On thermodynamically consistent models and gradient structures for thermoplasticity

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Dedicated to Hans-Dieter Alber on the occasion of his sixtieth birthday

1 Introduction

While there is a vast mathematical literature for theory of time-dependent isothermal plasticity, the corresponding temperature-dependent theory is just starting to develop, see e.g. [BaR08, Rou10, BaR10]. However, it is restricted to the small-strain setting. The isothermal theory is developed along two threads of research, namely (1) via monotone operators and variational inequalities [Alb98, HaR99] for the small-strain situation and (ii) via incremental minimization for the finite-strain situation based on the multiplicative decomposition of the strains [OrR99, CHM02, MiM06, MaM09].

The latter theory is reminiscent to the theory of geometric evolution in metric spaces, see [Mie09], and it is the purpose of this note to prepare the grounds for similar approaches in the non-isothermal case. We want to give simple modeling approaches to such systems based on basic physical principles. The main idea is to extend the gradient structure for the heat equation (see [Ott01, AGS05]) to include plasticity as well. A similar theory was derived successfully for the thermodynamically consistent phase-field equations was achieved via the Penrose-Fife model in [PeF90], which we will address also in Section 2.3.

In situations where the internal variables contains gradient terms there seems to be some confusion about thermodynamically consistent models, and we hope to clear up this issue here. The main point is that one has to use the differential of the entropy functional as a driving force for the dissipative internal variables, rather than the previously used differential of the free energy (cf. [PeF93]). This idea was the crucial step in the Penrose-Fife model [PeF90], and a similar concept was used also in temperature-dependent semiconductor models and reaction-diffusion systems, see [AGH02, Mie10b].

In thermomechanics of elastic solids this issue seems to be les known. The theory is here more difficult, since the stress balance is obtained from minimizing the free energy, while the the plastic flow rule and the heat transport are driven by the entropy functional. In Section 2.1 we explain these structures starting from the GENERIC framework introduced in [GrÖ97] and adapted to solid mechanical problems in [Mie10a].

2 Thermomechanical modeling

General thermomechanical models contain reversible mechanical behavior such as elastic waves as well as dissipative behavior like heat conduction or internal friction. A proper modeling of the interplay between these phenomena is important, in particular the thermodynamic consistency. The latter asks for the existence of suitable thermodynamic quantities such as temperature, internal energy, and entropy as well as the relations between them. All constitutive modeling of a material should satisfy the fundamental laws such as the first and second law of thermodynamics at each material point.

Throughout this note we will study closed systems only, where the total energy $\mathcal{E}$ will be conserved and the total entropy $\mathcal{S}$ will be increasing.

2.1 GENERIC

The framework GENERIC is an acronym for General Equations for Non-Equilibrium Reversible Irreversible Coupling, see [GrÖ97, Ött05]. We consider a state variable X (containing displacement, velocity, internal variables, temperature field) in the state space $\mathcal{X}$ driven by the equation

$$\dot{X} = J(X)\mathrm{D}\mathcal{E}(X) + K(X)\mathrm{D}\mathcal{S}(X). \tag{2.1}$$

Here the functional $\mathcal{E}$ is the total energy and $\mathcal{S}$ is the total entropy. The mappings $J(X), K(X) : \mathrm{T}_X^* \mathcal{X} \to \mathrm{T}_X \mathcal{X}$ define geometric structures on the state space. Usually they are assumed to be linear, but for plasticity we will generalize the linearity of $K(X)$ to subdifferentials of convex entropy-production potential $\mathcal{K}^*$, i.e. the linear mapping $\xi \mapsto K(X)\xi$ will be replaced by the nonlinear, but monotone mapping $\xi \mapsto \partial_\xi \mathcal{K}^*(X;\xi)$.

The structure conditions on J and K are the following: the reversible dynamics is given by J which defines a co-symplectic structure, which means that $J(X) = -J(X)^*$ and that the Jacobi identity holds for the corresponding Poisson bracket $\{\mathcal{F}, \mathcal{G}\} := \langle \mathrm{D}\mathcal{F}, J\mathrm{D}\mathcal{G}\rangle$. In contrast, the irreversible part is driven by a dissipative structure K satisfying $K(X) = K(X)^* \geq 0$.

The crucial assumption of GENERIC is the mutual non-interaction condition

$$J(X)\mathrm{D}\mathcal{S}(X) = 0 \quad \text{and} \quad K(X)\mathrm{D}\mathcal{E}(X) = 0 \quad \text{for all } X \in \mathcal{X}. \tag{2.2}$$

It reflects the first and the second law of thermodynamics. In particular, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(X(t)) = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(X(t)) = \langle \mathrm{D}\mathcal{S}(X), K(X)\mathrm{D}\mathcal{S}(X)\rangle \geq 0.$$

2.2 Generalized gradient systems

For quasistatic systems, where inertia is neglected there are no reversible effects any more. So there is hope that after elimination of the elastic variables from the equilibrium equation, the problem can be written as a gradient system. We consider generalized gradient systems $(\mathcal{Y}, \Phi, \Psi)$, where $\mathcal{Y}$ is a Banach space, $\Phi : \mathcal{Y} \times \mathbb{R}_\infty$ is the driving potential, and $\Psi : \mathrm{T}\mathcal{Y} \to [0, \infty]$ is the dissipation potential. For a classical gradient system we have $\Psi(y, v) = \frac{1}{2}\langle G(y)v, v\rangle$, while for generalized gradient systems $\Psi(y, \cdot) : \mathcal{Y} \to [0, \infty]$ may be a general convex and lower semicontinuous functional.

The generalized gradient flow is given in the form

$$0 \in \partial_{\dot{y}} \Psi(y, \dot{y}) + \mathrm{D}\Phi(y) \quad \text{in } \mathrm{T}_z^* \mathcal{Y} \sim \mathcal{Y}^*. \tag{2.3}$$

An equivalent formulation is obtained by using the Legendre transform $\Psi^*(y, \cdot) = \mathcal{L}[\Psi(y, \cdot)]$, namely $\Psi^*(y, \eta) = \sup\{\langle \eta, v \rangle - \Psi(y, v) \mid v \in \mathcal{Y}\}$. Then, (2.3) is equivalent to the rate equation

$$\dot{y} = \partial_\eta \Psi^*(y, -\mathrm{D}\Phi(y)). \tag{2.4}$$

In our applications to thermomechanical systems the driving functional will be the (negative) entropy $\mathcal{S}$ and there will be an additional energy functional $\mathcal{E}$ which has to conserved along solutions. For this we will use the following notations $(\mathcal{Y}, \mathcal{S}, \mathcal{E}, \mathcal{K})$, where $\mathcal{K}$ is called the entropy-production potential. In our applications we will have $y = (z, \theta)$ where z is an internal variable and θ is the temperature. The entropy-driven evolution takes the form

$$\dot{y} = \partial_\eta \mathcal{K}^*(y, \mathrm{D}\mathcal{S}(y)), \qquad \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(y(t)) = 0. \tag{2.5}$$

The latter condition is not to be posed in addition, but will follow from a structural condition on $\mathcal{K}$, namely

$$\forall\, y \in \mathcal{Y}, \ \eta \in \mathcal{Y}^*, \ \lambda \in \mathbb{R}: \quad \mathcal{K}^*(y, \eta + \lambda \mathrm{D}\mathcal{E}(y)) = \mathcal{K}^*(y, \eta). \tag{2.6}$$

This condition can be seen as a remainder of $(2.2)_2$ and has the implication $\mathcal{K}(y, v) = \infty$ if $\langle \mathrm{D}\mathcal{E}(y), v \rangle \neq 0$.

2.3 The Penrose-Fife model

This model combines a phase-field variable z and the temperature θ defined on a domain $\Omega \subset \mathbb{R}^d$. The free energy is given in the form $\psi = \overline{\psi}(z, \nabla z, \theta) = -c\theta(\log \theta - 1) + \psi_0(z) + \theta\left(\psi_1(z) + \frac{1}{2}\kappa |\nabla z|^2\right)$. The functionals are

$$\mathcal{E}(z, \theta) = \int_\Omega c\theta + \psi_0(z) \, \mathrm{d}x \quad \text{and} \quad \mathcal{S}(z, \theta) = \int_\Omega c \log \theta - \psi_1(z) - \frac{k}{2}|\nabla z|^2 \, \mathrm{d}x.$$

The dual entropy-production potential $\mathcal{K}^*$ takes the form

$$\mathcal{K}^*(\xi_z, \xi_\theta) = \int_\Omega \frac{M(z, \theta)}{2}\left(\xi_z - \frac{\psi_0'(z)}{c}\xi_\theta\right)^2 + \frac{\kappa(z, \theta)}{2}|\nabla \xi_\theta|^2 \, \mathrm{d}x.$$

Obviously (2.6) holds and $(\dot{z}, \dot{\theta}) = \partial \mathcal{K}^*(z, \theta, \mathrm{D}\mathcal{S}(z, \theta))$ gives the Penrose-Fife system

$$\dot{z} = M(z, \theta)\left(k\Delta z - \psi_1'(z) - \frac{\psi_0'(z)}{\theta}\right), \quad \dot{\theta} + \frac{\psi_0'(z)}{c}\dot{z} = \operatorname{div}\left(\frac{c\kappa(z, \theta)}{\theta^2}\nabla\theta\right).$$

Note that the right-hand side of the the first equation is given in terms of M times $\mathrm{D}_z\mathcal{S} - \frac{1}{\theta}\mathrm{D}_z\mathcal{E}$, which is not a multiple of the differential of the free energy, see the discussion in [PeF93] (where previous phase-field models where shown to be thermodynamically inconsistent). The driving force $\mathrm{D}_z\mathcal{S} - \frac{1}{\theta}*\mathrm{D}_z\mathcal{E}$ will be fundamental in Section 3.2. We also refer to [AGH02, Mie10a] for more discussion.

3 Thermoplasticity

In this section we treat the system of thermoplasticity, where we neglect inertia terms and viscoelastic effects but take temperature into account. For the treatment of more general cases we refer to [Mie10a], where the details are worked out in the GENERIC framework. For plasticity we allow for rate-independent as well as viscoplastic terms. In fact, we will not use any specific properties of plasticity, but rather treat general *dissipative materials*, also called *generalized standard materials* with an internal variable $z : \Omega \to \mathbb{R}^m$, which can contain the plastic strain, hardening variables, but also magnetization, polarization or any other dissipative internal variable.

3.1 Variational and other derivatives of densities

To write the balance equations in an efficient way we introduce the following notations. For a function $g(w, \nabla w)$ and smooth functions $w, \widetilde{w} : \Omega \to \mathbb{R}^k$ we write

$$\Delta_w g[\widetilde{w}] := \partial_w g(w, \nabla w) \cdot \widetilde{w} + \partial_{\nabla w} g(w, \nabla w) : \nabla \widetilde{w} : \Omega \to \mathbb{R},$$

$$\delta_w g := \partial_w g(w, \nabla w) - \mathrm{div}\left(\partial_{\nabla w} g(w, \nabla w)\right) : \Omega \to \mathbb{R}^k,$$

where the latter is the standard variational derivative. For $\alpha : \Omega \to \mathbb{R}$ we will also need the following nonstandard definition:

$$\alpha * \delta_w g := \alpha \partial_w g(w, \nabla w) - \mathrm{div}\left(\alpha \partial_{\nabla w} g(w, \nabla w)\right) : \Omega \to \mathbb{R}^k,$$

where the multiplication with α occurs *under* the divergence. Thus, this notion is defined only for variational derivatives! The following divergence identity will be crucial for the subsequent derivations:

$$\alpha * \delta_w g \cdot \widetilde{w} = \alpha \Delta_w g[\widetilde{w}] + \mathrm{div}\left(\alpha \partial_{\nabla w} g(w, \nabla w) \cdot \widetilde{w}\right). \tag{3.1}$$

Hence, the mapping $\alpha \mapsto \alpha * \delta_w g$ can be seen as an adjoint of the mapping $\widetilde{w} \mapsto \Delta_w g[\widetilde{w}]$.

3.2 The coupled balance equations

We consider a body $\Omega \subset \mathbb{R}^d$ on which the deformation $\phi : \Omega \to \mathbb{R}^d$, the internal variable $z : \Omega \to \mathbb{R}^m$, and the temperature field $\theta : \Omega \to]0, \infty[$ are defined. Throughout, we assume that the system is closed in such a way that all integrations by parts can be done without generating contributions, so we neglect them for notational simplicity.

The free energy ψ will be given in the form $\psi = \overline{\psi}(\phi, \nabla \phi, z, \nabla z, \theta)$, where the possible dependence on x is suppressed. The dependence on ϕ appears for maximal generality and notational consistency. Moreover, this allows for the inclusion of an external volume loading f_{ext} with an additive term $-f_{\mathrm{ext}}(x) \cdot \phi$. The entropy s and the internal energy e are defined in the usual way, namely $\overline{s} := -\partial_\theta \overline{\psi}$ and $\overline{e} := \overline{\psi} + \theta \overline{s}$. The balance equations are now given in the standard form:

elastic force balance	$0 = \delta_\phi \overline{\psi},$	(3.2a)
internal force balance	$0 \in \partial_{\dot{z}} R_{\mathrm{pl}}(z, \theta; \dot{z}) + \delta_z \overline{s} - \dfrac{1}{\theta} * \delta_z \overline{e},$	(3.2b)
energy balance	$\dfrac{\mathrm{d}}{\mathrm{d}t} \overline{e} = \Delta_\phi \overline{\psi}[\dot{\phi}] - \mathrm{div}\left(\kappa \nabla\left(\dfrac{1}{\theta}\right)\right),$	(3.2c)

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where κ/θ^2 is the standard heat conduction coefficient. The plastic entropy-production potential R_{pl} may contain rate-independent and viscous terms, e.g.

$$R_{\mathrm{pl}}(z, \theta; v) = \frac{\sigma_{\mathrm{yield}}(z, \theta)}{\theta}|v| + \frac{1}{2}v \cdot V(z, \theta)v.$$

The energy balance (3.2c) reflects the fact that the internal energy only changes because of the mechanical work $\Delta_\phi \overline{\psi}[\dot{\phi}]$ and the heat flow $-\operatorname{div}\left(\kappa \nabla\left(\frac{1}{\theta}\right)\right)$.

The special form of the driving force in the internal force balance is justified as in the Penrose-Fife model as follows. Note that it cannot be written in the often used form $-\frac{1}{\theta}\delta_z \overline{\psi}$, which leads to thermodynamically inconsistent models [PeF93]. However, using $\overline{s} - \frac{1}{\theta}\overline{e} = -\overline{\psi}/\theta$ it has the form $-\delta_z(\overline{\psi}/\theta) = -\frac{1}{\theta}*\delta_z\overline{\psi}$. Because our aim is to use energy and entropy functionals, we prefer the formulation using $\overline{s}$ and $\overline{e}$. Moreover, we find

$$\frac{\mathrm{d}}{\mathrm{d}t}s = \left(\Delta_z\overline{s} - \frac{1}{\theta}\Delta_z\overline{e}\right)[\dot{z}] + \frac{\kappa}{\theta}|\nabla\left(\frac{1}{\theta}\right)|^2 - \operatorname{div}\left(\frac{\kappa}{\theta}\nabla\left(\frac{1}{\theta}\right)\right).$$

Using (3.1) the first term on the right-hand side can be written as $(\delta_z\overline{s} - \frac{1}{\theta}*\delta_z\overline{e}) \cdot \dot{z} - \operatorname{div}(\dots)$. Using (3.2b) the first term gives the plastic entropy production

$$\partial_{\xi_z}R_{\mathrm{pl}}^*(z, \theta, \delta_z\overline{s} - \frac{1}{\theta}*\delta_z\overline{e}) \cdot (\delta_z\overline{s} - \frac{1}{\theta}*\delta_z\overline{e}) \geq 0,$$

while the divergence term $\operatorname{div}(\dots)$ contributes to the entropy flux.

Our plastic driving force in (3.2b) is different from the one in [Rou10], where $\delta_z\overline{\psi}$ is used and the entropy production is defined as a function of $\dot{z}$. There, a local entropy equation is used instead of our local energy balance (3.2c). We expect that (3.2c) does not hold under the situation considered in [Rou10].

3.3 General thermodynamic variables

To understand the structure of our coupled system (3.2) better, it is advantageous to use a general thermodynamic variable τ, which can either be θ, s, e, or any monotone function of it (like the enthalpy $w = h_0(\theta)$ in [BaR10]). We then have constitutive functions

$$e = E(\phi, \nabla\phi, z, \nabla z, \tau) \quad \text{and} \quad s = S(\phi, \nabla\phi, z, \nabla z, \tau).$$

Using the abbreviations $w = (\phi, z)$ and $W = (w, \nabla w)$ we have the relations

$$\theta = \Theta(W, \tau) = \frac{\partial_\tau E(W, \tau)}{\partial_\tau S(W, \tau)}, \quad \partial_W \overline{\psi}(W, \Theta(W, \tau)) = \partial_W E(W, \tau) - \Theta(W, \tau)\partial_W S(W, \tau).$$

We now formulate the coupled balance equations (3.2) in abstract form via the functionals

$$\mathcal{E}(\phi, z, \tau) = \int_\Omega E(\phi, \nabla\phi, z, \nabla z, \tau)\,\mathrm{d}x \quad \text{and} \quad \mathcal{S}(\phi, z, \tau) = \int_\Omega S(\phi, \nabla\phi, z, \nabla z, \tau)\,\mathrm{d}x.$$

By using the identifications $\mathrm{D}_w\mathcal{E} = \delta_w E$ we arrive at the form

$$0 = \mathrm{D}_\phi\mathcal{E}(\phi, z, \tau) - \frac{\mathrm{D}_\tau\mathcal{E}}{\mathrm{D}_\tau\mathcal{S}} * \mathrm{D}\mathcal{S}(\phi, z, \tau), \tag{3.3a}$$

$$\dot{z} = \partial_{\xi_z}R_{\mathrm{pl}}^*\left(z, \tau; \mathrm{D}_z\mathcal{S} - \frac{\mathrm{D}_\tau\mathcal{S}}{\mathrm{D}_\tau\mathcal{E}} * \mathrm{D}_z\mathcal{E}\right), \tag{3.3b}$$

$$\dot{\tau} = \frac{1}{\mathrm{D}_\tau\mathcal{E}}\left(-\frac{\mathrm{D}_\tau\mathcal{E}}{\mathrm{D}_\tau\mathcal{S}}\Delta_\phi S[\dot{\phi}] - \Delta_z E[\dot{z}] - \operatorname{div}\left(\kappa\nabla\left(\frac{\mathrm{D}_\tau\mathcal{S}}{\mathrm{D}_\tau\mathcal{E}}\right)\right)\right). \tag{3.3c}$$

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This formulation displays the different contributions of the energy and the entropy in a clear fashion. Note that we have eliminated θ via $\frac{D_\tau \mathcal{E}}{D_\tau \mathcal{S}} = \frac{\partial_\tau E}{\partial_\tau S}$. The term $-\frac{1}{\partial_\tau S}\Delta_\phi S[\dot\phi]$ in (3.3c) expresses the exchange of latent heat, see also [Mie10a].

We can easily check the conservation of the total energy via

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{E} = \langle \mathrm{D}_\phi \mathcal{E}, \dot\phi \rangle + \langle \mathrm{D}_z \mathcal{E}, \dot z \rangle + \langle \mathrm{D}_\tau \mathcal{E}, \dot\tau \rangle$$

$$= \langle \theta * \mathrm{D}_\phi \mathcal{S}, \dot\phi \rangle + \langle \mathrm{D}_z \mathcal{E}, \dot z \rangle - \int_\Omega \theta \, \Delta_\phi S[\dot\phi] + \Delta_z E[\dot z] + \mathrm{div}(...) \, \mathrm{d}x = 0,$$

because the first and second terms on the right-hand side cancel the third and fourth terms, respectively.

3.4 The gradient structure based on entropy

We introduce the dual entropy-production potential, acting on z and τ only, via

$$\mathcal{K}^*(\phi, z, \tau; \xi_z, \xi_\tau) = \int_\Omega R_{\mathrm{pl}}^*\left(z, \tau; \xi_z - \frac{\xi_\tau}{D_\tau \mathcal{E}(\phi, z, \tau)} * D_z \mathcal{E}(\phi, z, \tau)\right) \mathrm{d}x$$

$$+ \int_\Omega \frac{\kappa(z, \tau)}{2}\left|\nabla \frac{\xi_\tau}{D_\tau \mathcal{E}(\phi, z, \tau)}\right|^2 \mathrm{d}x.$$

The derivatives with respect to ξ_z and ξ_τ take the form

$$\partial_{\xi_z} \mathcal{K}^*(\phi, z, \tau; \xi_z, \xi_\tau) = \partial_\zeta R_{\mathrm{pl}}^*\left(z, \tau; \xi_z - \frac{\xi_\tau}{D_\tau \mathcal{E}(\phi, z, \tau)} * D_z \mathcal{E}(\phi, z, \tau)\right),$$

$$\partial_{\xi_\tau} \mathcal{K}^*(\phi, z, \tau; \xi_z, \xi_\tau) = \frac{-1}{D_\tau \mathcal{E}}\Delta_z E\left[\partial_\zeta R_{\mathrm{pl}}^*\left(z, \tau; \xi_z - \frac{\xi_\tau}{D_\tau \mathcal{E}} * D_z \mathcal{E}\right)\right] - \frac{1}{D_\tau \mathcal{E}} \mathrm{div}\left(\kappa \nabla\left(\frac{\xi_\tau}{D_\tau \mathcal{E}}\right)\right).$$

Hence it is straightforward to see that (3.3) takes the abstract form

$$0 = \mathrm{D}_\phi \mathcal{E}(\phi, z, \tau) - \frac{D_\tau \mathcal{E}}{D_\tau \mathcal{S}} * D\mathcal{S}(\phi, z, \tau), \tag{3.4a}$$

$$\dot z = \partial_{\xi_z} \mathcal{K}^*(\phi, z, \tau; \mathrm{D}_z \mathcal{S}, \mathrm{D}_\tau \mathcal{S}), \tag{3.4b}$$

$$\dot\tau = -\frac{1}{D_\tau \mathcal{S}}\Delta_\phi S[\dot\phi] + \partial_{\xi_\tau} \mathcal{K}^*(\phi, z, \tau; \mathrm{D}_z \mathcal{S}, \mathrm{D}_\tau \mathcal{S}). \tag{3.4c}$$

Hence, we clearly see that role of the entropy functional $\mathcal{S}$ as a driving potential and the entropy-production potential $\mathcal{K}$ as the dissipation mechanism.

The latter system can be reduced to a gradient system, if we choose $\tau = s$ leading to

$$S(W, s) = s, \quad \theta = \Theta(W, s) = \partial_s E(W, s), \quad \text{and } \partial_W \overline\psi(W, \theta) = \partial_W E(W, s).$$

Moreover, we may assume that $\phi = \Phi(z, s)$ is obtained locally as the (local) minimizer of $\mathcal{E}(\cdot, z, s)$ depending smoothly on z and s. Thus, (3.4a) is satisfied. Since $\Delta_\phi S \equiv 0$, we immediately see that (3.4c) and (3.4c) are equivalent to the *gradient system*

$$\dot z = \partial_{\xi_z}\widetilde{\mathcal{K}}^*(z, s; \mathrm{D}\widetilde{\mathcal{S}}(z, s)), \quad \dot s = \partial_{\xi_s}\widetilde{\mathcal{K}}^*(z, s; \mathrm{D}\widetilde{\mathcal{S}}(z, s)), \tag{3.5}$$

where $\widetilde{\mathcal{K}}^*(z, s; \xi) = \mathcal{K}^*(\Phi(z, s), z, s; \xi)$ and $\mathrm{D}\widetilde{\mathcal{S}}(z, s) = (\mathrm{D}_z\widetilde{\mathcal{S}}(z, s), \mathrm{D}_s\widetilde{\mathcal{S}}(z, s)) = (0, 1) = (\mathrm{D}_z\mathcal{S}(\phi, z, s), \mathrm{D}_s\mathcal{S}(\phi, z, s))$.

The reduction of (3.4) to (3.5) also works for general τ as long as $\mathcal{S}$ does not depend on ϕ, i.e. $\Delta_\phi S[\cdot] \equiv 0$. Moreover, the final gradient system is energy conserving in the form

$$\widetilde{\mathcal{K}}^*(z, \tau; \xi + \lambda \mathrm{D}\widetilde{\mathcal{E}}(z, \tau)) = \widetilde{\mathcal{K}}^*(z, \tau; \xi) \quad \text{for all } z, \tau, \xi, \lambda,$$

where $\widetilde{\mathcal{E}}(z, \tau) = \mathcal{E}(\Phi(z, \tau), z, \tau)$. For this use the corresponding property of $\mathcal{K}^*$ and (3.4a) giving $\mathrm{D}_z\widetilde{\mathcal{E}}(z, \tau) = \mathrm{D}_z\mathcal{E}(\Phi(z, \tau), z, \tau)$ and $\mathrm{D}_\tau\widetilde{\mathcal{E}}(z, \tau) = \mathrm{D}_\tau\mathcal{E}(\Phi(z, \tau), z, \tau)$.

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