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Free energy, free entropy, and a gradient structure for thermoplasticity

Dedicated to Michael Ortiz on the occasion of his sixtieth birthday

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ABSTRACT

In the modeling of solids the free energy, the energy, and the entropy play a central role. We show that the free entropy, which is defined as the negative of the free energy divided by the temperature, is similarly important. The derivatives of the free energy are suitable thermodynamical driving forces for reversible (i.e. Hamiltonian) parts of the dynamics, while for the dissipative parts the derivatives of the free entropy are the correct driving forces. This difference does not matter for isothermal cases nor for local materials, but it is relevant in the non-isothermal case if the densities also depend on gradients, as is the case in gradient thermoplasticity.

Using the total entropy as a driving functional, we develop gradient structures for quasistatic thermoplasticity, which again features the role of the free entropy. The big advantage of the gradient structure is the possibility of deriving time-incremental minimization procedures, where the entropy-production potential minus the total entropy is minimized with respect to the internal variables and the temperature.

We also highlight that the usage of an auxiliary temperature as an integrating factor in [YSO06] serves exactly the purpose to transform the reversible driving forces, obtained from the free energy, into the needed irreversible driving forces, which should have been derived from the free entropy. This reconfirms the fact that only the usage of the free entropy as driving functional for dissipative processes allows us to derive a proper variational formulation.

1 Introduction

The mathematical theory of plasticity has its origin in the 1970s based on the work Moreau [Mor74], Johnson [Joh76], and Gröger [Grö78], which treated the small-strain case with quadrtic energies and fixed elastic domains. They developed a rich theory based on convex analysis and monotone operators which allowed for significant generalizations, but still staying in the small-strain regime, see e.g. [Alb98]. Finite-strain elastoplasticity also plays a fundamental role in engineering applications, and many algorithms were derived starting in the 1980s, see e.g. [SiO85, MiS92]. A major breakthrough was the discovery in [OrR99, OrS99] that incremental problems in finite-strain elastoplasticity can be formulated as minimization problems jointly for the elastic and the plastic updates. This means that elastoplasticity can be formulated in terms of a generalized gradient system with a dissipation potential $\mathcal{R}$ and a free energy $\mathcal{F}$ such that it reads

$$\mathrm{D}_u \mathcal{F}(t, u, z) = 0, \quad 0 \in \partial_{\dot{z}} \mathcal{R}(u, z; \dot{z}) + \mathrm{D}_z \mathcal{F}(t, u, z),$$

where u is the displacement, and z contains all internal (dissipative) variables. This theory even led to the first mathematical existence results for the rate-independent case, see [GM*06, MaM09, MiR15].

However, the whole theory remained restricted to the isothermal case, and it remains a challenging problem to find a corresponding mechanical and mathematical theory for thermoplasticity. The major difference arises from the fact, that the mechanics is quite

different. In the isothermal case there is one free energy, and time-incremental minimization procedures can be formulated by minimizing the sum of the free energy plus the dissipation in the time step. In the non-isothermal case one has to take care of the mechanical forces still given by the free energy, but instead of dissipation one now has to model entropy production. A time-incremental minimization procedure should involve the entropy production minus the total entropy. A first step in this direction was done in [YSO06], and here we connect our work [Mie11a, Mie11b] with the latter.

The major observation is that one has to formulate thermoplasticity in a suitable thermodynamically consistent way, in order to recast it in variational form. For this, we start from the GENERIC framework (General Equations for Non-Equilibrium Reversible Irreversible Coupling) providing the form (cf. [Mie11a])

$$\rho \ddot{u} = -\big(D_u \mathcal{E}(q) - \Theta * D_u \mathcal{S}(q)\big) \qquad = -D_u \overline{\mathcal{F}}(u, z, \Theta(u, z, r)),$$

$$\dot{z} = \partial_{\xi_z} \mathcal{P}_z^* \big(q, D_z \mathcal{S}(q) - \frac{1}{\Theta} * D_z \mathcal{E}(q)\big) \quad = \partial_{\xi_z} \mathcal{P}_z^* \big(q, D_z \overline{\mathcal{H}}(u, z, \Theta(u, z, r))\big),$$

$$\dot{r} = -\frac{\Delta_u S(q)[\dot{u}]}{\partial_r S(q)} - \frac{\Delta_z E(q)[\dot{z}]}{\partial_r E(q)} - \frac{1}{\partial_r E} \operatorname{div}\Big(\kappa(q) \nabla \frac{\partial_r S}{\partial_r E}\Big),$$

where $\overline{\mathcal{F}}$ and $\overline{\mathcal{H}}$ are the total free energy and total free entropy expresses in terms of the temperature $\theta = \Theta(u, z, r)$, where r is an arbitrary scalar thermodynamic variable, such that Gibbs' relation $\theta = \Theta(u, z, r) = \frac{D_r \mathcal{E}(u, z, r)}{D_r \mathcal{S}(u, z, r)}$ holds.

The above form clearly shows the role of the free energy as the driving functional for the reversible elastodynamics, while the free entropy

$$\overline{\mathcal{H}}(u, z, \theta) = \int_\Omega \overline{H}(u, \nabla u, z, \nabla z, \theta) \, dx \quad \text{with } H(W, \theta) = \frac{-S(W, \theta)}{\theta}$$

is the driving functional for the dissipative variables z (like the plastic tensor or the hardening variables). Locally the free entropy is simply given as 'minus the free energy divided by the temperature', but for functional derivatives, which involve integration by parts, new terms appear and the naive relation $D_z \overline{\mathcal{H}}(u, z, \theta) = -\frac{1}{\theta} D_z \overline{\mathcal{F}}(u, z, \theta)$ may be wrong. More precisely we have

$$D_z \overline{\mathcal{H}}(u, z, \theta) = -\frac{1}{\theta} D_z \overline{\mathcal{F}}(u, z, \theta) + \partial_{\nabla z} \overline{F}(u, \nabla u, z, \nabla z, \theta) \nabla\big(\frac{1}{\theta}\big).$$

The last term vanishes in two important cases: (i) in the isothermal case where $\nabla \theta \equiv 0$ and (ii) in the case "local case" where $\overline{F}$ does not depend on ∇z. In these two cases, it is correct to use the derivative of the free energy and put the factor θ into the dual entropy-production potential (thus turning it into a dual dissipation potential). However, in all other cases, one has to distinguish the free energy and the free entropy as driving functionals. Moreover, the inverse tmeperature $1/\theta$ is the driving force for heat transfer:

driving force for revers. dynamics: $D_u \overline{\mathcal{F}}(u, z, \theta) = D_u E(u, z, r) - \Theta(u, z, r) * D_u S(u, z, r),$

driving force for dissip. dynamics: $D_z \overline{\mathcal{H}}(u, z, \theta) = D_z S(u, z, r) - \frac{1}{\Theta(u, z, r)} * D_z E(u, z, r),$

driving force for energy transport: $1/\theta = 1/\Theta(u, z, r) = \frac{\partial_r S(u, z, r)}{\partial_r E(u, z, r)}.$

An important fact is that the terms on the right-hand side are independent of the choice of the thermodynamical variable r, see Theorem 3.3, which gives a great flexibility in the mathematical approaches.

Turning to the quasistatic case, we drop the interia term $\rho\ddot{u}$ and rewrite the remaining system in the form

$$
\begin{aligned}
0 &= \mathrm{D}_u\mathcal{E}(q) - A(q)\mathrm{D}_r\mathcal{E}(q), \qquad \dot{z} = \partial_{\eta_z}\mathcal{P}_Z^*\Big(q; \mathrm{D}_z\mathcal{S}(q) - B(q)\mathrm{D}_r\mathcal{S}(q)\Big), \\
\dot{r} &= -A(q)^*\dot{u} - B(q)^*\dot{z} - C(q)^*\operatorname{div}\big(\kappa(q)\nabla(C(q)\mathrm{D}_r S(q))\big) \text{ with} \\
A(q)\xi_r &= \Big(\tfrac{\xi_r}{\mathrm{D}_r\mathcal{S}(q)}\Big)*\mathrm{D}_u\mathcal{S}(q), \quad B(q)\xi_r = \Big(\tfrac{\xi_r}{\mathrm{D}_r\mathcal{E}(q)}\Big)*\mathrm{D}_z\mathcal{E}(q), \quad C(q)\xi_r = \tfrac{\xi_r}{\mathrm{D}_r\mathcal{E}(q)}.
\end{aligned}
\tag{1.1}
$$

Assuming that the first relation, which is static, can be solved in the form $u = \mathrm{U}(z,r)$, Theorem 3.4 shows that this system can be formulated as a gradient system as follows

$$
\begin{pmatrix} \dot{z} \\ \dot{r} \end{pmatrix} = \partial_{\boldsymbol{\xi}}\mathfrak{P}^*\big(z,r;\mathrm{D}\mathfrak{S}(z,r)\big) \text{ with } \mathfrak{S}(z,r) = \mathcal{S}(\mathrm{U}(z,r),z,r),
$$

where $\mathfrak{P}^*$ is a suitably reduced dual entropy-production potential, and the reduced energy $\mathfrak{E}(z,r) = \mathcal{E}(\mathrm{U}(z,r),z,r)$ is conserved.

In general, this gradient structure is highly nonlocal, where $\mathfrak{P}^*$ involves the derivatives $\mathrm{D}_z\mathrm{U}(z,r)$ and $\mathrm{D}_r\mathrm{U}(z,r)$, and thus less useful. However, in the case $A(u,z,r) \equiv 0$, which occurs for a choice of r such that $\mathrm{D}_u\mathcal{S}(u,z,r) \equiv 0$, one obtains a system that allows for local approaches. Thus, the freedom of choosing r as freely as possible is essential. For that case, we propose the time-incremental minimization procedure

$$
\begin{aligned}
\begin{pmatrix} z^{k+1} \\ r^{k+1} \end{pmatrix} &\in \operatorname*{Arg\,min}_{(z,r)} \Big\{ \tau\,\mathcal{P}\Big(q^k; \tfrac{1}{\tau}\begin{pmatrix} z-z^k \\ r-r^k \end{pmatrix}\Big) - \mathcal{S}(u^k,z,r) \Big\}, \\
u^{k+1} &\in \operatorname*{Arg\,min}_{u}\mathcal{E}(u,z^{k+1},r^{k+1}),
\end{aligned}
\tag{1.2}
$$

where $\mathcal{P}$ is the primal entropy-production potential obtained from $\mathcal{P}^*(u,z,r;\xi_z,\xi_r) = \mathcal{P}_Z^*(q;\xi_z - B(q)\xi_r) + \tfrac{1}{2}\int_\Omega \nabla(C(q)\xi_r)\cdot\kappa(q)\nabla(C(q)\xi_r)\,\mathrm{d}x$ by Legendre-Fenchel transform.

We discuss the abstract along specific thermomechanical examples. The simplest is a spring-damper system, see Examples 3.5 and 3.7. Section 4.1 discusses the Penrose-Fife model and shows how in [MiS15] the gradient structure is exploited to do a rigorous homogenization, where the effective entropy functional is obtained by averaging of the free energy density. Section 4.2 treats a time-dependent thermoplastic model where the gradient structure in terms of the entropy involves a time-dependent entropy-production because of the elimination $u(t) = \mathbf{U}(z(t),\ell(t))$, where ℓ is the mechanical loading. Finally, a plastic model with thermal expansion is considered in Section 4.3.

For all these models we need a specific and problem-dependent choice of the thermodynamic variable r, which highlights the importance of a clear modeling in terms of the free energy and free entropy giving the driving forces $\mathrm{D}_u E(u,z,r) - \Theta(u,z,r)*\mathrm{D}_u S(u,z,r)$, $\mathrm{D}_z S(u,z,r) - \tfrac{1}{\Theta(u,z,r)}*\mathrm{D}_z E(u,z,r)$, and $1/\theta = \tfrac{\partial_r S(u,z,r)}{\partial_r E(u,z,r)}$.

2 Heat equation as a starting example

As a first example we treat the heat equation with energy density e and heat flux $\mathbf{q}$:

$$
\dot{e} + \operatorname{div}\mathbf{q} = 0 \quad \text{in } \Omega, \qquad \mathbf{q}\cdot n = 0 \text{ on } \partial\Omega.
$$

Subsequently, we will drop all boundary conditions (like $\mathbf{q} \cdot n = 0$) and assume that we have no-flux boundary conditions for all quantities, such that the system is thermodynamically closed. We describe the energy density by an arbitrary scalar field r, which may be the energy density e itself, the absolute temperature θ, the coldness $1/\theta$, or the entropy density s. This means that we have constitutive functions

$$\theta = \Theta(r), \quad e = E(r), \quad s = S(r).$$

Of course, by the Gibbs relation $\theta \mathrm{d}s = \mathrm{d}e$ we have the compatibility $\Theta(r) = E'(r)/S'(r)$. Often this last relation is seen as the definition of the temperature. Note that already here the inverse of the absolute temperature plays the role of an integrating factor such that $1/\theta \, \mathrm{d}e$ is the total differential $\mathrm{d}s$, cf. [Car09].

In the classical form of the heat equation, the heat flux $\mathbf{q}$ is a linear function of the temperature gradient, which is called Fourier's law. In terms of r we arrive at

$$E'(r)\dot{r} - \mathrm{div}\big(k(r)\nabla\Theta(r)\big) = 0, \tag{2.1}$$

where $k \in \mathbb{R}^{d \times d}$ is the symmetric and positive definite heat conductivity matrix. However, for a proper coupling to other mechanical effects, we want to have a gradient flow formulation in terms of the total entropy $\mathcal{S}$ as a driving functional, while the total energy $\mathcal{E}$ should be conserved

$$\mathcal{S}(r) = \int_\Omega s(r(x)) \, \mathrm{d}x \quad \text{and} \quad \mathcal{E}(r) = \int_\Omega E(r(x)) \, \mathrm{d}x.$$

Hence, an *entropic gradient structure* must have the form

$$\dot{r} = \mathbb{K}(r)\mathrm{D}\mathcal{S}(r), \tag{2.2}$$

where $\mathbb{K}$ is a selfadjoint positive definite operator that maps the field $\xi_r = \mathrm{D}\mathcal{S}(r)$ to the rate $\dot{r}$, where ξ_r is the thermodynamical driving force associated with r. The operator $\mathbb{K}$ will be called *Onsager operator*, since Onsager showed that such linear operators should be symmetric. Indeed, in [Ons31] the symmetry $\mathbb{K} = \mathbb{K}^*$ is called "reciprocal relation".

The positive semidefiniteness $\langle \xi_r, \mathbb{K}(r)\xi_r \rangle \geq 0$ guarantees that the second law of thermodynamics is satisfied. Note that energy conservation needs the relation $\mathbb{K}(r)\mathrm{D}\mathcal{E}(r) \equiv 0$. Using the variational derivative $\mathrm{D}\mathcal{E}(r) \equiv E'(r)$ we see that the only Onsager operators which are compatible with the usual heat equation (2.1) and the gradient structure (2.2) have the form

$$\mathbb{K}(r)\xi_r = -\frac{1}{E'(r)} \mathrm{div}\Big(\kappa(r)\nabla\big(\frac{\xi_r}{E'(r)}\big)\Big),$$

where $\kappa(r) \in \mathbb{R}^{d \times d}_{\mathrm{spd}}$ still can be chosen suitably.

As a result we see that the heat equation takes the general structure

$$\dot{r} = -\frac{1}{E'(r)} \mathrm{div}\Big(\kappa(r)\nabla\big(\frac{S'(r)}{E'(r)}\big)\Big) = \mathbb{K}(r)\mathrm{D}\mathcal{S}(r),$$

since $\mathrm{D}\mathcal{S}(r) \equiv S'(r)$. In this general form we see that $S'(r)/E'(r) = 1/\Theta(r)$ is the function under the spatial gradient, i.e. the heat flux has the form

$$\mathbf{q} = \kappa(r)\nabla\big(1/\theta\big) = -k\nabla\theta \quad \text{with } \kappa(r) = k(r)\Theta(r)^2.$$

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Thus, we see that κ has to be chosen as $k(r)\Theta(r)^2$. More importantly, we see that the inverse temperature $1/\theta$ is the *driving force for energy flow*, independently of the choice of the scalar thermodynamical variable r.

To connect our theory to the work in [YSO06] we introduce the *dual entropy-production potential (EPP)*, also called kinetic potential there, namely

$$\mathcal{P}^*(r,\xi) := \frac{1}{2}\langle\xi,\mathbb{K}(r)\xi\rangle = \frac{1}{2}\int_\Omega \nabla\Big(\frac{\xi}{E'(r)}\Big)\cdot\kappa(r)\nabla\Big(\frac{\xi}{E'(r)}\Big)\,\mathrm{d}x.$$

By Legendre transform we can also define the (primal) entropy-production potential via

$$\mathcal{R}(r,\dot{r}) = \sup_\xi\langle\xi,\dot{r}\rangle - \mathcal{P}^*(r,\xi) = \sup_\xi\int_\Omega \xi\dot{r} - \frac{1}{2}\nabla\tfrac{\xi}{E'}\cdot\kappa\nabla\tfrac{\xi}{E'}\,\mathrm{d}x,$$

which is nonlocal in $\dot{r}$, since the maximizer is obtained by solving $-\mathrm{div}\big(\kappa\nabla(\xi/E')\big) = \dot{r}E'$.

The gradient flow $\dot{r} = \mathbb{K}(r)\mathrm{D}\mathcal{S}(r)$ can be rewritten in the four fully equivalent forms:

(i) $\dot{r} = \partial_\xi\mathcal{P}^*(r,\mathrm{D}\mathcal{S}(r))$, 　　　　(ii) $\dot{r} = \mathrm{Arg\,min}_v\,\mathcal{P}(r,v) - \langle\mathrm{D}\mathcal{S}(r),v\rangle$,

(iii) $\partial_{\dot{r}}\mathcal{P}(r,\dot{r}) = \mathrm{D}\mathcal{S}(r)$, 　　　　(iv) $\mathrm{D}\mathcal{S}(r) \in \mathrm{Arg\,min}_\xi\,\mathcal{P}^*(r,\xi) - \langle\xi,\dot{r}\rangle$.

Here the equivalence of (i) and (iii) is the Fenchel equivalence for the Legendre transformation, while (ii) and (iv) are simply equivalent to (i) and (iii), respectively, using the convexity of the EPPs $\mathcal{P}$ and $\mathcal{P}^*$. To calculate the rate $\dot{r}$ from the nonlocal minimum principle (ii), the following local inf-sup formulation was introduced in [YSO06]:

$$(\widehat{\xi},\dot{r}) \quad\text{solves}\quad \inf_v\Big(\sup_\xi\big(\langle\xi,v\rangle - \mathcal{R}^*(r,\xi) - \langle\mathrm{D}\mathcal{S}(r),v\rangle\big)\Big).$$

3　Non-isothermal dissipative material models

We now consider general elastic materials with internal parameters describing dissipative effects such as plasticity, phase transformation, damage, magnetization, or polarization, see e.g. [MiR15]. We follow the approach presented in [Mie11a] but do not emphasize the very useful framework GENERIC. This framework stands for *General Equations for Non-Equilibrium Reversible Irreversible Coupling* (cf. [GrÖ97, Ött05]), and highlights the distinction between reversible (i.e. Hamiltonian) and dissipative driving forces.

We consider a body in the reference configuration Ω, which is a bounded domain with Lipschitz boundary. The displacement is denoted by $u : \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$, and $\mathbf{e}(u) = \frac{1}{2}(\nabla u+\nabla u^\mathsf{T})$ is the linearized strain tensor. All the internal variables (also called dissipative variables) are included in the variable $z : \Omega \to \mathbb{R}^m$, which may include plastic strains, phase indicators, or damage variables. By a general scalar field $r : \Omega \to \mathbb{R}$ we describe the thermodynamical properties, e.g. r can be either the temperature θ, the internal energy density e, or the entropy density s.

We consider a closed system, which means that we have no-flux boundary conditions. The total energy and total entropy are given by

$$\mathcal{E}_{\mathrm{kin\text{-}pot}}(u,\dot{u},z,r) = \mathcal{E}_{\mathrm{kin}}(\dot{u}) + \mathcal{E}(u,z,r) \quad\text{and}\quad \mathcal{S}(u,z,r) = \int_\Omega S(\nabla u,z,\nabla z,r)\,\mathrm{d}x$$

where $\mathcal{E}_{\mathrm{kin}}(\dot{u}) := \int_\Omega \frac{\rho}{2}|\dot{u}|^2\,\mathrm{d}x$ and $\mathcal{E}(u,\dot{u},z,r) = \int_\Omega E(u,\nabla u,z,\nabla z,r)\,\mathrm{d}x,$

where the consitutive laws E and S are related by Gibbs' relation $\theta = \Theta(q) := \frac{\partial_r E(q)}{\partial_r S(q)}$.

3.1 Free energy and free entropy as driving functionals

Before we discuss the equations of motions for such material models, we introduce the free energy f and the free entropy s and discuss their role in continuum mechanics:

$$\begin{aligned}\text{free energy } \ f &= e - \theta s & \text{(Gibbs 1873, Helmholtz 1882)}, \\ \text{free entropy } h &= -f/\theta = s - e/\theta & \text{(Massieu 1869)}.\end{aligned}$$

As is common for the free energy, we also consider the free entropy only as a function of $r = \theta$ and use the densities (where $W = (u, \nabla u, z, \nabla z)$)

$$f = \overline{F}(W, \theta) = \overline{E}(W, \theta) - \theta\, \overline{S}(W, \theta), \quad h = \overline{H}(W, \theta) = -\frac{\overline{F}(W, \theta)}{\theta} = \overline{S}(W, \theta) - \frac{\overline{E}(W, \theta)}{\theta}$$

as fields on the body Ω and define total free energy $\overline{\mathcal{F}}$ and the total free entropy $\overline{\mathcal{H}}$ via

$$\overline{\mathcal{F}}(u, z, \theta) = \int_\Omega \overline{F}(u, \nabla u, z, \nabla z, \theta)\, \mathrm{d}x \ \text{ and } \ \overline{\mathcal{H}}(u, z, \theta) = \int_\Omega \overline{H}(u, \nabla u, z, \nabla z, \theta)\, \mathrm{d}x.$$

The major point we want to address here is that $\overline{\mathcal{F}}$ and $\overline{\mathcal{H}}$ can serve as driving functionals, since their partial derivatives with respect to any of the variables $W = (W_1, ..., W_k) = (u, \nabla u, z, \nabla z)$ are independent of the particular choice of the thermodynamic quantity r. The physical requirement for a driving force is that it takes the same physical value, independent of the choice of the thermodynamic quantity. The main observation is the following lemma which relies on the Gibbs relation.

Lemma 3.1 *Consider smooth functions* $E : (W, r) \mapsto E(W, r)$ *and* $S : (W, r) \mapsto S(W, r)$ *such that* $\Theta(W, r) := \partial_r E(W, r)/\partial_r S(W, r) > 0$. *Consider any transformation* $r = R(W, \rho)$ *with* $\partial_r R(W, r) \neq 0$ *and define*

$$\widetilde{E}(W, \rho) = E(W, R(W, \rho)) \ \text{ and } \ \widetilde{S}(W, \rho) = S(W, R(W, \rho)).$$

Then, we have the identities

$$\mathrm{D}_W E(W, r) - \Theta(W, r)\mathrm{D}_W S(W, r) = \mathrm{D}_W \widetilde{E}(W, \rho) - \widetilde{\Theta}(W, \rho)\mathrm{D}_W \widetilde{S}(W, \rho)$$

$$\text{and } \ \widetilde{\Theta}(W, \rho) = \frac{\partial_\rho \widetilde{E}(W, \rho)}{\partial_\rho \widetilde{S}(W, \rho)} = \Theta(W, R(W, \rho)) \quad \text{if } r = R(W, \rho).$$

In particular, for $R(W, \rho) = \Theta(W, \theta) = \theta$ *and* $\overline{F}(W, \theta) = \overline{E}(W, \theta) - \theta\overline{S}(W, \theta)$ *we obtain*

$$\mathrm{D}_W \overline{F}(W, \theta) = \mathrm{D}_W E(W, \rho) - \theta\mathrm{D}_W S(W, \rho), \quad \text{if } \theta = \Theta(W, \rho) = \frac{\partial_\rho E(W, \rho)}{\partial_\rho S(W, \rho)}.$$

Proof: For the first result, we first establish the Gibbs relation using the chain rule:

$$\frac{\partial_\rho \widetilde{E}(W, \rho)}{\partial_\rho \widetilde{S}(W, \rho)} = \frac{\partial_r E(W, R(W, r))\partial_\rho R(W, \rho)}{\partial_r S(W, R(W, r))\partial_\rho R(W, \rho)} = \frac{\partial_r E(W, R(W, r))}{\partial_r S(W, R(W, r))} = \Theta(W, R(W, \rho)).$$

For the driving forces for W we again use the chain rule to obtain

$$\mathrm{D}_W \widetilde{E}(W, \rho) = \mathrm{D}_W E(W, R(W, \rho)) + \partial_r E(W, R(W, \rho)) \mathrm{D}_W R(W, \rho),$$
$$\mathrm{D}_W \widetilde{S}(W, \rho) = \mathrm{D}_W S(W, R(W, \rho)) + \partial_r S(W, R(W, \rho)) \mathrm{D}_W R(W, \rho).$$

Thus, taking the linear combination $\mathrm{D}_W \widetilde{E} - \widetilde{\Theta} \mathrm{D}_W \widetilde{S}$ and using the Gibbs relation for $\widetilde{\Theta}$ we see that all terms involving $\mathrm{D}_W R$ cancel and the result follows.

Finally choosing $R(W, \rho) = \Theta(W, \rho) =: \theta$ and setting $\overline{F}(W, \theta) = E(W, \theta) - \theta S(W, \theta)$ we obtain the desired result since for $\overline{\Theta}(W, \theta) = \theta$ we have $\mathrm{D}_W \overline{\Theta}(W, \theta) \equiv 0$. ∎

To highlight the result of the previous lemma we consider the following simple example.

Example 3.2 *We consider* $\overline{E}(z, \theta) = \frac{2}{3} a(z) \theta^{3/2}$ *and* $\overline{S}(z, \theta) = a(z) \theta^{1/2}$, *which gives the free energy* $\overline{F}(z, \theta) = -\frac{1}{3} a(z) \theta^{3/2}$ *and the free entropy* $\overline{H}(z, \theta) = \frac{1}{3} a(z) \theta^{1/2}$.

Now consider r *such that* $\theta = R(z, r) = b(z)^2 r^2$ *giving* $E(z, r) = \frac{2}{3} ab^3 r^3$ *and* $S(z, r) = abr$. *We can easily check the identity* $\theta = b^2 r^2 = \Theta(z, r) = \partial_r E / \partial_r S$. *Moreover, we find*

$$\partial_z E(z, r) - \Theta(z, r) \partial_z S(z, r) = \frac{1}{3} a'(z) b(z)^3 r^3 = \partial_z \overline{F}(z, b(z)^2 r^2),$$

i.e. the driving forces coincide as desired. However, for $b'(z) \neq 0$ *we have*

$$\partial_z E(z, r) \neq \partial_z \overline{E}(z, b(z)^2 r^2), \ \partial_z S(z, r) \neq \partial_z \overline{S}(z, b(z)^2 r^2), \ \text{and} \ \partial_z F(z, r) \neq \partial_z \overline{F}(z, b(z)^2 r^2)$$

where $F(z, r) = E(z, r) - \Theta(z, r) S(z, r)$ *is the free energy expressed in* r.

As a consequence of the previous theorem we see that the only mechanically relevant driving forces must be the derivative of the free energy $\mathrm{D}_W \overline{F}(W, \theta) = \mathrm{D}_W E(w, r) - \Theta(W, r) \mathrm{D}_W S(W, r)$ or the temperature $\theta = \partial_r E(W, r) / \partial_r S(W, r)$ or any W-independent combination of these two. In fact, we will see that the following three combinations are the most common:

driving force for reversible dynamics: $\ \mathrm{D}_W \overline{F}(W, \theta) = \mathrm{D}_W E(W, r) - \Theta(W, r) \mathrm{D}_W S(W, r),$

driving force for dissipative dynamics: $\ \mathrm{D}_W \overline{H}(W, \theta) = \mathrm{D}_W S(W, r) - \dfrac{\mathrm{D}_W E(W, r)}{\Theta(W, r)},$

driving force for energy transport: $\ \dfrac{1}{\theta} = \dfrac{1}{\Theta(W, r)} = \dfrac{\partial_r S(W, r)}{\partial_r E(W, r)}.$

However, there is still a major issue when considering fields over a body Ω and considering the total free energy $\overline{\mathcal{F}}$ and the total free entropy $\overline{\mathcal{H}}$. If we consider variations of these functionals the variational derivatives involve integrations by part, namely

$$\mathrm{D}_z \overline{\mathcal{H}}(u, z, \theta) = \delta_z \overline{H}(u, \nabla u, z, \nabla z, \theta) = \partial_z \overline{H}(u, \nabla u, z, \nabla z, \theta) - \mathrm{div}\left(\partial_{\nabla z} \overline{H}(u, \nabla u, z, \nabla z, \theta)\right).$$

Now using the relation $\overline{H} = -\overline{F}/\theta$ we see that the differentials of $\overline{\mathcal{F}}$ and $\overline{\mathcal{H}}$ are not simply related by multiplying with temperature, since we have

$$\mathrm{D}_z \overline{\mathcal{H}}(u, z, \theta) = -\frac{1}{\theta} \mathrm{D}_z \overline{\mathcal{F}}(u, z, \theta) + \partial_{\nabla z} \overline{F}(u, \nabla u, z, \nabla z, \theta) \nabla\left(\frac{1}{\theta}\right).$$

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The last term, which destroys the naive relation $D_z \overline{\mathcal{H}}(u, z, \theta) = -\frac{1}{\theta} D_z \overline{\mathcal{F}}(u, z, \theta)$, vanishes in two important cases: (i) in the isothermal case where $\nabla \theta \equiv 0$ and (ii) in the case "local case" where $\overline{F}$ does not depend on ∇z. *In all other cases, we have to be careful and distinguish the free energy and the free entropy as driving functionals.*

In many situations it is helpful to use other thermodynamical fields r instead of θ, in particular the internal-energy density $e = \overline{E}(W, \theta)$ or the entropy density $s = \overline{S}(W, \theta)$ are often relevant. For these situations it is better to use the total energy $\mathcal{E}$ and the total entropy $\mathcal{S}$ as function of (u, z, r). Hence, we need to adapt the nice cancellation properties derived in Lemma 3.1 by introducing a multiplication "$*$" for scalar fields α and variational derivatives $\delta_z G$ as follows:

$$\Big(\alpha * \delta_z G(z, \nabla z) \Big)(x) := \alpha(x) \partial_z G(z(x), \nabla z(x)) - \mathrm{div}\big(\alpha \partial_{\nabla z} G(z, \nabla z) \big)(x).$$

We also write $\alpha * D_z \mathcal{G}(u, z, r)$ for $\alpha * \delta_z G(u, \nabla u, z, \nabla z, r)$ and obtain the important identities (3.1) below. We should consider "$\alpha * \delta_z$" or "$\alpha * D_z$" as one operator acting on functions G or functionals $\mathcal{G}$, respectively; see [MiR15, Ch. 5.3] for a fully abstract definition.

Theorem 3.3 *Using the above definitions we have*

$$D_u \overline{\mathcal{F}}(u, z, \Theta(u, z, r)) = D_u \mathcal{E}(u, z, r) - \Theta(u, z, r) * D_u \mathcal{S}(u, z, r), \tag{3.1a}$$

$$D_z \overline{\mathcal{H}}(u, z, \Theta(u, z, r)) = D_z \mathcal{S}(u, z, r) - \frac{1}{\Theta(u, z, r)} * D_z \mathcal{E}(u, z, r). \tag{3.1b}$$

Proof: The right-hand side in the first line can be written in full detail as

$$\mathrm{RHS} := \partial_u E(W, r) - \Theta(W, r) \partial_u S(W, r) - \mathrm{div}\big(\partial_{\nabla u} E(W, r) - \Theta(W, r) \partial_{\nabla z} S(W, r) \big),$$

where $W = (u, \nabla u, z, \nabla z)$. Using Lemma 3.1 we can apply the relation for ∂_u and $\partial_{\nabla u}$ independently and find

$$\mathrm{RHS} = \partial_u \overline{F}(W, \Theta(W, r)) - \mathrm{div}\big(\partial_{\nabla u} \overline{F}(W, \Theta(W, r)) \big)$$
$$= \delta_u \overline{F}(W, \theta))|_{\theta = \Theta(W, r)} = D_u \overline{\mathcal{F}}(u, z, \Theta(u, z, r)).$$

This proves (3.1a), and the relation (3.1b) follows analogously. ∎

The importance of the formulas in Theorem 3.3 is that we are able to choose an arbitrary thermodynamics field r of describing the heat effects in our material model. This will allows us to find new mathematical formulations that cannot be accessed by using the temperature θ, the energy density e, or the entropy density s, only.

We remark that in many papers and textbooks only the free energy is used as driving functionals and that $D_z \overline{\mathcal{F}}(u, z, r)$ is used as the driving force for the dissipative variable. This is correct for the cases of isothermal models or if $\overline{F}$ is local, i.e. $\partial_{\nabla z} \overline{F} \equiv 0$. In these two cases one has the relation $D_z \overline{\mathcal{H}} = -\frac{1}{\theta} D_z \overline{\mathcal{F}}$, and the factor $-1/\theta$ can be compensated in the dissipation potential, see [YSO06] for the relevance of the "integrating factor θ".

However, in other cases the usage of $D_z \overline{\mathcal{F}}$ leads to equations that are thermodynamically inconsistent for the local balance laws, while the total energy conservation and total entropy production may still be valid, see the discussion in [Mie11a, Rem. 4.1].

3.2 The balance equations for dissipative material models

Acording to [Mie11a, HüS12] the GENERIC framework suggests to write the coupling of elastodynamics for u, dissipative dynamics for z, and energy transport for r in the form

$$\rho\ddot{u} = -\big(D_u\mathcal{E}(q)-\Theta*D_u\mathcal{S}(q)\big) \qquad = -D_u\overline{\mathcal{F}}(u,z,\Theta(u,z,r)),$$

$$\dot{z} = \partial_{\xi_z}\mathcal{P}_z^*\big(q, D_z\mathcal{S}(q)-\frac{1}{\Theta}*D_z\mathcal{E}(q)\big) \quad = \partial_{\xi_z}\mathcal{P}_z^*\big(q, D_z\overline{\mathcal{H}}(u,z,\Theta(u,z,r))\big),$$

$$\dot{r} = -\frac{\Delta_u S(q)[\dot{u}]}{\partial_r S(q)} - \frac{\Delta_z E(q)[\dot{z}]}{\partial_r E(q)} - \frac{1}{\partial_r E}\,\mathrm{div}\Big(\kappa(q)\nabla\frac{\partial_r S}{\partial_r E}\Big),$$

where the directional derivatives $\Delta_u S(q)[\dot{u}]$ and $\Delta_z E(q)[\dot{z}]$ are defined via

$$\Delta_w G(w)[v] := \partial_w G(w,\nabla w)\cdot v + \partial_{\nabla w}G(w,\nabla w){:}\nabla v.$$

Here the first equation described elastodynamics and contains the Hamiltonian part. In particular, we see that the reversible (i.e. Hamiltonian) part of the dynamics is driven by the derivative $D_u\overline{\mathcal{F}}(u,z,\Theta(u,z,r))$ of the free energy $\overline{\mathcal{F}}$. In contrast, the dissipative effects described by the internal variable z and the thermodynamical field r are driven by $D_z\overline{\mathcal{H}}(u,z,\Theta(u,z,r))$ and $1/\Theta = \partial_r S/\partial_r E$, respectively. In particular, we can define a joint dual entropy-production potential (EPP) $\mathcal{P}^*$ via

$$\mathcal{P}^*(u,z,r;\xi_u,\xi_z,\xi_r) = \mathcal{P}_0^*(u,z,r;\mathbf{M}(u,z,r)(\xi_z,\xi_r)^{\mathsf{T}})\ \text{with}$$

$$\mathcal{P}_0^*(u,z,r;\eta_z,\eta_r) = \mathcal{P}_z^*(u,z,r;\eta_z) + \int_\Omega \frac{1}{2}\nabla\eta_r\cdot\kappa\nabla\eta_r\,\mathrm{d}x\ \text{ and}$$

$$\mathbf{M}(u,z,r) = \begin{pmatrix} I & \frac{-\square}{\partial_r E(\ldots)}*D_z\mathcal{E}(u,z,r) \\ 0 & \frac{\square}{\partial_r E(\ldots)} \end{pmatrix},$$

where $\square$ indicates the slot, where the corresponding argument (here ξ_r) has to be inserted.

We now discuss the two first terms on the right-hand side of the energy balance for r, namely $\Delta_u S(u,z,r)[\dot{u}]/\partial_r S$ and $\Delta_z E(u,z,r)[\dot{z}]/\partial_r E$. The first term $\Delta_u S(u,z,r)[\dot{u}]/\partial_r S$ can be seen as the latent-heat production term that is dual to the term $\frac{\partial_r E}{\partial_r S}*D_u\mathcal{S}$ in the linear momentum balance and thus belongs to the reversible (=Hamiltonian) part of dynamics. In particular it disappears completely if we choose $r = s$, which means that it does not change the entropy. We refer to [Mie11a] for more details. In contrast, the second term $\Delta_z E(u,z,r)[\dot{z}]/\partial_r E$ is an entropy-production term that is dual to the term $\frac{\partial_r S}{\partial_r E}*D_z\mathcal{E}$ appearing in $\mathcal{P}_z^*$. We can now rewrite the system for (z,r) in the form

$$\begin{pmatrix} \dot{z} \\ \dot{r} \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{\Delta_u S[\dot{u}]}{\partial_r S} \end{pmatrix} + \mathbf{M}(u,z,r)^*\partial_{\boldsymbol{\xi}}\mathcal{P}_0^*\Big(u,z,r;\mathbf{M}(u,z,r)\begin{pmatrix} D_z\mathcal{S}(u,z,r) \\ D_r\mathcal{S}(u,z,r) \end{pmatrix}\Big) \qquad (3.2)$$

Before restricting to the quasistatic case with $\rho = 0$ we look at the total energy balance and the total entropy production using the given abstract form. First we observe that

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along solutions $q(t) = (u(t), z(t), r(t))$ we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\int_\Omega \frac{\rho}{2}|\dot{u}|^2 \,\mathrm{d}x + \mathcal{E}(q(t)) \Big)$$

$$= \int_\Omega \rho \ddot{u} \cdot \dot{u} \,\mathrm{d}x + \langle \mathrm{D}_u \mathcal{E}(q), \dot{u} \rangle + \langle \mathrm{D}_z \mathcal{E}(q), \dot{z} \rangle + \langle \mathrm{D}_r \mathcal{E}(q), \dot{r} \rangle$$

$$\overset{(1)}{=} -\langle \Theta * \mathrm{D}_u \mathcal{S}, \dot{u} \rangle + \Big\langle \big(\begin{smallmatrix} \mathrm{D}_z \mathcal{E} \\ \partial_r E \end{smallmatrix}\big), \big(\begin{smallmatrix} 0 \\ -\frac{\Delta_u S[\dot{u}]}{\partial_r S} \end{smallmatrix}\big) + \mathbf{M}(q)^* \partial_{\boldsymbol{\eta}} \mathcal{P}_0^* \big(q, \mathbf{M}(q)\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \partial_r S \end{smallmatrix}\big)\big) \Big\rangle$$

$$\overset{(2)}{=} 0 + 0 + \Big\langle \mathbf{M}(q)\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{E} \\ \mathrm{D}_r \mathcal{E} \end{smallmatrix}\big), \partial_{\boldsymbol{\eta}} \mathcal{P}_0^* \big(q, \mathbf{M}\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \partial_r S \end{smallmatrix}\big)\big) \Big\rangle \overset{(3)}{=} 0,$$

where we used the momentum balance and (3.2) in (1). Equality (2) follows from Gibbs relation $\Theta = \partial_r E / \partial_r S$ and the definition of "$*$", whereas (3) uses $\mathbf{M}(q)(\mathrm{D}_z \mathcal{E}, \mathrm{D}_r \mathcal{E})^\mathsf{T} = (0,1)^\mathsf{T}$ and the energy conservation property $\mathcal{P}_0^*(q, \boldsymbol{\eta} + \lambda(0,1)^\mathsf{T}) = \mathcal{P}_0^*(q, \boldsymbol{\eta})$.

Similarly, the total entropy production can be calculated as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{S}(q(t)) = \langle \mathrm{D}_u \mathcal{S}(q), \dot{u} \rangle + \langle \mathrm{D}_z \mathcal{S}(q), \dot{z} \rangle + \langle \mathrm{D}_r \mathcal{S}(q), \dot{r} \rangle$$

$$\overset{(i)}{=} \langle \mathrm{D}_u \mathcal{S}(q), \dot{u} \rangle + \Big\langle \big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \partial_r S \end{smallmatrix}\big), \big(\begin{smallmatrix} 0 \\ -\frac{\Delta_u S[\dot{u}]}{\partial_r S} \end{smallmatrix}\big) + \mathbf{M}(q)^* \partial_{\boldsymbol{\eta}} \mathcal{P}_0^* \big(q, \mathbf{M}(q)\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \partial_r S \end{smallmatrix}\big)\big) \Big\rangle$$

$$= 0 + 0 + \Big\langle \mathbf{M}(q)\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \mathrm{D}_r \mathcal{S} \end{smallmatrix}\big), \partial_{\boldsymbol{\eta}} \mathcal{P}_0^* \big(q, \mathbf{M}\big(\begin{smallmatrix} \mathrm{D}_z \mathcal{S} \\ \partial_r S \end{smallmatrix}\big)\big) \Big\rangle \overset{(ii)}{\geq} 0,$$

where we used (3.2) for (i) and the fact that $\mathcal{P}_0^*$ is a dual dissipation potential in (ii), i.e. $\mathcal{P}_0^*(\boldsymbol{\eta}) \geq \mathcal{P}_0^*(0) = 0$ and convexity of $\mathcal{P}_0^*$ imply $\langle \boldsymbol{\eta}, \partial \mathcal{P}_0^*(\boldsymbol{\eta}) \rangle \geq 0$.

3.3 A gradient structure for the quasistatic case

Subsequently we choose the quasistatic approximation and neglect the kinetic energy, i.e. we set the density $\rho = 0$. It was shown already in [Mie11b] that, after elimination of the displacement u, the remaining equation for (z, r) is a gradient system if one uses the specific choice $r = s$ (the density of the entropy). Here we follow [Mie11a] and show that the result holds for any choice of r, which is extremely helpful, since traditionally one prefers $r = \theta$ (the temperature) and more recently also the choice $r = e$ (the density of the internal energy), but general r gives more flexibility, see e.g. Sections 4.2 and 4.3. To simplify the formulas we restrict our subsequent discussion to the simpler case

$$\mathcal{P}_0^*(q; \eta_z, \eta_r) = \mathcal{P}_Z^*(q; \eta_z) + \int_\Omega \frac{1}{2} \nabla \eta_r \cdot \kappa(q) \nabla \eta_r \,\mathrm{d}x.$$

The quasistatic thermomechanical system for $q = (u, z, r)$ takes the form

$$0 = \mathrm{D}_u \mathcal{E}(q) - \Theta(q) * \mathrm{D}_u \mathcal{S}(q), \tag{3.3a}$$

$$\dot{z} = \partial_{\eta_z} \mathcal{P}_Z^* \Big(q; \mathrm{D}_z \mathcal{S}(q) - \frac{1}{\Theta(q)} * \mathrm{D}_z \mathcal{E}(q) \Big), \tag{3.3b}$$

$$\dot{r} = -\frac{\Delta_u S(q)[\dot{u}]}{\partial_r S(q)} - \frac{\Delta_z E(q)[\dot{z}]}{\partial_r E(q)} - \frac{1}{\partial_r E} \,\mathrm{div}\big(\kappa(q) \nabla \frac{\partial_r S}{\partial_r E}\big), \tag{3.3c}$$

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still displaying the driving forces in terms of free energy and free entropy. However, the *special GENERIC structure* discussed in [Mie11a, Sec. 2.4] guides us to write the system in the form

$$0 = D_u \mathcal{E}(q) - A(q) D_r \mathcal{E}(q), \tag{3.4a}$$

$$\dot{z} = \partial_{\eta_z} \mathcal{P}_Z^* \Big(q; D_z \mathcal{S}(q) - B(q) D_r \mathcal{S}(q) \Big), \tag{3.4b}$$

$$\dot{r} = -A(q)^* \dot{u} - B(q)^* \dot{z} - C(q)^* \operatorname{div} \big(\kappa(q) \nabla (C(q) D_r S(q)) \big), \tag{3.4c}$$

where the operators A, B, and C are defined via

$$A(q)\xi_r = \big(\frac{\xi_r}{D_r \mathcal{S}(q)} \big) * D_u \mathcal{S}(q), \quad B(q)\xi_r = \big(\frac{\xi_r}{D_r \mathcal{E}(q)} \big) * D_z \mathcal{E}(q), \quad C(q)\xi_r = \frac{\xi_r}{D_r \mathcal{E}(q)}. \tag{3.4d}$$

By definition we have the following identities

$$\begin{aligned} AD_r\mathcal{E} &= \Theta * D_u\mathcal{S}, & BD_r\mathcal{E} &= D_z\mathcal{E}, & CD_r\mathcal{E} &= 1, \\ AD_r\mathcal{S} &= D_u\mathcal{S}, & BD_r\mathcal{S} &= \big(\tfrac{1}{\Theta} \big) * D_z\mathcal{E}, & CD_r\mathcal{S} &= 1/\Theta. \end{aligned} \tag{3.5}$$

For the following we assume that (3.3a) or (3.4a) can be solved uniquely in the form $u = U(z,r)$. As a shorthand, we also write $q = Q(z,r) = (U(z,r), z, r)$.

Theorem 3.4 *Assume that the mapping $\xi_r \mapsto \xi_r + D_r U(z,r)^* A(Q(z,r))\xi_r$ is invertible and denote the inverse by $\mathbf{J}(z,r)$. Defining the functionals*

$$\mathfrak{S}(z,r) = \mathcal{S}(U(z,r), z, r), \quad \mathfrak{E}(z,r) = \mathcal{E}(U(z,r), z, r), \quad \text{and}$$

$$\mathfrak{P}^*(z,r;\xi_z,\xi_r) = \mathcal{P}_Z^* \Big(Q(z,r); \xi_z - \mathbf{B}(z,r)\xi_r \Big) + \int_\Omega \frac{1}{2} \nabla \big(\mathbf{C}(z,r)\xi_r \big) \cdot \kappa(Q) \nabla \big(\mathbf{C}(z,r)\xi_r \big) \, dx,$$

$$\mathbf{B}(z,r) = \big(B(Q(z,r)) + D_z U(z,r)^* A(Q(z,r)) \big) \mathbf{J}(z,r) \quad \text{and} \quad \mathbf{C}(z,r) = C(Q(z,r)) \mathbf{J}(z,r),$$

we obtain the following gradient structure:

$$(3.3a)–(3.3c) \quad \Longleftrightarrow \quad \Big(u = U(z,r) \text{ and } \frac{d}{dt} \begin{pmatrix} z \\ r \end{pmatrix} = \partial_{\boldsymbol{\xi}} \mathfrak{P}^*(z,r; D\mathfrak{S}(z,r)) \Big),$$

and we have energy conservation via $\frac{d}{d\lambda} \mathfrak{P}^*(z,r;\boldsymbol{\xi} + \lambda D\mathfrak{E}(z,r)) = 0$.

Proof: The last relation follows from the definition of $\mathfrak{P}^*$ and the identities

$$\mathbf{J}D_r\mathfrak{E} = D_r\mathcal{E}(Q), \quad \mathbf{C}D_r\mathfrak{E}(z,r) = C(Q)D_r\mathcal{E}(Q) \equiv 1, \text{ and}$$

$$D_z\mathfrak{E} - \mathbf{B}D_r\mathfrak{E} = D_z U^* D_u\mathcal{E} + D_z\mathcal{E} - (B + D_z U^* A)D_r\mathcal{E})$$

$$= D_z U^* (D_u\mathcal{E} - \Theta * D_u\mathcal{S}) + D_z\mathcal{E} - BD_r\mathcal{E} = 0,$$

where we used (3.3a) and (3.5)$_2$, respectively.

To see the equivalence between the evolution equations, first note

$$\dot{z} = \partial_{\xi_z} \mathfrak{P}^*(z,r; D\mathfrak{S}(z,r)) = \partial_{\eta_z} \mathcal{P}_Z^*(Q; D_z\mathfrak{S} - \mathbf{B}D_r\mathfrak{S}).$$
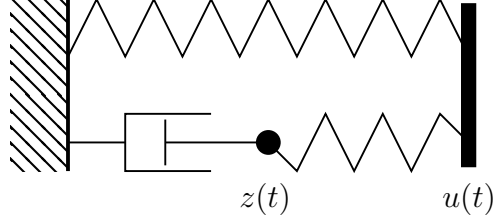
Figure 1: A system with two springs and one damper. The upper spring undergoes thermal expansion.

Proceeding as for $D_z\mathfrak{E}-\mathbf{B}D_r\mathfrak{E}$ we obtain the relation $D_z\mathfrak{S}-\mathbf{B}D_r\mathfrak{S} = D_z\mathcal{S}-BD_r\mathcal{S}|_{q=Q(z,r)}$, which is the physically correct driving force, namely the derivative of the free entropy. Thus, the equation for z is identical to (3.4b).

For the r-equation we first observe $\mathbf{C}D_r\mathfrak{S} = CD_r\mathcal{S}(Q) = 1/\Theta(Q)$, which is the correct driving force for heat conduction. Thus, the gradient-flow equation for r yields

$$\dot{r} = -\mathbf{B}^*\partial_{\xi_z}\mathfrak{P}^*(..) - \mathbf{C}^*\operatorname{div}\big(\kappa\nabla(1/\Theta)\big) = \mathbf{J}^*\Big(-(A^*D_z\mathrm{U}+B^*)\dot{z} - C^*\operatorname{div}\big(\kappa\nabla(1/\Theta)\big)\Big).$$

Now we use that by definition $\mathbf{J}^*$ is the inverse of $I + A^*D_r\mathrm{U}$. Thus, we can rewrite the last equation in the form

$$\dot{r} = -A(Q)^*(\mathrm{U}(z,r)\dot{z}+D_r\mathrm{U}(z,r)\dot{r}) - B(Q)^*\dot{z} - C(Q)^*\operatorname{div}\big(\kappa(Q)\nabla(1/\Theta(Q))\big),$$

which is the desired equation (3.4c), because of $\dot{u} = D_z\mathrm{U}(z,r)\dot{z} + D_r\mathrm{U}(z,r)\dot{r}$. ∎

Before going into more details, we present a simple finite-dimensional example, where the reduction and the induced gradient structure can be calculated explicitly.

Example 3.5 *We explain the derivation of the gradient structure by considering a simple mass-spring-damper system, where we assume energy conservation, i.e. the damping mechanics heats up the device, which additionally contains some thermal expansion, see Figure 1. To keep the model as simple as possible we choose the free energy*

$$F(u, z, \theta) = \frac{1}{2}u^2 + \alpha u\theta + \frac{1}{2}(u-z)^2 - \frac{4c}{3}\theta^{3/2},$$

where α is the thermal expansion coefficient. The classical force balances are

$$0 = \partial_u F(u, z, \theta) = u + \alpha\theta + u - z \quad \text{and} \quad 0 = \mu\dot{z} + z - u.$$

The evolution of θ will be determined by energy conservation.

For this we will transform the system into the above structure. First observe that

$$E(u, z, \theta) = \frac{1}{2}u^2 + \frac{1}{2}(u-z)^2 + \frac{2c}{3}\theta^{3/2} \quad \text{and} \quad S(u, z, u) = 2c\theta^{1/2} - \alpha u.$$

The driving force for the damper is the derivative of the free entropy with respect to z, which is

$$\partial_z H(u, z, \theta) = \partial_z S(u, z, \theta) - \theta\partial_z E(u, z, \theta) = (u-z)/\theta.$$

This is consistent with the choice of the EPP which differs from the dissipation potential $\mathcal{R}(\dot{z}) = \frac{\mu}{2}\dot{z}^2$ by a factor of temperature, namely $\mathcal{P}(\theta;\dot{z}) = \frac{\mu}{2\theta}\dot{z}^2$ and $\mathcal{P}^*(\theta;\xi) = \frac{\theta}{2\mu}\xi^2$.

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Together, the equations take the form (3.4), namely

$$0 = D_u F(u, z, \theta) = 2u - z + \alpha\theta,$$

$$\dot{z} = \frac{\theta}{\mu} \partial_z H(u, z, \theta) = \frac{1}{\mu}(u - z),$$

$$\dot{\theta} = -A(u, z, \theta)^* \dot{u} - B(u, z, \theta)^* \dot{z}, \text{ where } A(q) = -\frac{\alpha\theta^{1/2}}{c} \text{ and } B(q) = \frac{z - u}{c\theta^{1/2}}.$$

There is no heat conduction term, since the temperature is the same in the whole system.

For the reduction we immediately find $u = U(z, \theta) = \frac{1}{2}(z - \alpha\theta)$. Inserting this relation into the above system we see that the reduced ODE is given by

$$\dot{z} = \frac{-1}{2\mu}(z + \alpha\theta) \quad \text{and} \quad \left(1 + \frac{\alpha^2}{2c}\theta^{1/2}\right)\dot{\theta} = \frac{-z}{2c\theta^{1/2}}\dot{z}, \tag{3.6}$$

where the last equation is equivalent to $\frac{d}{dt}\mathfrak{E}(z(t), \theta(t)) = 0$ after multiplication with $c\theta^{1/2}$.

On the other hand, Theorem 3.4 provides a gradient structure via

$$\mathfrak{E}(z, \theta) = \frac{1}{4}z^2 + \frac{\alpha^2}{4}\theta^2 + \frac{2c}{3}\theta^{3/2}, \quad \mathfrak{S}(z, \theta) = -\frac{\alpha}{2}z + \frac{\alpha^2}{2}\theta + 2c\theta^{1/2},$$

$$\mathfrak{P}^*(\theta; \xi_z, \xi_\theta) = \frac{\theta}{2\mu}\left(\xi_z - \mathbf{B}(z, \theta)\xi_\theta\right)^2, \quad \mathbf{B}(z, r) = \frac{z}{2c\theta^{1/2} + \alpha^2\theta}.$$

It is easily checked that the gradient flow

$$\dot{z} = \partial_{\xi_z}\mathcal{P}^*\left(\theta; D_z\mathfrak{S}(z, r) - \mathbf{B}(z, \theta)D_\theta\mathfrak{S}(z, \theta)\right) \quad \text{and} \quad \dot{r} = -\mathbf{B}(z, \theta)\dot{z}$$

is the same as (3.6), while the individual driving forces $D_z\mathfrak{S}(z, \theta) = -\alpha/2$ and $D_\theta\mathfrak{S}(z, \theta) = c/\theta^{1/2} + \alpha^2/2$ are quite different from what one might naively expect. $\square$

The above abstract result is a beautiful and mathematically clean reduction of the quasistatically coupled system of elastostatics and dissipative material behavior to a perfect gradient system driven by the physical entropy $\mathfrak{S}$. However, in practice it is of limited use because of the involved nonlocal functionals. In particular, $U(z, r)$ depends nonlocally on (z, r), since it is obtained by solving an elliptic boundary value problem. As a consequence, the operators $\mathbf{J}$, $\mathbf{B}$, and $\mathbf{C}$ are nonlocal as well.

Fortunately, there are cases, where the nonlocality disappears or is reduced to a minimum. The most important case occurs if the entropy functional is independent of u:

$$\alpha * D_u\mathcal{S}(u, z, r) = 0 \text{ for all } \alpha \quad \Longrightarrow \quad A(q) \equiv 0.$$

As a consequence we obtain $\mathbf{B}(z, r) = B(Q(z, r))$, $\mathbf{C}(z, r) = C(Q(z, r))$, and $\mathbf{J} = \text{id}$. Moreover, the elastostatic equation reduces to $D_u\mathcal{E}(u, z, r) = 0$. Here we see the advantage of using general thermodynamical variables r, since the form of $A(u, z, r)$ strongly depends on r: We have $A(u, z, r) \equiv 0$ only for specific choices, see Example 3.7 and Sections 4.2 and 4.3.

3.4 A time-incremental minimization procedure

If we are able to find a formulation with $\alpha * \mathrm{D}_u \mathcal{S} \equiv 0$, we can take advantage of the gradient structure derived in Theorem 3.4, even without eliminating u explicitly. Hence, we start with system (3.4), but now under the simplifying assumption $A(q) = 0$.

We first construct the (primal) entropy-production potential $\mathcal{P}(u, z, r; \dot{z}, \dot{r})$. For this we introduce the dual potential for the heat transfer, which is quadratic, namely

$$\mathcal{P}^*_{\text{heat}}(q; \xi_r) := \frac{1}{2} \int_\Omega \nabla\big(C(q)\xi_r\big) \cdot \kappa(q)\nabla\big(C(q)\xi_r\big)\,\mathrm{d}x$$

and denote by $\mathcal{P}_{\text{heat}}$ its Legendre transform, i.e. $\mathcal{P}_{\text{heat}}(q; \dot{r}) = \sup_{\xi_r} \big(\int_\Omega \xi_r \dot{r}\,\mathrm{d}x - \mathcal{P}^*_{\text{heat}}(q; \xi_r)\big)$. Since $\mathcal{P}^*_{\text{heat}}(q; \mathrm{D}_r\mathcal{S})$ corresponds to an H^1 norm of $C(q)\mathrm{D}_r\mathcal{S} = 1/\Theta$, the quadratic form $\mathcal{P}_{\text{heat}}(q; \dot{r})$ corresponds to an H^{-1} norm of $\partial_r E(q)\dot{r}$.

Recall that the full dual EPP has the form $\mathcal{P}^*(q; \xi_z, \xi_r) = \mathcal{P}^*_Z(q; \xi_z - B(q)\xi_r) + \mathcal{P}^*_{\text{heat}}(\xi_r)$; hence the associated primal EPP reads

$$\mathcal{P}(q; \dot{z}, \dot{r}) = \mathcal{P}_Z(q; \dot{z}) + \mathcal{P}_{\text{heat}}(q; \dot{r} + B(q)^* \dot{z}).$$

Using the Fenchel equivalence $\xi \in \partial \mathcal{P}(v) \iff v \in \mathcal{P}^*(\xi)$, we find that the system (3.4) with $A(q) \equiv 0$ for $q = (u, z, r)$ can be rewritten as follows:

$$\mathrm{D}_u\mathcal{E}(q) = 0, \qquad \begin{pmatrix} \mathrm{D}_z\mathcal{S}(q) \\ \mathrm{D}_r\mathcal{S}(q) \end{pmatrix} \in \partial_{(\dot{z},\dot{r})}\mathcal{P}(q; \dot{z}, \dot{r}) = \begin{pmatrix} I & B(q) \\ 0 & I \end{pmatrix} \begin{pmatrix} \partial\mathcal{P}_Z(q; \dot{z}) \\ \partial\mathcal{P}_{\text{heat}}(q; \dot{r} + B^*\dot{z}) \end{pmatrix}.$$

We see that both relations are variational in the sense that derivatives of functionals determine the solutions.

In particular, we can discretize the system in time such that we obtain time-incremental minimization principles that are useful for proving existence of solutions or for numerical simulation of concrete models.

Time-incremental minimization procedure for the case $A \equiv 0$**:** *Consider a time step* $\tau > 0$ *and assume that the initial condition* $q^0 = (u^0, z^0, r^0)$ *is given such that* $\mathrm{D}_u\mathcal{E}(q^0) = 0$. *We define* q^k *for* $k \in \mathbb{N}$ *incrementally as follows:*

$$\text{(TIMP)} \quad \begin{cases} \begin{pmatrix} z^{k+1} \\ r^{k+1} \end{pmatrix} &\in \underset{(z,r)}{\operatorname{Arg\,min}} \left\{ \tau\mathcal{P}\Big(q^k; \frac{1}{\tau}\begin{pmatrix} z-z^k \\ r-r^k \end{pmatrix}\Big) - \mathcal{S}(u^k, z, r) \right\}, \\ u^{k+1} &\in \underset{u}{\operatorname{Arg\,min}} \mathcal{E}(u, z^{k+1}, r^{k+1}). \end{cases} \tag{3.7}$$

Note that we do not enforce energy conservation, which could be done as well. However, it is better to use the errors in the energy conservation as quality control for the numerical accuracy, see the example below.

Remark 3.6 *It may be tempting to write a similar time-incremental minimization procedure also in the case* $A(q) \neq 0$. *However, we see that the term* $A(q)^*\dot{u}$ *needs to be approximated. One way would be to use the consistent tangents* $\mathrm{D}_z\mathrm{U}$ *and* $\mathrm{D}_r\mathrm{U}$ *and to replace the term by* $A(q^k)\big(\mathrm{D}_z\mathrm{U}(z^k, r^k)\dot{z} + \mathrm{D}_r\mathrm{U}(z^k, r^k)\dot{r}\big)$ *before discretizing the derivatives by time increments. However, the numerical calculation of the tangents* $\mathrm{D}_z\mathrm{U}$ *and* $\mathrm{D}_r\mathrm{U}$ *seems to be very inefficient. Moreover, it is not clear, whether the update* $u^{k+1} = u^k + \tau\big(\mathrm{D}_z\mathrm{U}(z^k, r^k)(z^{k+1} - z^k) + \mathrm{D}_r\mathrm{U}(z^k, r^k)(r^{k+1} - r^k)\big)$ *is consistent enough with the elastostatic equation* $\mathrm{D}_u\mathcal{E}(q) - A(q)\mathrm{D}_r\mathcal{E}(q) = 0$.

To highlight the usefulness of the algorithm we return to the spring-damper model treated in Example 3.5. We will take advantage of using a suitable thermodynamic variable r, namely $r = s$.

Example 3.7 (Continuation of Example 3.5) *The model is originally formulated in (u, z, θ) but $\partial_u S(u, z, \theta) = -\alpha$ does not vanish, so the model cannot be treated with these variables. Thus, we will use the entropy density s as the thermodynamical variable r:*

$$s = R(z, \theta) := 2c\theta^{1/2} - \alpha u \quad \rightsquigarrow \quad \theta = \Theta(u, s) = \left(\frac{s + \alpha u}{2c}\right)^2.$$

Hence, we find the following relations

$$\widetilde{E}(u, z, s) = \frac{1}{2}u^2 + \frac{1}{2}(u-z)^2 + \widetilde{e}(s + \alpha u) \text{ with } \widetilde{e}(y) = \begin{cases} y^3/(12c^2) & \text{for } y \geq 0, \\ \infty & \text{for } y < 0, \end{cases}$$

$$\widetilde{S}(u, z, s) = s, \qquad \widetilde{A}(u, z, s) = 0, \qquad \widetilde{B}(u, z, s) = 4c^2 \frac{z-u}{(s+\alpha u)^2} = \frac{z-u}{\Theta(u, s)}.$$

The full coupled system takes the form

$$0 = \mathrm{D}_u \widetilde{E}(u, z, s) = 2u - z + \frac{\alpha}{4c^2}(s+\alpha u)^2, \tag{3.8a}$$

$$\dot{z} = \frac{\Theta(u, s)}{\mu}\left(\partial_z \widetilde{S} - \widetilde{B}\partial_s \widetilde{S}\right) = \frac{\Theta}{\mu}\left(0 - \widetilde{B}(u, z, s)\,1\right) = \frac{u-z}{\mu}, \tag{3.8b}$$

$$\dot{s} = -\widetilde{A}(u, z, s)\,\dot{u} - \widetilde{B}(u, z, s)\dot{z} = 0 + \frac{\Theta}{\mu}\left(\widetilde{B}(u, z, s)\right)^2. \tag{3.8c}$$

Since the dual EPP $\mathcal{P}^*$ has the form $\mathcal{P}^*(\theta; \xi_z, \xi_s) = \frac{\Theta}{2\mu}(\xi_z - \widetilde{B}\xi_s)^2$ the primal EPP reads

$$\mathcal{P}(u, z, s; \dot{z}, \dot{s}) = \begin{cases} \dfrac{\mu}{2\Theta(u, s)}|\dot{z}|^2 & \text{if } \dot{s} + \widetilde{B}(u, z, s)\dot{z} = 0, \\ \infty & \text{else.} \end{cases}$$

Using the explicit constraint $\dot{s} = \widetilde{B}(u, z, s)\dot{z}$, the time-incremental minimization procedure of (3.7) takes the explicit form:

Find (z^{k+1}, s^{k+1}) as minimizer of $\dfrac{\mu}{2\Theta(u^k, s^k)}\dfrac{1}{\tau}(z - z^k)^2 - s$

subject to $s - \widetilde{B}(u^k, z^k, s^k)z = s^k - \widetilde{B}(u^k, z^k, s^k)z^k$,

find u^{k+1} as minimizer of $E(u, z^{k+1}, s^{k+1})$.

Here the first minimization problem is quadratic, and the explicit solution can be determined. In the second minimization problem the functional is cubic in u, so the unique minimizer $u^{k+1} = \mathrm{U}(z^{k+1}, s^{k+1})$ can be obtained by solving (3.8a). Thus, we find the incremental update formulas

$$z^{k+1} = z^k + \tau\frac{\Theta(q^k)}{\mu}\widetilde{B}(q^k), \quad s^{k+1} = s^k + \tau\frac{\Theta(q^k)}{\mu}\widetilde{B}(q^k)^2, \quad u^{k+1} = \mathrm{U}(z^{k+1}, s^{k+1}). \tag{3.9}$$

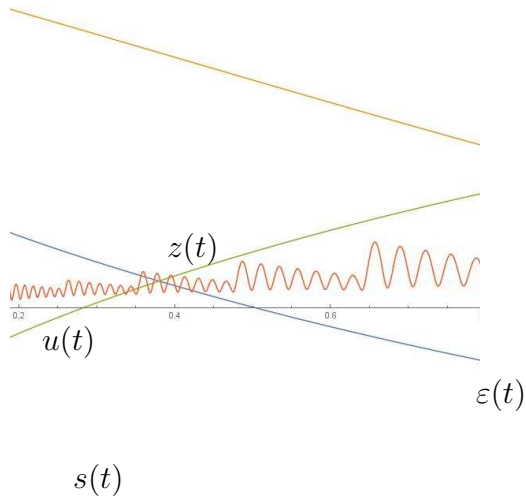Figure 2: Numerical solution $q(t) = (u(t), z(t), s(t))$ of the ODE (3.8) for parameters $\mu = \alpha = 1$ and $c = 1/2$. Here $\varepsilon(t) = 10^6(\widetilde{E}(q(t)) - \widetilde{E}(q(0)))$.
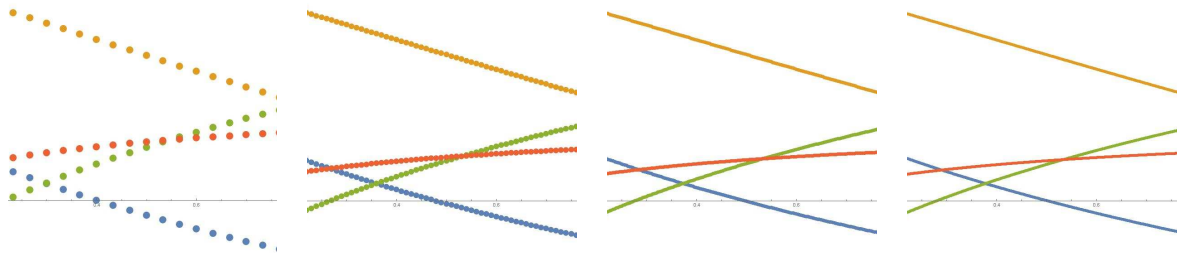

Figure 3: Numerical simulation via (3.9) for time steps $\tau = 1/30$, $1/100$, $1/300$, $1/1000$. Energy conservation is checked via $\varepsilon_\tau(k\tau) = (\widetilde{E}(q^k) - \widetilde{E}(q^0))/(\tau\widetilde{E}(q^0))$, hence $\varepsilon_\tau(1) \approx 5\tau$.

Inserting the explicit form of $\widetilde{B}$ we find the relation $z^{k+1} = z^k + \frac{\tau}{\mu}(u^k - z^k)$, which is an explicit discretization of (3.8b). Nevertheless, by construction of our algorithm we know that it is entropy increasing. Figure 2 shows the numerical solution of the ODE (3.8), while Figure 3 shows numerical approximations obtain via the TIMP (3.7), which yields (3.9). We observe that the scheme is only of first order in the time step. However, we expect that it is stable even when treating fully nonlinear thermomechanical systems. □

4 Gradient structures for thermomechanical systems

In this section we give three examples of temperature dependent models that can be rewritten in terms of entropic gradient flows.

4.1 Homogenization of the Penrose-Fife system

This model is without any elastic deformation, so there is no need to eliminate the variable u and the condition $D_u \mathcal{S} \equiv 0$ is trivially satisfied.

The Penrose-Fife model was introduced in [PeF90] to resolve a long-lasting debate concerning thermodynamically correct couplings between phase transitions models and the heat equation, see [PeF93, Mie13] and [Mie11a, Rem. 4.1] for details. Typically the free energy $F(z, \nabla z, \theta) = -c\theta \log \theta + \psi_0(z) + \theta\psi_1(z) + \theta\frac{\alpha}{2}|\nabla z|^2$ is used which leads to

$$E(z, \theta) = c\theta + \psi_0(z) \quad \text{and} \quad S(z, \nabla z, \theta) = c \log \theta + c - \psi_1(z) - \frac{\nu}{2}|\nabla z|^2. \tag{4.1}$$

The equations in the variables z and θ take the form

$$\text{(PF)} \quad \begin{cases} \dot{z} = m\big(\delta_z S(z,\theta) - \frac{1}{\theta}\partial_z E\big) \;=\; m\big(\nu\Delta z - \psi_1'(z) - \frac{1}{\theta}\psi_0'(z)\big) \\ c\dot{\theta} = -\psi_0'(z)\dot{z} + \text{div}\,\big(k(z,\theta)\nabla\theta\big). \end{cases} \tag{4.2}$$

Almost all mathematical work is restricted to the case $E(z, \theta) = c\theta + \lambda z$, which is physically only relevant in a small temperature range. In particular, the logarithmic entropy $\sigma(\theta) = c \log \theta$ is only good for gases, while for solids one should have $\sigma(0) = 0$, e.g. $\sigma(\theta) = c\theta^\alpha$ for $\alpha \in\,]0, 1[$ is more appropriate.

In [MiS15] we consider the internal energy e as thermodynamic variable $r = e$, namely $\mathcal{E}(z, e) = \int_\Omega e(x)\,dx$ and $\mathcal{S}(z, e) = \int_\Omega \widehat{S}(z, \nabla z, e)\,dx$. Indeed, the above case (4.1) can be rewritten in terms of e via $s = \widehat{S}(z, \nabla z, e) = c\log(e - \psi_0(z)) - c\log c - \psi_1(z) - \frac{\alpha}{2}|\nabla z|^2$, but much more general functions $\widehat{S}$ are possible.

The Penrose-Fife system (4.2) can be formulated as gradient system via the EPP

$$\mathcal{P}^*(z, e; \xi_z, \xi_e) = \frac{1}{2}\langle\boldsymbol{\xi}, \mathbb{K}(z, e)\boldsymbol{\xi}\rangle = \frac{1}{2}\int_\Omega m(x, z, e))\xi_z(x)^2 + \nabla\xi_e(x)\cdot\kappa(z, e)\nabla\xi_e(e)\,dx.$$

In particular, one has the explicit form

$$\text{(PF)} \iff \begin{pmatrix} \dot{z} \\ \dot{e} \end{pmatrix} = \mathbb{K}(z, e)D\mathcal{S}(z, e) = \partial_{\boldsymbol{\xi}}\mathcal{P}^*\big(z, e; D\mathcal{S}(z, e)\big) = \begin{pmatrix} m & 0 \\ 0 & -\text{div}(\kappa\nabla\square) \end{pmatrix}\begin{pmatrix} \delta_z S \\ \partial_e S \end{pmatrix}.$$

There is one special case where the gradient system can be rewritten as an *evolutionary variational inequality (EVI)*, cf. [AGS05, Mie14]. For this we have to assume that $\mathbb{K}$ (or equivalently $\mathcal{P}^*$) does not depend on the state (z, e). Moreover, one needs to assume that $(z, e) \mapsto -\mathcal{S}(z, e)$ is λ-convex, i.e. for some $\lambda \in \mathbb{R}$ the function $(z, e) \mapsto -\mathcal{S}(z, e) - \lambda\mathcal{P}(z, e)$ is convex, where $\mathcal{P}$ is the primal EPP. Under these assumptions, a curve $q = (z, e) : [0, T] \mapsto \mathbf{X}_{\text{PF}} := H^1(\Omega) \times L^1(\Omega)$ is a solution of (PF), if and only if

$$\text{(EVI)} \quad e^{\lambda(t-s)}\mathcal{P}(q(t) - w) + \mathcal{P}(q(s) - w) \le \int_0^{t-s} e^{\lambda r}\,dr\,\big(\mathcal{S}(q(t)) - \mathcal{S}(w)\big)$$

$$\text{for all } 0 \le s < t \text{ and all } w = (\widetilde{z}, \widetilde{e}) \in \mathbf{X}_{\text{PF}}.$$

This variational formulation of the Penrose-Fife model is ideal for coarse graining. Assuming that the entropy density $\widehat{S}$, the mobility m, and the heat conduction tensor κ depend periodically on a microscopical variable in the form

$$\widehat{S}_\varepsilon = \mathbb{S}(\frac{1}{\varepsilon}x, z, e) - \frac{1}{2}\nabla z \cdot \mathbb{A}(\frac{1}{\varepsilon}x)\nabla z, \quad m_\varepsilon(x) = \mathbb{M}(\frac{1}{\varepsilon}x), \quad \kappa_\varepsilon(x) = \mathbb{H}(\frac{1}{\varepsilon}x),$$

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one can pass to the homogenization limit $\varepsilon \to 0$ using the abstract methods for evolutionary Γ-convergence described in [Mie14]. In [MiS15] it is shown that solutions $(z^\varepsilon, e^\varepsilon)$ for the gradient system $(\mathbf{X}_{\mathrm{PF}}, \mathcal{S}_\varepsilon, \mathcal{P}_\varepsilon)$ converge to the unique solution (z^0, e^0) of the limiting gradient system $(\mathbf{X}_{\mathrm{PF}}, \mathcal{S}_0, \mathcal{P}_0)$, if this is true for the initial conditions.

The effective entropy functional $\mathcal{S}_0$ and the effective EPP $\mathcal{P}_0$ are

$$\mathcal{S}_0(z, e) = \int_\Omega S_{\mathrm{eff}}(z, e) - \tfrac{1}{2} \nabla z \cdot A_{\mathrm{hom}} \nabla z \, dx, \quad \mathcal{P}_0^*(\xi_z, \xi_e) = \tfrac{1}{2} \int_\Omega m_{\mathrm{harm}} \xi_z^2 + \nabla \xi_e \cdot H_{\mathrm{hom}} \nabla \xi_e \, dx.$$

Here A_{hom} and H_{hom} are the classical homogenized effective tensors obtained from the periodic functions $\mathbb{A}$ and $\mathbb{H}$, respectively. Moreover, m_{harm} is the harmonic mean of $\mathbb{M}$. More interesting is the homogenization of the nonlinear function $\mathbb{S}$ to obtain S_{eff}. Here one takes advantage of the concavity of the mapping $e \mapsto \mathbb{S}(y, z, e)$. Doing a partial Legendre transform of $-\mathbb{S}$ with dual variable τ, one obtains the free energy evaluated at $\theta = -1/\tau$. After simply averaging $\mathbb{F}(y, z, -1/\tau)$ over the periodicity cell, one can reverse the Legendre transform and obtains $S_{\mathrm{eff}}(z, e)$. We refer to [MiS15] for more details.

4.2 A time-dependent thermoplasticity model

We consider a special case of a linearized non-isothermal elastoplastic material, where the coupling between the strain $\mathbf{e}(u)$ and the temperature is only indirect via the plastic tensor z, cf. [BaR08]. In contrast to the theory so far, we also allow for a time-dependent loading $\ell(t)$. Hence, we consider the functionals

$$\mathcal{E}(t, u, z, \theta) = \int_\Omega \frac{1}{2} |\mathbf{e}(u) - z|_{\mathbb{C}}^2 + \Phi(z, \theta) \, dx - \langle \ell(t), u \rangle \quad \text{and} \quad \mathcal{S}(u, z, \theta) = \int_\Omega S(z, \theta) \, dx,$$

where $|\mathbf{e}|_{\mathbb{C}}^2 = \mathbf{e} : \mathbb{C} \mathbf{e}$ and Gibbs relation $\partial_\theta \Phi = \theta \partial_\theta S$. Setting $E(e, z, \theta) = \frac{1}{2} |\mathbf{e} - z|_{\mathbb{C}}^2 + \Phi(z, \theta)$, we will explicitly use the decouplings $\partial_{\mathbf{e}} \partial_\theta E = 0 = \partial_{\mathbf{e}} S$.

We note that $\mathrm{D}_u \mathcal{S} \equiv 0$ implies that the elastic equilibrium takes the form

$$0 = \mathrm{D}_u \mathcal{E}(t, u, z, \theta) - \theta * \mathrm{D}_u \mathcal{S}(u, z, \theta) = \mathrm{D}_u \mathcal{E}(t, u, z, \theta) = -\operatorname{div}\left(\mathbb{C}(\mathbf{e}(u) - z)\right) - \ell(t).$$

In particular, we are able to solve this equation for u as a nonlocal function of z and the loading $\ell(t)$, namely $u(t) = \mathbf{U}(z(t), \ell(t))$, where $\mathbf{U} : \mathrm{L}^2(\Omega; \mathbb{R}^{d \times d}_{0, \mathrm{sym}}) \times (\mathrm{H}^1_{\mathrm{D}}(\Omega; \mathbb{R}^d))^* \to \mathrm{H}^1_{\mathrm{D}}(\Omega; \mathbb{R}^d)$ is a bounded linear operator.

Respecting the energy conservation, we can take the dual EPP $\mathcal{P}^*$ in the form

$$\mathcal{P}^*(q; \xi_u, \xi_z, \xi_\theta) = \mathcal{P}_0^*\left(q; \xi_z - \frac{\xi_\theta}{\partial_\theta \Phi(z, \theta)} * \mathrm{D}_z \mathcal{E}(t, q), \frac{\xi_\theta}{\partial_\theta \Phi(z, \theta)}\right),$$

which clearly satisfies $\mathcal{P}^*(q; \boldsymbol{\xi} + \lambda \mathrm{D}\mathcal{E}(t, q)) = \mathcal{P}^*(q, \boldsymbol{\xi})$.

Defining the reduced energy $\widehat{\mathcal{E}}(t, z, \theta) := \mathcal{E}(t, \mathbf{U}(z, \ell(t)), \theta)$ we find the relations

$$\widehat{\mathcal{E}}(t, z, \theta) = \int_\Omega \frac{1}{2} z : \mathbf{A} z + \Phi(z, \theta) \, dx - \langle z, a(t) \rangle,$$

where $\mathbf{A}$ is a bounded, symmetric, and non-negative linear operator from $\mathrm{L}^2(\Omega; \mathbb{R}^{d \times d}_{0, \mathrm{sym}})$ into itself and $a(t) = \mathbf{K} \ell(t)$ for a suitable bounded linear operator $\mathbf{K}$. Thus, Theorem 3.4

yields the gradient-flow equation

$$\begin{pmatrix} \dot{z} \\ \dot{\theta} \end{pmatrix} = \partial_{\boldsymbol{\xi}} \mathcal{P}^*(z, \theta; \mathrm{D}\mathcal{S}(z, \theta)) = \begin{pmatrix} I & 0 \\ \frac{-1}{\partial_\theta \Phi} \mathrm{D}_z \widehat{\mathcal{E}} & \frac{1}{\partial_\theta \Phi} \end{pmatrix} \partial_{\boldsymbol{\xi}} \mathcal{P}_0^* \Big(z, \theta; \begin{pmatrix} I & \frac{-1}{\partial_\theta \Phi} * \mathrm{D}_z \widehat{\mathcal{E}} \\ 0 & \frac{1}{\partial_\theta \Phi} \end{pmatrix} \begin{pmatrix} \mathrm{D}_z \mathcal{S} \\ \mathrm{D}_\theta \mathcal{S} \end{pmatrix} \Big).$$

We emphasize here that the transformation inside $\partial_{\boldsymbol{\xi}} \mathcal{P}^*$ via $\mathrm{D}_z \widehat{\mathcal{E}} = \mathbf{A}z + \partial_z \Phi(z, \theta) - a(t)$ is time-dependent and nonlocal because of $\mathbf{A}$.

To simplify the gradient structure we reformulate it using the internal energy

$$e(x) := \frac{1}{2} z(x) : (\mathbf{A}z)(x) + \Phi(z(x), \theta(x)),$$

where we note that the nonlocal operator $\mathbf{A}$ has to be taken with care. This relation can be inverted to express the temperature as function of z and e as follows. Denote by $\theta = \widetilde{\Theta}(z, \widetilde{e})$ the unique solution of $\widetilde{e} = \Phi(z, \theta)$ and define $\widetilde{S}(z, \widetilde{e}) = S(z, \widetilde{\Theta}(z, \widetilde{e}))$, which gives $\partial_{\widetilde{e}} \widetilde{S}(z, \widetilde{e}) = 1/\widetilde{\Theta}(z, \widetilde{e})$ by Gibbs relation $\partial_\theta \Phi = \theta \partial_\theta S$. Then, with $\widetilde{e} = e - \frac{1}{2} z : \mathbf{A}z$, the total energy, total entropy, and the dual EPP read

$$\widetilde{\mathcal{E}}(t, z, e) = \int_\Omega e - a(t){:}z \, \mathrm{d}x, \qquad \widetilde{\mathcal{S}}(z, e) = \int_\Omega \widetilde{S}(z, e - \tfrac{1}{2} z{:}\mathbf{A}z) \, \mathrm{d}x, \quad \text{and}$$

$$\widetilde{\mathcal{P}}^*(t, z, e; \xi_z, \xi_e) := \widetilde{\mathcal{P}}_0^*(z, e; \xi_z + \xi_e a(t), \xi_e) = \widetilde{\mathcal{P}}_0^* \Big(z, e; \begin{pmatrix} I & a(t) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \xi_z \\ \xi_e \end{pmatrix} \Big).$$

The energy balance $\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(t, z(t), e(t)) = \partial_t \mathcal{E}(t, z(t), e(t))$ along solutions still follows from the relation $\widetilde{\mathcal{P}}_0^*(z, e; \boldsymbol{\xi} + (0, \lambda)^{\mathsf{T}}) = \widetilde{\mathcal{P}}_0^*(z, e; \boldsymbol{\xi})$ for all constants $\lambda \in \mathbb{R}$.

The primal EPP $\widetilde{\mathcal{P}}$ takes a similar time-dependent form

$$\widetilde{\mathcal{P}}(t, z, e; \dot{z}, \dot{e}) = \widetilde{\mathcal{P}}_0(z, e; \dot{z}, \dot{e} - a(t){:}\dot{z}) = \widetilde{\mathcal{P}}_0\big(z, e; \mathbf{N}(t)\big(\begin{smallmatrix} \dot{z} \\ \dot{e} \end{smallmatrix}\big)\big) \text{ with } \mathbf{N}(t) := \begin{pmatrix} I & 0 \\ -a(t){:}\square & 1 \end{pmatrix},$$

where $\mathcal{P}_0(z, e; v, w) = \infty$ if $\int_\Omega w \, \mathrm{d}x \neq 0$, which enforces energy conservation.

In total, the generalized gradient flow for this simple thermoplastic model can be written in the following two equivalent forms

$$\begin{pmatrix} \dot{z} \\ \dot{e} \end{pmatrix} = \mathbf{N}(t)^{-1} \partial_{\boldsymbol{\xi}} \widetilde{\mathcal{P}}_0^* \Big(z, e; \begin{pmatrix} \mathrm{D}_z \widetilde{\mathcal{S}} + \mathrm{D}_e \widetilde{\mathcal{S}} \, a(t) \\ \mathrm{D}_e \widetilde{\mathcal{S}}(z, e) \end{pmatrix} \Big) \quad \Longleftrightarrow$$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} \in \mathbf{N}(t)^* \partial_{\mathbf{v}} \widetilde{\mathcal{P}}_0\Big(z, e; \mathbf{N}(t)\begin{pmatrix} \dot{z} \\ \dot{e} \end{pmatrix}\Big) - \begin{pmatrix} \mathrm{D}_z \widetilde{\mathcal{S}}(z, e) \\ \mathrm{D}_e \widetilde{\mathcal{S}}(z, e) \end{pmatrix}.$$

We consider a specially simple case of thermo-viscoplastic gradient plasticity by choosing

$$\widetilde{\mathcal{P}}_0(z, e; v, w) = \sigma_{\text{yield}} \|v\|_{\mathrm{L}^1} + \frac{\mu}{2} \|v\|_{\mathrm{L}^2}^2 + \frac{\kappa}{2} \|w\|_{\mathrm{H}^{-1}}^2 \quad \text{and}$$

$$\widetilde{\mathcal{S}}(z, e) = \int_\Omega \widetilde{S}(z, e - \frac{1}{2} z{:}\mathbf{A}z) - \frac{\nu}{2} |\nabla z|^2 \, \mathrm{d}x,$$

where $\|w\|_{\mathrm{H}^{-1}}^2 = \|\nabla \phi\|_{\mathrm{L}^2}^2$ if $\Delta \phi = w$ in Ω and $\nabla \phi \cdot n = 0$ on $\partial \Omega$. This leads to the generalized gradient flow equation

$$\begin{aligned} 0 &= \sigma_{\text{yield}} \operatorname{Sign}(\dot{z}) + \mu \dot{z} + \partial_z \widehat{S}(z, e - \tfrac{1}{2} z{:}\mathbf{A}z) - \tfrac{1}{2}\big(\Xi\,(\mathbf{A}z) + \mathbf{A}(\Xi z)\big) + \nu \Delta z, \\ 0 &= \dot{e} - a(t){:}\dot{z} - \kappa \Delta \Xi, \qquad \text{where } \Xi = \partial_{\widetilde{e}} \widetilde{S}\big(z, e - \tfrac{1}{2} z{:}\mathbf{A}z\big). \end{aligned} \tag{4.3}$$

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Here $\Xi = \partial_{\widetilde{e}}\widetilde{S}$ denotes the inverse temperature $1/\theta$.

In particular, the second formulation gives rise to a simple time-incremental minimization procedure, which is well-known in isothermal elastoplasticity (cf. [OrR99, OrS99, CHM02, Mie03, DDM06, MaM09, DDS11]), but is new for the non-isothermal case:

$$(\text{TIMP})_* \qquad \begin{pmatrix} z^{k+1} \\ e^{k+1} \end{pmatrix} \in \underset{(z,e)}{\text{Arg min}} \; (t^{k+1}-t^k)\widetilde{\mathcal{P}}_0\Big(z^k, e^k; \tfrac{1}{t^{k+1}-t^k}\mathbf{N}(t^k)\begin{pmatrix} z-z^k \\ e-e^k \end{pmatrix}\Big) - \widetilde{\mathcal{S}}(z,e).$$

We emphasize that $(\text{TIMP})_*$ is not equivalent to the one proposed in (3.7), since here we eliminated u beforehand by using the nonlocal operator $\mathbf{A}$. So, $(\text{TIMP})_*$ should be preferable if $\mathbf{A}$ is available. Again, we observe that the concavity of $\widetilde{\mathcal{S}}$ implies that the minimum problem is convex. In the case of viscoplasticity, $\widetilde{\mathcal{P}}_0$ is even strictly convex, so there is a unique minimizer in each time step. Thus, it should be possible to show existence of solutions for the thermo-viscoplastic system in (4.3). Unfortunately, the methods developed in [MiS15] and based on the (EVI) are not applicable because of the nonquadratic behavior of $\widetilde{\mathcal{P}}_0$ due to $\sigma_{\text{yield}} > 0$.

4.3 A thermoplastic model with thermal expansion

Finally, we consider a classical plasticity model (see e.g. [BaR10]) where thermal expansion leads to a stronger coupling of elastostatics and heat conduction. As usual we again start with a free energy containing a thermal expansion tensor $\mathbb{E} \in \mathbb{R}^{d\times d}_{\text{sym}}$ in the form

$$F(\nabla u, z, \nabla z, \theta) = \frac{1}{2}|\mathbf{e}(u){-}z|^2_{\mathbb{C}} + \psi_1(\theta)\mathbb{E}{:}\mathbf{e}(u) + H(z) + \frac{\sigma\theta}{2}|\nabla z|^2 - \frac{c}{\alpha(1{+}\alpha)}\theta^{1+\alpha},$$

with $c > 0$ and $\alpha \in]0, 1[$. We obtain the energy and entropy functionals

$$\mathcal{E}(u, z, \theta) = \int_\Omega \frac{1}{2}|\mathbf{e}(u){-}z|^2_{\mathbb{C}} + \widetilde{\psi}_1(\theta)\mathbb{E}{:}\mathbf{e}(u) + H(z) + \frac{c\theta^{1+\alpha}}{1+\alpha} \, \mathrm{d}x,$$

$$\mathcal{S}(u, z, \theta) = \int_\Omega \frac{c}{\alpha}\theta^\alpha - \psi'_1(\theta)\mathbb{E}{:}\mathbf{e}(u) - \frac{\nu}{2}|\nabla z|^2 \, \mathrm{d}x,$$

where $\widetilde{\psi}_1(\theta) = \psi_1(\theta) - \theta\psi'_1(\theta)$. Clearly, $\alpha * \mathrm{D}_u\mathcal{S}(u, z, \theta) = -\operatorname{div}(\alpha\psi'_1(\theta)\mathbb{E})$ is non-zero, so the reduction to a local gradient system is not possible, unless we replace the temperature θ by a more convenient thermodynamically variable r. A possible choice is

$$r = R(\mathbf{e}(u), \theta) := \frac{c}{\alpha}\theta^\alpha - \psi'_1(\theta)\mathbb{E}{:}\mathbf{e}(u).$$

Since we also need the inverse transformation $\theta = \Theta(\mathbf{e}(u), r)$, we assume $\psi_1(\theta) = \theta$ for notational simplicity. Then $\widetilde{\psi}_1 \equiv 0$ and $\theta = \Theta(\mathbf{e}, r) = \big(\alpha(r{+}\mathbb{E}{:}\mathbf{e})/c\big)^{1/\alpha}$, and the functionals take the form

$$\mathcal{E}(u, z, r) = \int_\Omega \frac{1}{2}|\mathbf{e}(u){-}z|^2_{\mathbb{C}} + H(z) + \frac{\alpha c_\alpha}{1+\alpha}\big(r{+}\mathbb{E}{:}\mathbf{e}(u)\big)^{1+1/\alpha} \, \mathrm{d}x,$$

$$\mathcal{S}(u, z, r) = \int_\Omega r - \frac{\nu}{2}|\nabla z|^2 \, \mathrm{d}x, \; \text{where } c_\alpha = (\alpha/c)^{1/\alpha}.$$

This choice now guarantees that $A(u, z, r) \equiv 0$ and the reduction to a local gradient system for (z, r) can be done as described at the end of Section 3.3. In particular the solution $u = \mathrm{U}(z, r)$ can be obtained as the unique minimizer of the convex functional $u \mapsto \mathcal{E}(u, z, r)$. The corresponding Euler-Lagrange equation reads

$$- \operatorname{div}\left(\mathbb{C}(\mathbf{e}(u) - z) + c_\alpha(r + \mathbb{E}{:}\mathbf{e}(u))^{1/\alpha}\mathbb{E} \right) = 0.$$

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