigma_{\mathsf{prod}}^{\mathsf{entr}}\,\mathrm{d}x = \langle \mathrm{D}(X), \mathscr{K}(X;\mathrm{D}\mathscr{S}(X))\rangle,$$

where the dual entropy-production potential $\mathscr{K}$ is given in terms of $\mathscr{K}_0$ and $N_{\mathscr{E}}$ as follows:

$$\begin{aligned}\mathscr{K}(X;\xi_{\boldsymbol{\phi}},\xi_{\boldsymbol{p}},\xi_z,\xi_\tau) &= \mathscr{K}_0(X;N_{\mathscr{E}}(X)(\xi_{\boldsymbol{\phi}},\xi_{\boldsymbol{p}},\xi_z,\xi_\tau)^{\mathsf{T}})\\ &= \mathscr{K}_0\big(X;\nabla\xi_{\boldsymbol{p}} - \tfrac{\xi_\tau}{\partial_\tau U}\dot{\boldsymbol{F}}, \xi_z - \tfrac{\xi_\tau}{\partial_\tau U}{*}\delta_z U, \tfrac{\xi_\tau}{\partial_\tau U}\big)\end{aligned} \tag{4.16}$$

4.5 Small-strain thermoelastoplasticity

As an example of the above theory we consider the well-established small-strain case. This means that instead of the deformation $\boldsymbol{\phi}$ we consider the displacement $\boldsymbol{u} : x \mapsto \boldsymbol{\phi}(x) - x$. Moreover, the relevant strain measure is the linearized strain tensor $\mathbf{e} = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^{\mathsf{T}})$, which replaces $\boldsymbol{F} = \nabla\boldsymbol{\phi}$ used above. Finally the plastic variables includes the plastic strain tensor $\boldsymbol{\pi}(x) \in \mathbb{R}^{d\times d}_{\mathrm{dev}} := \{A \in \mathbb{R}^{d\times d} \,|\, A = A^{\mathsf{T}},\ \operatorname{tr} A = 0\}$. For simplicity we restrict ourselves to kinematic hardening where no further plastic variable is needed. However, the theory works equally well, if further variables like hardening parameters are included. We refer to [BaR08, BaR10] and the references therein for thermoelastoplastic models with small strains. There, existence results for the fully coupled system are derived for linearized elastoplasticity.

The classical modeling uses the variables $X = (\boldsymbol{u}, \boldsymbol{p}, \boldsymbol{\pi}, \theta)$ and the free energy in the form (2.10), namely

$$\overline{\psi}(\mathbf{e}, \boldsymbol{\pi}, \theta) = -c\theta(\log\theta - 1) + \frac{1}{2}(\mathbf{e}-\boldsymbol{\pi}){:}\mathbb{C}{:}(\mathbf{e}-\boldsymbol{\pi}) + \frac{1}{2}\boldsymbol{\pi}{:}\mathbb{H}{:}\boldsymbol{\pi} + \theta\mathbb{A}{:}\mathbf{e}, \tag{4.17}$$

where $\mathbb{C}$, $\mathbb{H}$, and $\mathbb{A}$ are the elasticity tensor, the kinematic hardening tensor, and the thermal expansion tensor, respectively. The first are assumed to be uniformly positive definite and all of them may be bounded measurable functions on Ω. According to Example 2.2 we obtain the functionals

$$\overline{\mathscr{E}}(X) = \int_\Omega \frac{1}{2\rho}|\boldsymbol{p}|^2 + c\theta + \frac{1}{2}(\mathbf{e}-\boldsymbol{\pi}){:}\mathbb{C}{:}(\mathbf{e}-\boldsymbol{\pi}) + \frac{1}{2}\boldsymbol{\pi}{:}\mathbb{H}{:}\boldsymbol{\pi}\,\mathrm{d}x, \quad \overline{\mathscr{S}}(X) = \int_\Omega c\log\theta - \mathbb{A}{:}\mathbf{e}\,\mathrm{d}x.$$

The Poisson structure $\overline{L}(X)$ takes the form as is $M_{\overline{\mathscr{S}}} L_0 M^*_{\overline{\mathscr{S}}}$ with L_0 from (4.13b). We obtain the latent-heat transfer operator $\overline{\mathscr{A}}(X)\xi_\theta = \mathrm{div}\big(\frac{\theta\xi_\theta}{c}\mathbb{A}\big)$, where we used $\partial_\theta\overline{s} = c/\theta$ and $\partial_{\mathbf{e}}\overline{s} = \mathbb{A}$. Using the heat capacity $\partial_\theta\overline{u} = c$ the dual entropy-production potential takes the form

$$\begin{aligned}\overline{\mathscr{K}}(X; \xi_{\boldsymbol{u}}, \xi_{\boldsymbol{p}}, \xi_{\boldsymbol{\pi}}, \xi_\theta) = \int_\Omega & \tfrac{\theta}{2}\big(\nabla\xi_{\boldsymbol{p}} - \tfrac{\xi_\theta}{c}\dot{\mathbf{e}}\big){:}\Lambda_{\mathsf{vis}}(\mathbf{e}, \boldsymbol{\pi}, \theta){:}\big(\nabla\xi_{\boldsymbol{p}} - \tfrac{\xi_\theta}{c}\dot{\mathbf{e}}\big)\\ &+ K_{\mathsf{plast}}\big(\mathbf{e}, \boldsymbol{\pi}, \theta; \xi_{\boldsymbol{\pi}} - \tfrac{\xi_\theta}{c}\boldsymbol{\Sigma}_{\mathsf{pl}}\big) + \tfrac{\theta^2\kappa(\mathbf{e},\boldsymbol{\pi},\theta)}{2}\big|\nabla\tfrac{\xi_\theta}{c}\big|^2\,\mathrm{d}x,\end{aligned}$$

where $\boldsymbol{\Sigma}_{\mathsf{pl}} \overset{\mathsf{def}}{=} \partial_{\boldsymbol{\pi}}\overline{u} = \mathbb{C}(\boldsymbol{\pi}-\mathbf{e}) + \mathbb{H}\boldsymbol{\pi}$. As a conclusion we see that the reversible part of the generalized GENERIC system $\dot{X} = \overline{L}(X)\mathrm{D}\overline{\mathscr{E}}(X) + \partial_\xi\overline{\mathscr{K}}(X, \mathrm{D}\overline{\mathscr{S}}(X))$ is given by

$$\overline{L}\mathrm{D}\overline{\mathscr{E}} = \begin{pmatrix} 0 & I & 0 & 0\\ -I & 0 & 0 & \overline{\mathscr{A}}(X)\\ 0 & 0 & 0 & 0\\ 0 & -\overline{\mathscr{A}}(X)^* & 0 & 0\end{pmatrix}\begin{pmatrix} -\mathrm{div}\big(\mathbb{C}(\mathbf{e}-\boldsymbol{\pi})\big)\\ \frac{1}{\rho}\boldsymbol{p}\\ \mathbb{C}(\boldsymbol{\pi}-\mathbf{e}) + \mathbb{H}\boldsymbol{\pi}\\ c\end{pmatrix} = \begin{pmatrix}\dot{\boldsymbol{u}}\\ \mathrm{div}\big(\mathbb{C}(\mathbf{e}-\boldsymbol{\pi}) + \theta\mathbb{A}\big)\\ 0\\ \frac{\theta}{c}\mathbb{A}{:}\dot{\mathbf{e}}\end{pmatrix}..$$

Using $\mathrm{D}\overline{\mathscr{S}}(X) = (\mathrm{div}\,\mathbb{A}, 0, 0, c/\theta)$, the entropic part is

$$\partial_\xi\overline{\mathscr{K}}(X, \mathrm{D}\overline{\mathscr{S}}(X)) = \begin{pmatrix} 0\\ \mathrm{div}\big(\Lambda_{\mathsf{vis}}\dot{\mathbf{e}}\big)\\ \partial_\zeta K_{\mathsf{plast}}(\mathbf{e}, \boldsymbol{\pi}, \theta; -\frac{1}{\theta}\boldsymbol{\Sigma}_{\mathsf{pl}})\\ \frac{1}{c}\dot{\mathbf{e}}{:}\Lambda_{\mathsf{vis}}\dot{\mathbf{e}} - \frac{1}{c}\partial_\zeta K_{\mathsf{plast}}(\ldots; -\frac{1}{\theta}\boldsymbol{\Sigma}_{\mathsf{pl}}){:}\boldsymbol{\Sigma}_{\mathsf{pl}} + \frac{1}{c}\mathrm{div}\big(\kappa\nabla\theta\big)\end{pmatrix}.$$

Clearly, we obtain the classical equations for thermoelastoplasticity with temperature as the thermodynamics independent variable, see [BaR08, BaR10].

5 Quasistatic models as entropy-driven systems

We first treat the quasistatic approximation first on the abstract level and then apply it to thermoviscoplasticity. We restrict to the case that there is no viscoelastic damping, since otherwise the analysis gets much more involved.

5.1 The abstract quasistatic limit

We consider a GENERIC systems for $X=(q,p,z,\tau)$ with total energy and entropy $\mathscr{E}(X)=\frac{1}{2\varepsilon}\langle M^{-1}p,p\rangle+\Phi(q,z,\tau)$ and $\mathscr{S}(X)=\mathscr{S}(q,z,\tau)$. In the quasistatic limit we neglect inertia terms by assuming that the density $\rho=\varepsilon$, which then is sent to 0. Thus, p will be eliminated.

We use the abbreviation $w=(z,\tau)$ and consider a GENERIC system where L and K have the block structures

$$L(X)=\begin{pmatrix} 0 & I & 0 \\ -I & 0 & A(q,w) \\ 0 & -A(q,w)^* & 0 \end{pmatrix},\quad K(X)=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & K_{ww}(q,w) \end{pmatrix}.$$

Assuming that K has only one block clearly excludes viscoelasticity, but it allows for thermoviscoplasticity.

For the quasistatic limit we assume $p=O(\varepsilon)$ and are left with the equations

$$0=-\mathrm{D}_q\Phi(q,w)+A(q,w)\mathrm{D}_w\Phi(q,w),\quad \dot w=-A(q,w)^*\dot q+K_{ww}(q,w)\mathrm{D}_w\mathscr{S}(q,w). \tag{5.1}$$

We first observe that solutions $t\mapsto(q(t),w(t))$ of this systems satisfy $\Phi(q(t),w(t))\equiv$ const., where we use the GENERIC structure condition $K\mathrm{D}\mathscr{E}\equiv 0$, viz. $K_{ww}\mathrm{D}_w\Phi\equiv 0$:

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\Phi(q(t),w(t)) &= \langle \mathrm{D}_q\Phi,\dot q\rangle+\langle \mathrm{D}\Phi_w,\dot w\rangle \\ &= \langle \mathrm{D}_q\Phi,\dot q\rangle+\langle \mathrm{D}\Phi_w,-A(q,w)^*\dot q+K_{ww}\mathrm{D}_w\mathscr{S}(q,w)\rangle \\ &= \langle \mathrm{D}_q\Phi-A(q,w)\mathrm{D}\Phi_w,\dot q\rangle+\langle K_{ww}\mathrm{D}\Phi_w,\mathrm{D}_w\mathscr{S}(q,w)\rangle=0+0.\end{aligned}$$

(We may also assume to have a driven system in the form $\mathscr{E}_{\mathsf{driv}}(t,X)=\mathscr{E}(X)-\langle\ell(t),q\rangle$, then we find $\frac{\mathrm{d}}{\mathrm{d}t}\Phi(q(t),w(t))=-\langle\dot\ell(t),q\rangle$.)

We now assume that the static equation $0=-\mathrm{D}_q\Phi(q,w)+A(q,w)\mathrm{D}_w\Phi(q,w)$ can be solved (at least locally) in the form $q=Q(w)$ and define the quasistatic, reduced entropy function $\mathscr{S}^{\mathsf{qs}}$ via $\mathscr{S}^{\mathsf{qs}}(w)\overset{\text{def}}{=}\mathscr{S}(Q(w),w)$. For its differential we have

$$\mathrm{D}\mathscr{S}^{\mathsf{qs}}(w)=\mathrm{D}Q(w)^*\mathrm{D}_q\mathscr{S}(Q(w),w)+\mathrm{D}_w\mathscr{S}(Q(w),w)=(I+B(w))^*\mathrm{D}_w\mathscr{S}(Q(w),w)$$

with $B(w)\overset{\text{def}}{=}A(Q(w),w)^*\mathrm{D}Q(w)$, where we have used $L\mathrm{D}\mathscr{S}\equiv 0$. Thus, the second equation in (5.1) gives $\dot w=-B(w)\dot w+K_{ww}\mathrm{D}_w\mathscr{S}$, and we find the desired entropy-driven system

$$\dot w=K^{\mathsf{qs}}(w)\mathrm{D}\mathscr{S}^{\mathsf{qs}}(w),\quad \text{where } K^{\mathsf{qs}}(w)=(I+B(w))^{-1}K_{ww}(Q(w),w)(I+B(w))^{-*}. \tag{5.2}$$

If we start from a generalized GENERIC system, where K is not a linear operator, we can proceed the same way by using the dual entropy-production potential $\mathscr{K}:(q,w,\xi_w)\mapsto\mathscr{K}(q,w;\xi_w)$. As above,the final equation for w is the generalized gradient system

$$\dot w=\partial_\mu\mathscr{K}^{\mathsf{qs}}(w;\mathrm{D}\mathscr{S}^{\mathsf{qs}}(w)),\quad \text{where } \mathscr{K}^{\mathsf{qs}}(w;\mu)\overset{\text{def}}{=}\mathscr{K}(Q(w),w;(I+B(w))^{-*}\mu). \tag{5.3}$$

Defining the reduced energy functional Φ_{red} via $\Phi_{\mathrm{red}}(w)\overset{\text{def}}{=}\Phi(Q(w),w)$ and using $\mathrm{D}\Phi_{\mathrm{red}}(w)=(I+B(w))^*\mathrm{D}_w\Phi(Q(w),w)$ we obtain from $\mathscr{K}(q,w;\zeta+\lambda\mathrm{D}_w\Phi(q,w))=\mathscr{K}(q,w;\zeta)$ the noninteraction condition

$$\mathscr{K}^{\mathsf{qs}}(w;\mu+\lambda\mathrm{D}\Phi_{\mathrm{red}}(w))=\mathscr{K}^{\mathsf{qs}}(w;\mu).$$

This confirms that Φ_{red} is constant along solutions of (5.3).

5.2 Quasistatic small-strain thermoviscoplasticity

Our aim is to derive a generalized gradient structure for quasistatic small-strain thermoviscoplasticity, where the entropy $\mathscr{S}$ is the driving functional, i.e. the state W evolves according to

$$\dot{W} = \partial_\zeta \Psi^*(W, +\mathrm{D}\mathscr{S}(W)) \iff 0 \in \partial_{\dot{W}} \Psi(W, \dot{W}) - \mathrm{D}\mathscr{S}(W).$$

We follow that abstract approach from the previous subsection for a thermoviscoplastic system as given in Subsection 4.5, but without viscoelasticity, i.e. $\mathbf{\Lambda} = 0$. We start with the thermodynamic variable $\tau = s$, such that $\mathscr{A} \equiv 0$. We consider the situation of Section 4.5 with displacement $\boldsymbol{u} : \Omega \to \mathbb{R}^d$, small strains $\mathbf{e}(\boldsymbol{u})$, and the plastic variable $z = \boldsymbol{\pi}$. The entropy and potential energy are

$$\widetilde{\mathscr{S}}(\boldsymbol{u}, z, s) = \int_\Omega s \,\mathrm{d}x \;\text{ and }\; \widetilde{\Phi}(\boldsymbol{u}, z, s) = \int_\Omega \widetilde{u}(\mathbf{e}(\boldsymbol{u}), \boldsymbol{\pi}, s) \,\mathrm{d}x,$$

where we assume that $\widetilde{u}$ depends strictly convex on $\mathbf{e}$, which holds for the case given in (4.17) after doing the transformation in Example 2.2. In the quasistatic setting the elastic displacement $\boldsymbol{u}$ is minimized out such that $\boldsymbol{u} = Q(\boldsymbol{\pi}, s) = \mathrm{argmin}\{\, \widetilde{\Phi}(\boldsymbol{u}, \boldsymbol{\pi}, s) \,|\, \boldsymbol{u} \in \mathrm{H}^1_0(\Omega) \,\}$. The solution is unique since the integrand of $\widetilde{\Phi}$ is uniformly convex in $\mathbf{e}$. This solution solves the (static) equilibrium of linear momentum, since $\delta_{\boldsymbol{u}} \overline{\psi} = \delta_{\boldsymbol{u}} \widetilde{u}$ because of $\delta_{\boldsymbol{u}} \widetilde{s} \equiv 0$.

From the dual entropy-production potential (4.16) for $\tau = s$ and with $\mathbf{\Lambda} = 0$ we derive the quasistatic dual potential $\widetilde{\mathscr{K}}^{\mathsf{qs}}$ via (5.3) and $B \equiv 0$ as follows:

$$\widetilde{\mathscr{K}}^{\mathsf{qs}}(z, s; \xi_{\boldsymbol{\pi}}, \xi_s) = \textstyle\int_\Omega K_{\mathsf{plast}}(\ldots; \xi_{\boldsymbol{\pi}} - \frac{\xi_s}{\theta} \partial_{\boldsymbol{\pi}} \widetilde{u}) + \frac{\theta^2 \kappa}{2} \big|\nabla(\frac{\xi_s}{\theta})\big|^2 \,\mathrm{d}x,$$

where $\theta = \partial_s \widetilde{u}(\mathbf{e}(Q(\boldsymbol{\pi}, s)), \boldsymbol{\pi}, s)$. Together with $\widetilde{\mathscr{S}}^{\mathsf{qs}}(\boldsymbol{\pi}, s) = \widetilde{\mathscr{S}}(0, 0, s) = \int_\Omega s \,\mathrm{d}x$, this defines the generalized gradient system for $(\boldsymbol{\pi}, s)$, namely

$$\begin{pmatrix} \dot{\boldsymbol{\pi}} \\ \dot{s} \end{pmatrix} = \mathrm{D}_\mu \widetilde{\mathscr{K}}^{\mathsf{qs}}(..; \tbinom{0}{1}) = \begin{pmatrix} \partial_\zeta K_{\mathsf{plast}}(.., -\frac{1}{\theta} \partial_{\boldsymbol{\pi}} \widetilde{u}(..)) \\ \partial_\zeta K_{\mathsf{plast}}(..; -\frac{1}{\theta} \partial_{\boldsymbol{\pi}} \widetilde{u}(..)) : (-\partial_{\boldsymbol{\pi}} \widetilde{u}(..)) + \frac{1}{\theta} \operatorname{div}\big(\kappa \nabla \theta\big) \end{pmatrix}. \tag{5.4}$$

The structure of the equation reveals that the first equation is the plastic flow rule, while the entropy balance shows the entropy production and flux through plastic changes and through heat conduction.

Often the formulation in terms of $w = (\boldsymbol{\pi}, \theta)$ is more desirable. This is easily obtained by using the transformation $(\boldsymbol{\pi}, s) = (z, \overline{s}(\mathbf{e}, \boldsymbol{\pi}, \theta))$, where $\mathbf{e} = \mathbf{e}(\boldsymbol{u})$ is now obtained as a function of $(\boldsymbol{\pi}, \theta)$ via solving the static balance of linear momentum $0 = \delta_{\boldsymbol{u}} \overline{\psi} = \delta_{\boldsymbol{u}} \overline{u} - \theta {*} \delta_{\boldsymbol{u}} \overline{s}$.

For simplicity we now assume that $\overline{\psi}$ is given in the form (4.17). Then, the equation for $\boldsymbol{u}$ reads $0 = \mathrm{div}(\mathbb{C}(\mathbf{e}(\boldsymbol{u}) - \boldsymbol{\pi}) + \theta \mathbb{A})$. Thus, the dependence $\boldsymbol{u} = Q(\boldsymbol{\pi}, \theta)$ is linear. More specifically, we define the bounded linear operator $\mathscr{L}$ mapping $\mathrm{L}^2(\Omega; \mathbb{R}^{d \times d})$ into itself via solving $0 = \mathrm{div}(\mathbb{C}\mathbf{e}(\boldsymbol{u}) - \mathbb{M})$ for $\boldsymbol{u}_{\mathbb{M}}$ as a linear function of $\mathbb{M}$ and then setting $\mathscr{L}\mathbb{M} \overset{\mathsf{def}}{=} \mathbf{e}(\boldsymbol{u}_{\mathbb{M}})$. Obviously, $\mathscr{L}$ is a symmetric, nonlocal pseudo-differential operator of order 0 and satisfies the positivity relation

$$\int_\Omega \mathbb{M} : \mathscr{L}\mathbb{M} \,\mathrm{d}x = \int_\Omega \mathscr{L}\mathbb{M} : \mathbb{C} : \mathscr{L}\mathbb{M} \,\mathrm{d}x \geq 0.$$

With this construction the unique solution $\boldsymbol{u} = Q(\boldsymbol{\pi},\theta)$ satisfies $\mathbf{e}(\boldsymbol{u}) = \mathscr{L}(\mathbb{C}\boldsymbol{\pi} - \theta\mathbb{A})$.

Thus, we obtain the reduce entropy functional

$$\overline{\mathscr{S}}^{\mathsf{qs}}(\boldsymbol{\pi},\theta) = \int_\Omega c\log\theta + \mathbb{A}{:}\mathscr{L}(\theta\mathbb{A}) - \mathbb{A}{:}\mathscr{L}(\mathbb{C}\boldsymbol{\pi})\,\mathrm{d}x.$$

To transform the generalized gradient system $(\widetilde{\mathscr{S}}^{\mathsf{qs}},\widetilde{\mathscr{K}}^{\mathsf{qs}})$, see (5.4), from the variables $(\boldsymbol{\pi},s)$ into $(\boldsymbol{\pi},\theta)$ we use the derivative derivative

$$\mathrm{D}\binom{z}{\overline{s}}(\boldsymbol{\pi},\theta) = \begin{pmatrix} I & 0 \\ -\mathbb{A}{:}\mathscr{L}(\mathbb{C}\Box) & c/\theta + \mathbb{A}{:}\mathscr{L}(\Box\mathbb{A}) \end{pmatrix}.$$

The lower diagonal element defines a symmetric and invertible operator, because of $\int_\Omega \frac{c}{\theta}\beta^2 + \beta\mathbb{A}{:}\mathscr{L}(\beta\mathbb{A})\,\mathrm{d}x \geq \int_\Omega \frac{c}{\theta}\beta^2\,\mathrm{d}x > 0$. We denote the inverse operator by $\mathscr{B}_\theta$ and define

$$N^*(\boldsymbol{\pi},\theta) \overset{\mathsf{def}}{=} \mathrm{D}\binom{\boldsymbol{\pi}}{\overline{s}}(\boldsymbol{\pi},\theta)^{-*} = \begin{pmatrix} I & \mathbb{C}\mathscr{L}(\mathscr{B}_\theta\Box\mathbb{A}) \\ 0 & \mathscr{B}_\theta \end{pmatrix}.$$

With this we obtain the transformed dual entropy-production potential

$$\begin{aligned}\overline{\mathscr{K}}^{\mathsf{qs}}(\boldsymbol{\pi},\theta:\zeta_{\boldsymbol{\pi}},\zeta_\theta) &= \widetilde{\mathscr{K}}\big(\boldsymbol{\pi},\overline{s}(..);N^*(\boldsymbol{\pi},\theta)\big(\begin{smallmatrix}\zeta_\pi\\ \zeta_z\end{smallmatrix}\big)\big) = \widetilde{\mathscr{K}}\big(\boldsymbol{\pi},\overline{s}(..);\zeta_{\boldsymbol{\pi}} - \mathbb{C}\mathscr{L}(\mathscr{B}_\theta\zeta_\theta\mathbb{A}),\mathscr{B}_\theta\zeta_\theta\big) \\ &= \textstyle\int_\Omega K_{\mathsf{plast}}\big(\ldots;\zeta_z - \mathbb{C}\mathscr{L}(\mathscr{B}_\theta\zeta_\theta\mathbb{A}) - \frac{\mathscr{B}_\theta\zeta_\theta}{\theta}\partial_{\boldsymbol{\pi}}\widetilde{u}\big) + \frac{\kappa}{2}\big|\nabla\big(\frac{\mathscr{B}_\theta\zeta_\theta}{\theta}\big)\big|^2\,\mathrm{d}x.\end{aligned}$$

Thus, we have successfully derived the quasistatic generalized gradient system $(\overline{\mathscr{S}}^{\mathsf{qs}},\overline{\mathscr{K}}^{\mathsf{qs}})$ for the variables $(\boldsymbol{\pi},\theta)$, namely

$$\begin{pmatrix}\dot{\boldsymbol{\pi}}\\ \dot{\theta}\end{pmatrix} = \partial_{\boldsymbol{\xi}}\overline{\mathscr{K}}^{\mathsf{qs}}\big(\boldsymbol{\pi},\theta;\mathrm{D}\overline{\mathscr{S}}^{\mathsf{qs}}(\boldsymbol{\pi},\theta)\big) = \begin{pmatrix}\partial_{\boldsymbol{\xi}_\pi}\overline{\mathscr{K}}^{\mathsf{qs}}\big(\boldsymbol{\pi},\theta;\mathrm{D}\overline{\mathscr{S}}^{\mathsf{qs}}(\boldsymbol{\pi},\theta)\big)\\ \partial_{\boldsymbol{\xi}_\theta}\overline{\mathscr{K}}^{\mathsf{qs}}\big(\boldsymbol{\pi},\theta;\mathrm{D}\overline{\mathscr{S}}^{\mathsf{qs}}(\boldsymbol{\pi},\theta)\big)\end{pmatrix}.$$

Unfortunately, the nonlocal operators $\mathscr{L}$ and $\mathscr{B}_\theta$ make the analysis of the system quite involved.

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