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A multi-field incremental variational framework for gradient-extended standard dissipative solids

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ABSTRACT

The paper presents a constitutive framework for solids with dissipative micro-structures based on compact variational statements. It develops incremental minimization and saddle point principles for a class of gradient-type dissipative materials which incorporate micro-structural fields (micro-displacements, order parameters, or generalized internal variables), whose gradients enter the energy storage and dissipation functions. In contrast to classical local continuum approaches to inelastic solids based on locally evolving internal variables, these global micro-structural fields are governed by additional balance equations including micro-structural boundary conditions. They describe changes of the substructure of the material which evolve relatively to the material as a whole. Typical examples are theories of phase field evolution, gradient damage, or strain gradient plasticity. Such models incorporate non-local effects based on length scales, which reflect properties of the material micro-structure. We outline a unified framework for the broad class of first-order gradient-type standard dissipative solids. Particular emphasis is put on alternative multi-field representations, where both the microstructural variable itself as well as its dual driving force are present. These three-field settings are suitable for models with threshold- or yield-functions formulated in the space of the driving forces. It is shown that the coupled macro- and micro-balances follow in a natural way as the Euler equations of minimization and saddle point principles, which are based on properly defined incremental potentials. These multi-field potential functionals are outlined in both a continuous rate formulation and a time–space-discrete incremental setting. The inherent symmetry of the proposed multi-field formulations is an attractive feature with regard to their numerical implementation. The unified character of the framework is demonstrated by a spectrum of model problems, which covers phase field models and formulations of gradient damage and plasticity.

1. Introduction

The modeling of size effects in solids such as the width of moving phase interfaces, the width of shear bands due yo localized damage or the grain size dependence of the plastic flow in polycrystals (Hall–Petch effect), need to be based on non-standard continuum theories which incorporate length-scales. This is achieved by gradient-type dissipative solids, which incorporate at least the first-order spatial gradient of the micro-structural variable that describes the evolving dissipative mechanism. Typical examples are gradient theories of plasticity where the spatial gradients of the plastic strain field enter the

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constitutive functions. The aim of this work is to outline a *unified framework* for gradient theories for the broad class of standard dissipative solids, which are governed by only two scalar constitutive functions: the energy storage and the dissipation functions. It is shown that this type of solids exhibits an incremental variational structure of the coupled multi-field problem of evolving macro- and micro-structural variables. It generalizes incremental variational formulations for *local* dissipative solids proposed in Miehe (2002), Miehe et al. (2002, 2004) to *gradient-type* dissipative solids. A particular focus is put on *multi-field representations*, where both the microstructural variable itself and its dual driving force enter the framework. Such a setting is needed for models with threshold- or yield-functions. The proposed formulations are due to their inherent incremental potentials *symmetric* with respect to the involved fields. This feature is highly attractive with regard to the numerical implementation and considered to be the canonical approach to gradient theories of dissipative solids.

Non-standard continuum formulations for solids, which include independent variables accounting for length scales and long range effects of a material microstructure, can be traced back to the work by Cosserat and Cosserat (1909) on *micropolar theories*, where the material micro-structure has the property of rigid particles. We also refer to the classical works on generalized elasticity by Mindlin (1964) and Toupin (1964) in terms of vector-valid order parameters and the *micromorphic theories* based on tensorial order parameters, see for example Mindlin (1965) and Eringen and Kafadar (1976), where the material micro-structure possesses properties of deformable particles. These types of multi-field theories can be considered as specific classes for *continua with affine micro-structure* defined in Capriz et al. (1982). The book by Capriz (1989) outlines a general framework suitable for establishing order parameter-based models of continua with micro-structures. Recent comprehensive treatments in this spirit are the works by Svendsen (1999) and Mariano (2001). General *gradient-type dissipative solids* were considered in Maugin (1990) and Maugin and Muschik (1994a,b) by an extension of the classical local theory of internal variables, governed by the method of virtual power as reviewed in Maugin (1980). The monograph of Frémond (2002) outlines a treatment of first-order gradient-type dissipative solids in the full thermodynamic context. The recent work by Forest (2009) suggests a unified concept for the extension of standard local to generalized micromorphic theories. In all of these treatments, a critical aspect is to define the *working of microstructural processes* of the material. We refer to the works by Gurtin (1996, 2000, 2003) for a rigorous account of this viewpoint. These processes are described by the micro-structural fields (order parameters or generalized internal variables). Hence, substructural interactions are accompanied by explicit power expressions in the rate of the micro-structural variables, yielding *additional balance-type equations* associated with the micro-structure. As a consequence, standard macro-balances of mass and momentum are coupled with additional micro-balance equations, which govern micro-force-systems associated with the order parameters.

Typical examples of the above-mentioned theoretical frameworks are the treatments by Gurtin (1996) and Fried and Gurtin (1993) on diffusive *phase transformations*, the formulations by Frémond and Nedjar (1996) and Peerlings et al. (1996, 2004) on *gradient damage* and the approach of Miehe et al. (2010) on *diffusive fracture*. They all consider scalar fraction fields as micro-structural field variables and provide length scales such as finite widths of interfaces or localized zones. Recent important continuum theories with micro-structure concern models of *gradient plasticity*. These approaches incorporate size effects associated with lattice-curvature-based dislocation densities as outlined for example in Nye (1953), Kröner (1960), Ashby (1970), Fleck et al. (1994), Fleck and Hutchinson (1997), Nix and Gao (1998), Arzt (1998), and Gao et al. (1999). Strain-gradient theories for single crystal plasticity based on micro-force balances are proposed by Gurtin (2000, 2002), Svendsen (2002), and Evers et al. (2004). More phenomenologically based theories of gradient plasticity with micro-structural field variables are considered in the works by Aifantis (1987), Mühlhaus and Aifantis (1991), Gurtin (2003), Forest and Sievert (2003), Gudmundson (2004), Gurtin and Anand (2005), Reddy et al. (2008), and Fleck and Willis (2009a,b). These works take into account the working of micro-structural kinematics and derive additional balance equations which govern micro-structural changes. However, a unified embedding of the above-mentioned model theories into variational statements for dissipative solids is missing in literature.

The field equations of dissipative solids may be related to *rate-type incremental variational formulations*. We refer to the contributions on *local* plasticity by Hill (1950), Martin (1975), Han and Reddy (1999), Simó and Honein (1990), Ortiz and Stainier (1999), Miehe (2002), and Carstensen et al. (2002). In the recent works Miehe (2002) and Miehe et al. (2002, 2004), a variational framework for *local* dissipative solids with threshold-type dissipation functions was outlined and applied to variational-based definitions of homogenization and relaxation of dissipative solids. These variational principles may be considered as the canonically compact formulations of the boundary value problem for standard dissipative solids defined in Biot (1965), Ziegler (1963), Germain (1973) and Halphen and Nguyen (1975). However, the above-mentioned treatments are restricted to *local* theories, where the evolution of the order parameters is described by ordinary differential equations. First steps towards the generalization to gradient-type theories with balance-type evolution equations of the order parameters, as considered in Maugin (1990) and Maulin and Muschik (1994a,b), are outlined by Francfort and Mielke (2006) and Fleck and Willis (2009a,b) for gradient plasticity and Mielke and Roubicek (2006) for gradient damage mechanics. This work outlines a generalization towards a *unified variational framework for gradient-type dissipative solids in alternative multi-field representations*, which provides an embedding of those model problems under the roof of gradient-enhanced standard dissipative media. A central aspect is the construction of *incremental potentials*, which govern the boundary value problems of those solids. We develop characteristic types of multi-field variational principles, which are of practical importance and well suited for numerical implementations. These are

- *Two-field minimization principles*, formulated in terms of displacement and order parameter fields based on constitutive energy storage and dissipation functions.

- *Three-field saddle point principles*, incorporating the dissipative driving force as a third field and formulated in terms of energy and dual dissipation functions.
- *Four-field saddle point principles* for non-smooth, rate-independent problems based on energy and threshold functions, with a Lagrange parameter as the fourth field.

The four fields possibly involved are visualized in Fig. 1. We (i) focus on quasi-static problems by neglecting macro- and micro-inertia effects and (ii) restrict the treatment to first-order gradients. In the *canonical two-field formulation*, the constitutive response is defined in terms of energy storage and dissipation functions. They are assumed to depend on the macro- and micro-motions and their first gradients. Reduced constitutive functions are obtained from the argument of material frame invariance. The coupled two-field balances of gradient-type standard dissipative solids are derived from the concept of virtual power reviewed in Maugin (1980), which may conceptually be considered as an extension of the exploitation method by Coleman and Gurtin (1967) of the second axiom of thermodynamics from local to gradient-type dissipative solids. The statement postulates an equivalence of internal and external power along with the irreversibility constraint of the second axiom of thermodynamics. Hence, the derivation of the macro- and micro-structural balances is conceptually in line with the virtual power-based treatment of strain gradient plasticity by Gurtin (2002, 2003). For prescribed Dirichlet-type boundary conditions, we derive from this argument the coupled macro- and micro-structural balances along with the Neumann-type boundary conditions. The coupled field equations define a broad class of first-order gradient-type standard dissipative materials, which extend the classical local treatments by Biot (1965), Ziegler (1963), and Halphen and Nguyen (1975) to gradient-type theories. The *three-field setting* is based on the introduction of a dual dissipation function in terms of the force fields which drives the order parameters, obtained by a consistent Legendre transformation based on a local definition of the dissipation. These additional fields are defined by local evolution equations which accompany the coupled balances. The presence of the driving forces allow formulations in terms of threshold- or yield-functions. A non-smooth rate-independent setting needs in addition the introduction of a Lagrangian multiplier field within a *four-field setting*, which governs the local evolution equations. These three general settings cover important representations of gradient theories for inelastic solids.

The subsequent Sections 3 and 4 of the paper develop a rate-type variational structure of the multi-field problems. Section 3 outlines rate-potentials and associated variational principles which govern the *continuous evolution* of the macro- and micro-motions. Section 4 focuses on a *finite-step-sized incremental setting* with time-discrete fields. We start with the definition of incremental energy, dissipation and load functionals. With these functionals at hand, we first postulate an incremental potential for the canonical *two-field setting*. It is shown that the optimization of this potential with respect to the displacement and order parameter fields gives the coupled balances evaluated at a discrete time as the Euler equations. A finite element formulation is obtained in a straightforward manner in terms of coupled finite elements with discrete displacement and order parameters at the nodes. The associated algebraic setting highlights, as an advantage of the variational approach, the symmetry of the coupled system matrix within Newton-type iterative solvers. Next, we derive a saddle point principle for the extended *three-field setting* with the driving forces as a third field. The optimization of the associated incremental potential gives the coupled macro- and micro balances accompanied by time-discrete forms of the evolution equations for the order parameters as Euler equations. The spatial finite element discretization, based on coupled finite elements with discrete displacement, order parameters, and driving forces at the nodes, yields again a fully symmetric structure of the coupled system. Finally, we develop the variational structure of the *four-field setting* with an additional Lagrange parameter field. The associated non-smooth finite element formulation is treated by an active set search of the discrete Lagrange parameters at the nodes of a typical finite element, yielding a dynamic size of the symmetric algebraic system. This may be considered as a generalization of variational-based return mapping schemes, such as reviewed in Simó (1998) and Armero and Pérez-Foguet (2002), from local plasticity to gradient-type plasticity.

The formulations outlined in the three Sections 2–4 are very general and valid for a wide spectrum of problems. In order to show this, we consider in Section 5 model problems of gradient-type dissipative solids which address phenomena of *phase transitions*, *damage*, *and plasticity*. In this context, specific energy storage and dissipation functions form *model-inherent incremental potentials*, which enter the above outlined general settings. The subsequent treatment is then governed in a unified format by the variational structure discussed above. This underlines the power of the proposed framework. The first model problem is a smooth viscoelastic Kelvin solid, which provides the prototype of a gradient-dependent dissipation function. Next, we derive the incremental potential for a smooth Ginzburg–Landau-type phase field model. We then outline the variational structure of a non-smooth gradient-type damage model with energetic threshold function. Finally, variational settings of non-smooth gradient-type crystal and purely phenomenological plasticity are considered. The overall goal of this section is to point out the key importance of the incremental potentials per unit volume, which completely determine the coupled field equations as the Euler equations of the unified variational principles.

2. Multi-field formulations of dissipative solids

2.1. Basic geometry of a solid with microstructural changes

Let $\mathcal{B} \subset \mathcal{R}^d$ be the reference configuration of a material body with dimension $d \in [1,2,3]$ in space and $\partial\mathcal{B} \subset \mathcal{R}^{d-1}$ its surface as depicted in Fig. 1. We study the deformation of the material body under mechanical loading in the range $\mathcal{T} \subset \mathcal{R}$ of time and are interested in predicting the macroscopic displacement of material points $\boldsymbol{x} \in \mathcal{B}$ at time $t \in \mathcal{T}$. To this end, we focus on a

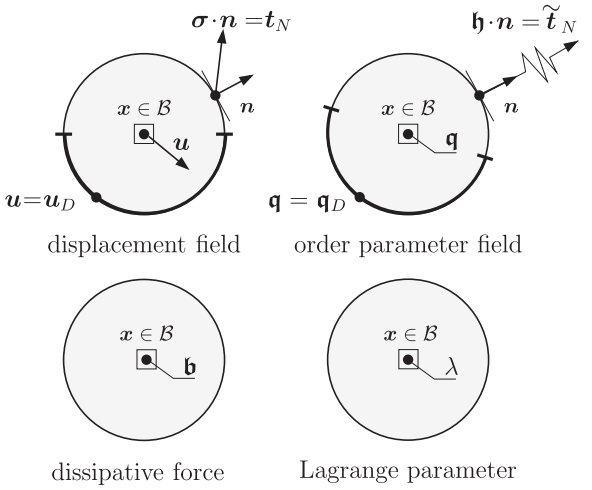

Fig. 1. Multi-field approach to gradient-type dissipative solids. The dual macro- and micro-motion fields $\boldsymbol{u}$ and $\mathfrak{q}$ defined on the solid domain $\mathcal{B}$ govern the basic *two-field setting*, where gradients of the latter account for length-scales l associated with a neighborhood $\mathcal{N}_{\boldsymbol{x}}$ of the material point $\boldsymbol{x}\in\mathcal{B}$. (a) The displacement field is constrained by the Dirichlet- and Neumann-type boundary conditions $\boldsymbol{u}=\boldsymbol{u}_D$ on $\partial\mathcal{B}_{\boldsymbol{u}}$ and $\boldsymbol{\sigma}\cdot\boldsymbol{n}=\bar{\boldsymbol{t}}_N$ on $\partial\mathcal{B}_{\boldsymbol{\sigma}}$ with $\partial\mathcal{B}=\partial\mathcal{B}_{\boldsymbol{u}}\cup\partial\mathcal{B}_{\boldsymbol{\sigma}}$. (b) The order parameter field is restricted by the conditions $\mathfrak{q}=\mathfrak{q}_D$ on $\partial\mathcal{B}_{\mathfrak{q}}$ and $\mathfrak{h}\cdot\boldsymbol{n}=\tilde{\mathfrak{t}}_N$ on $\partial\mathcal{B}_{\mathfrak{h}}$ with $\partial\mathcal{B}=\partial\mathcal{B}_{\mathfrak{q}}\cup\partial\mathcal{B}_{\mathfrak{h}}$. (c) The dissipative force field $\mathfrak{b}$ dual to the constitutive state $\mathfrak{c}:=\{\nabla_s\boldsymbol{u},\mathfrak{q},\nabla\mathfrak{q}\}$ is the third field in the *three-field setting* based on a dual dissipation potential $\phi^*(\mathfrak{b};\mathfrak{c})$. (d) The Lagrange parameter λ is the fourth field used in the rate-independent *four-field setting* based on threshold functions $f(\mathfrak{b};\mathfrak{c})$.

multi-scale viewpoint, which relates the dissipative effects to micro-structural mechanisms. In the phenomenological context, we account for these microstructural mechanisms by *micro-motion fields* as indicated in Fig. 1, which generalize the classical notion of locally evolving internal variables to global fields driven by additional micro-balances. This induces a multi-field treatment of continua with micro-structure in the spirit of the works by Capriz (1989), Mariano (2001), and Frémond (2002). In what follows, $\nabla(\cdot):=\partial_{\boldsymbol{x}}(\cdot)$ and $\dot{(\cdot)}:=\partial_t(\cdot)$ denote the spatial gradient and the time derivative of the field $(\cdot)$, respectively.

2.1.1. Macro-motion of the body

In the small-strain context, we describe the macroscopic motion of the body by the *macro-motion field*

$$\boldsymbol{u}:\begin{cases}\mathcal{B}\times\mathcal{T}\to\mathcal{R}^d,\\ (\boldsymbol{x},t)\mapsto\boldsymbol{u}(\boldsymbol{x},t).\end{cases}\tag{1}$$

$\boldsymbol{u}\in\mathcal{R}^d$ is the displacement of the material point $\boldsymbol{x}\in\mathcal{B}$ at time $t\in\mathcal{T}$. The exterior surface of the body is decomposed via $\partial\mathcal{B}=\partial\mathcal{B}_{\boldsymbol{u}}\cup\partial\mathcal{B}_{\boldsymbol{\sigma}}$ into a part $\partial\mathcal{B}_{\boldsymbol{u}}$, where the displacement is prescribed by Dirichlet-type boundary conditions

$$\boldsymbol{u}(\boldsymbol{x},t)=\boldsymbol{u}_D(\boldsymbol{x},t)\quad\text{at }\boldsymbol{x}\in\partial\mathcal{B}_{\boldsymbol{u}},\tag{2}$$

and a part $\partial\mathcal{B}_{\boldsymbol{\sigma}}$, where the macro-traction $\bar{\boldsymbol{t}}_N(\boldsymbol{x},t)$ is prescribed by a Neumann-type boundary condition as outlined below. Clearly, we have $\partial\mathcal{B}_{\boldsymbol{u}}\cap\partial\mathcal{B}_{\boldsymbol{\sigma}}=0$. In the interior domain $\mathcal{B}$, the strains are assumed to be small. Thus, the norm of the macroscopic displacement gradient

$$\|\boldsymbol{h}\|<\varepsilon\quad\text{with }\boldsymbol{h}:=\nabla\boldsymbol{u}\tag{3}$$

is bounded by a small number ε.

2.1.2. Micro-motion of the body

Microstructural changes of the body are described by additional fields which are not directly observable. These fields are related to the standard concept of internal variables, which describe dissipative mechanisms of the material. However, in contrast to standard treatments, we consider these fields to be driven by additional balance equations. We assemble in what follows these variables in the *micro-motion field* of the solid[1]

$$\mathfrak{q}:\begin{cases}\mathcal{B}\times\mathcal{T}\to\mathcal{R}^\delta,\\ (\boldsymbol{x},t)\mapsto\mathfrak{q}(\boldsymbol{x},t).\end{cases}\tag{4}$$

[1] *Remark on the notation.* The notation *micro-motion field* of $\mathfrak{q}$ used in this work is consistent with the treatment Frémond (2002). Alternative notations of $\mathfrak{q}$ may be *order parameter field* as used in Capriz (1989) or *generalized internal variable field* as used in Svendsen (1999). The micro-motion field $\mathfrak{q}$, or parts of it, may degenerate to standard local internal variables, if the gradient terms in the constitutive energy and dissipation functions are dropped for modeling rapid spatial changes at the microscale. See Section 5.5 for an example. Hence, the framework outlined here contains standard internal variable theories for dissipative response without length scales in the sense of Coleman and Gurtin (1967) as a special case.

$\boldsymbol{\mathfrak{q}} \in \mathcal{R}^{\delta}$ covers δ scalar internal variables at the material point $\boldsymbol{x} \in \mathcal{B}$ at time $t \in \mathcal{T}$. They constitute in a homogenized sense the micro-motion of the material due to structural changes on lower scales. We associate with $\boldsymbol{\mathfrak{q}}$ order parameters with possibly tensorial, geometric character, such as damage variables, phase fractions, inelastic strains, or hardening-softening variables. With respect to *each* micro-structural field, we decompose the surface of the solid via $\partial\mathcal{B} = \partial\mathcal{B}_{\mathfrak{q}} \cup \partial\mathcal{B}_{\mathfrak{h}}$ into a part $\partial\mathcal{B}_{\mathfrak{q}}$, where the micro-motion is prescribed by Dirichlet-type boundary conditions

$$\boldsymbol{\mathfrak{q}}(\boldsymbol{x},t) = \boldsymbol{\mathfrak{q}}_D(\boldsymbol{x},t) \quad \text{at } \boldsymbol{x} \in \partial\mathcal{B}_{\mathfrak{q}}, \tag{5}$$

and a part $\partial\mathcal{B}_{\mathfrak{h}}$, where *micro-tractions* $\tilde{\boldsymbol{t}}_N(\boldsymbol{x},t)$ are assumed as Neumann-type boundary conditions. We have $\partial\mathcal{B}_{\mathfrak{q}} \cap \partial\mathcal{B}_{\mathfrak{h}} = 0$. Note that this equation summarizes in an abstract setting the possible boundary condition of each separate field, which might be related to different parts of the surface. In contrast to the restriction (3) of the macro-displacement gradient in the small-strain context, the norm of the gradient $\|\nabla\boldsymbol{\mathfrak{q}}\|$ is not bounded.

2.1.3. Superimposed macroscopic rigid body motions

Consider a smooth time-dependent infinitesimal rigid rotation superimposed on the macroscopic displacement $\boldsymbol{u}$, governed by the expression

$$\boldsymbol{u}^{+}(\boldsymbol{x},t) \coloneqq \boldsymbol{u}(\boldsymbol{x},t) + \boldsymbol{w}(t)\boldsymbol{x} + \boldsymbol{c}(t). \tag{6}$$

Here, $\boldsymbol{w}(t)$ is a time-dependent skew second-order tensor with $\boldsymbol{w}^T = -\boldsymbol{w}$ and $\|\boldsymbol{w}\| < \varepsilon$, representing an *infinitesimal rotation* superimposed onto the displaced solid. The time-dependent vector $\boldsymbol{c}(t)$ characterizes a *translation* superimposed onto the displaced solid. With (6), the macroscopic displacement and velocity gradients transform by

$$\nabla\boldsymbol{u}^{+} \coloneqq \nabla\boldsymbol{u} + \boldsymbol{w} \quad \text{and} \quad \nabla\dot{\boldsymbol{u}}^{+} \coloneqq \nabla\dot{\boldsymbol{u}} + \dot{\boldsymbol{w}}. \tag{7}$$

The micro-motion is assumed to be independent of the superimposed rigid macro-motion. As a consequence, the internal variables are unaffected by the transformation (6). Thus, we have

$$\boldsymbol{\mathfrak{q}}^{+}(\boldsymbol{x},t) \coloneqq \boldsymbol{\mathfrak{q}}(\boldsymbol{x},t) \tag{8}$$

and therefore no changes of the gradients

$$\nabla\boldsymbol{\mathfrak{q}}^{+} \coloneqq \nabla\boldsymbol{\mathfrak{q}} \quad \text{and} \quad \nabla\dot{\boldsymbol{\mathfrak{q}}}^{+} \coloneqq \nabla\dot{\boldsymbol{\mathfrak{q}}} \tag{9}$$

of the microstructural fields.[2]

2.2. Energy storage and dissipation of gradient-type solids

2.2.1. Stored energy and dissipation potential functionals

We generalize ideas of standard dissipative materials such as outlined in Halphen and Nguyen (1975) to the multi-field context. To this end, we introduce two functionals related to energy storage and dissipative mechanisms, respectively. We denote

$$E(\boldsymbol{u},\boldsymbol{\mathfrak{q}}) \coloneqq \int_{\mathcal{B}} \psi \, dV \quad \text{and} \quad D(\dot{\boldsymbol{u}},\dot{\boldsymbol{\mathfrak{q}}};\boldsymbol{u},\boldsymbol{\mathfrak{q}}) \coloneqq \int_{\mathcal{B}} \phi \, dV \tag{10}$$

as the *stored energy functional* and the *dissipation potential functional*, respectively. E represents the free energy stored in the body $\mathcal{B}$ due to its coupled macro–micro-deformation. D is related to the power of internal dissipative mechanisms and is identical with the dissipation if the material is rate-independent. In the above definitions, ψ and ϕ are called the *energy storage function* and the *dissipation potential function*, respectively. They represent at a macroscopic point $\boldsymbol{x} \in \mathcal{B}$ the stored energy and the dissipation potential with respect to the unit volume. These functions are linked by a set of constitutive state variables to the macro- and micro-motions $\boldsymbol{u}$ and $\boldsymbol{\mathfrak{q}}$, respectively. Focusing on *simple materials of the grade one*, we consider a dependence of the stored energy function ψ on the macro- and micro-motions and their first gradients and a dependence of the dissipation potential function ϕ on the micro- and macro-velocities and their first gradients. Introducing the set of independent *constitutive state variables*

$$\mathfrak{c}_0 \coloneqq \{\boldsymbol{u},\nabla\boldsymbol{u},\boldsymbol{\mathfrak{q}},\nabla\boldsymbol{\mathfrak{q}}\}, \tag{11}$$

we start with the basic constitutive assumption

$$\psi = \psi(\mathfrak{c}_0) \quad \text{and} \quad \phi = \phi(\dot{\mathfrak{c}}_0;\mathfrak{c}_0). \tag{12}$$

Note that the dissipation potential function may depend beside the rate of the current state $\dot{\mathfrak{c}}_0$ also on the current state $\mathfrak{c}_0$ itself. For *heterogeneous solids*, both functions depend in addition on $\boldsymbol{x} \in \mathcal{B}$. In order to keep the notation compact, we do not point out this explicitly.

[2] *Remark on invariance.* This assumption is different from the treatment by Capriz (1989), where a particular transformation is assumed for vectorial and tensorial order parameter fields.

2.2.2. Material frame invariance and reduced forms

The constitutive functionals (10) must be invariant under arbitrary superimposed macroscopic rigid body motions (6). Thus, the stored energy and dissipation potential functions defined in (12) have to satisfy

$$\psi(\mathfrak{e}_0^+)=\psi(\mathfrak{e}_0) \quad \text{and} \quad \phi(\dot{\mathfrak{e}}_0^+;\mathfrak{e}_0^+)=\phi(\dot{\mathfrak{e}}_0;\mathfrak{e}_0) \tag{13}$$

with the definition $\mathfrak{e}_0^+ := \{\boldsymbol{u}+\boldsymbol{w}\boldsymbol{x}+\boldsymbol{c},\nabla\boldsymbol{u}+\boldsymbol{w},\mathfrak{q},\nabla\mathfrak{q}\}$ for *arbitrary* skew tensors $\boldsymbol{w}$ and vectors $\boldsymbol{c}$. The immediate consequence of the first condition is that the free energy function ψ cannot depend on the macro-motion $\boldsymbol{u}$ and the skew part *skew*$[\nabla\boldsymbol{u}]$ of its gradient. The second condition states that the dissipation function ϕ cannot depend on the macro-velocity $\dot{\boldsymbol{u}}$ and the skew part *skew*$[\nabla\dot{\boldsymbol{u}}]$ of its gradient. As a consequence, when introducing the set of *objective state variables*

$$\mathfrak{e} := \{\nabla_s\boldsymbol{u},\mathfrak{q},\nabla\mathfrak{q}\}, \tag{14}$$

the above demands of material frame invariance induce the *reduced forms* of (12)

$$\psi=\psi(\mathfrak{e}) \quad \text{and} \quad \phi=\phi(\dot{\mathfrak{e}};\mathfrak{e}), \tag{15}$$

which satisfy a priori the principle of material frame invariance. Recall that the symmetric part of the macroscopic displacement gradient is the classical small-strain tensor

$$\boldsymbol{\varepsilon} := \nabla_s\boldsymbol{u}=\tfrac{1}{2}[\boldsymbol{h}+\boldsymbol{h}^T]. \tag{16}$$

Note carefully that the principle of material frame invariance does not affect the dependence of the constitutive functions on the micro-motion $\mathfrak{q}$ and its gradient $\nabla\mathfrak{q}$.

2.2.3. Rate of energy storage and dissipation functionals

The above constitutive functions determine the powers of storage and dissipation mechanisms due to the deformation of the solid. The *rate of the energy storage* at a given state $\{\boldsymbol{u},\mathfrak{q}\}$ is per definition the time derivative of the energy storage functional $(10)_1$. We write

$$\mathcal{E}(\dot{\boldsymbol{u}},\dot{\mathfrak{q}};\boldsymbol{u},\mathfrak{q}) := \frac{d}{dt}E=\int_{\mathcal{B}}\partial_{\dot{\mathfrak{e}}}\psi\cdot\dot{\mathfrak{e}}\;dV=\int_{\mathcal{B}}[\delta_{\boldsymbol{u}}\psi\cdot\dot{\boldsymbol{u}}+\delta_{\mathfrak{q}}\psi\cdot\dot{\mathfrak{q}}]\;dV+\int_{\partial\mathcal{B}_\sigma}[(\partial_{\nabla_s\boldsymbol{u}}\psi)\cdot\boldsymbol{n}]\cdot\dot{\boldsymbol{u}}\,dA+\int_{\partial\mathcal{B}_\mathfrak{h}}[(\partial_{\nabla_\mathfrak{q}}\psi)\cdot\boldsymbol{n}]\cdot\dot{\mathfrak{q}}\,dA. \tag{17}$$

Here, we introduced the variational or functional derivatives of the free energy function ψ by the macro- and micro-motion fields

$$\delta_{\boldsymbol{u}}\psi := -\mathrm{div}[\partial_{\nabla_s\boldsymbol{u}}\psi] \quad \text{and} \quad \delta_{\mathfrak{q}}\psi := \partial_{\mathfrak{q}}\psi-\mathrm{div}[\partial_{\nabla\mathfrak{q}}\psi], \tag{18}$$

respectively. In contrast, the *dissipation functional* is not the time derivative of the dissipation functional $(10)_2$, but defined by the expression

$$\mathcal{D}(\dot{\boldsymbol{u}},\dot{\mathfrak{q}};\boldsymbol{u},\mathfrak{q}) := \int_{\mathcal{B}}\partial_{\dot{\mathfrak{e}}}\phi\cdot\dot{\mathfrak{e}}\;dV=\int_{\mathcal{B}}[\delta_{\dot{\boldsymbol{u}}}\phi\cdot\dot{\boldsymbol{u}}+\delta_{\dot{\mathfrak{q}}}\phi\cdot\dot{\mathfrak{q}}]\;dV+\int_{\partial\mathcal{B}_\sigma}[(\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi)\cdot\boldsymbol{n}]\cdot\dot{\boldsymbol{u}}\,dA+\int_{\partial\mathcal{B}_\mathfrak{h}}[(\partial_{\nabla_\mathfrak{q}}\phi)\cdot\boldsymbol{n}]\cdot\dot{\mathfrak{q}}\,dA. \tag{19}$$

at given state $\{\boldsymbol{u},\mathfrak{q}\}$. Here, we introduced functional derivatives of the dissipation function ϕ by the rates of the macro- and micro-motion fields

$$\delta_{\dot{\boldsymbol{u}}}\phi := -\mathrm{div}[\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi] \quad \text{and} \quad \delta_{\dot{\mathfrak{q}}}\phi := \partial_{\dot{\mathfrak{q}}}\phi-\mathrm{div}[\partial_{\nabla\dot{\mathfrak{q}}}\phi], \tag{20}$$

respectively. The total internal power of standard dissipative materials decomposes into the above storage and dissipative contributions according to

$$P_{int} := \mathcal{E}+\mathcal{D}, \tag{21}$$

and is governed by the two fundamental constitutive functions ψ and ϕ, respectively. Clearly, both contributions contain coupled effects from the macro- and micro-actions.

2.2.4. Irreversibility constraint and convexity

The central demand of the second axiom of thermodynamics is that the dissipative power (19) of the micro-structural changes is positive for all admissible thermodynamic processes. This demand of positive global dissipation of the solid

$$\mathcal{D}\geq 0 \tag{22}$$

is satisfied if the integrand of the volume integral (19) is positive for arbitrary arguments. Hence, the above inequality serves as a fundamental physically based constraint on the constitutive dissipation function ϕ. The above thermodynamic condition is a priori satisfied for *normalized*, *positive* dissipation functions with

$$\phi(0;\mathfrak{e})=0 \quad \text{and} \quad \phi(\dot{\mathfrak{e}};\mathfrak{e})\geq 0, \tag{23}$$

which are *convex* with respect to the rate of the constitutive state, i.e.

$$\alpha\phi(\dot{\mathfrak{e}}_1;\mathfrak{e})+(1-\alpha)\phi(\dot{\mathfrak{e}}_2;\mathfrak{e})>\phi(\alpha\dot{\mathfrak{e}}_1+(1-\alpha)\dot{\mathfrak{e}}_2;\mathfrak{e}) \tag{24}$$

for $\alpha\in[0,1]$. Taking these three conditions into account, it is easy to show that the integrand of (19) is always positive and condition (22) is satisfied.

2.3. Coupled two-field balances of gradient-type solids

The continuum with microstructure is assumed to be loaded by *macroscopic and microscopic* external field actions. As visualized in Fig. 1, we assume macro- and microscopic body force fields $\overline{\boldsymbol{\gamma}}$ and $\tilde{\boldsymbol{\gamma}}$ per unit volume of the domain $\mathcal{B}$. Furthermore, traction fields $\overline{\boldsymbol{t}}_N$ and $\tilde{\boldsymbol{t}}_N$ are defined on the surfaces $\partial\mathcal{B}_{\boldsymbol{\sigma}}$ and $\partial\mathcal{B}_{\mathfrak{y}}$, respectively, representing macro- and microscopic Neumann-type boundary conditions. Hence, the total power of external loading is assumed to decompose according to

$$P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t) := \overline{P}(\dot{\boldsymbol{u}};t)+\tilde{P}(\dot{\boldsymbol{\eta}};t) \tag{25}$$

into the macroscopic load functional

$$\overline{P}_{ext}(\dot{\boldsymbol{u}};t) := \int_{\mathcal{B}} \overline{\boldsymbol{\gamma}}(\boldsymbol{x},t)\cdot\dot{\boldsymbol{u}}\,dV+\int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} \overline{\boldsymbol{t}}_N(\boldsymbol{x},t)\cdot\dot{\boldsymbol{u}}\,dA \tag{26}$$

and the microscopic load functional

$$\tilde{P}_{ext}(\dot{\boldsymbol{\eta}};t) := \int_{\mathcal{B}} \tilde{\boldsymbol{\gamma}}(\boldsymbol{x},t)\cdot\dot{\boldsymbol{\eta}}\,dV+\int_{\partial\mathcal{B}_{\mathfrak{y}}} \tilde{\boldsymbol{t}}_N(\boldsymbol{x},t)\cdot\dot{\boldsymbol{\eta}}\,dA. \tag{27}$$

The loads are assumed to be *dead*, i.e. independent of the macro- and micro-motions $\boldsymbol{u}$ and $\boldsymbol{\eta}$. We derive the macro- and micro-balance equations from the standard argument of virtual power, see Maugin (1980, 1990) for a review. With the rate of energy storage functional (17), the dissipation functional (19) and the above external power functional (26) at hand, we demand that

$$0 \in \mathcal{E}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};\boldsymbol{u},\boldsymbol{\eta})+\mathcal{D}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};\boldsymbol{u},\boldsymbol{\eta})-P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t) \tag{28}$$

is satisfied at a given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$ at time t for all admissible, virtual rates $\dot{\boldsymbol{u}}$ and $\dot{\boldsymbol{\eta}}$ of the macro- and micro-motion, which satisfy the homogeneous form of the Dirichlet boundary conditions

$$\dot{\boldsymbol{u}} \in \mathcal{W}_u^0 := \{\dot{\boldsymbol{u}}\,|\,\dot{\boldsymbol{u}}=\boldsymbol{0} \text{ on } \partial\mathcal{B}_{\boldsymbol{u}}\} \quad \text{and} \quad \dot{\boldsymbol{\eta}} \in \mathcal{W}_{\boldsymbol{\eta}}^0 := \{\dot{\boldsymbol{\eta}}\,|\,\dot{\boldsymbol{\eta}}=\boldsymbol{0} \text{ on } \partial\mathcal{B}_{\boldsymbol{\eta}}\}. \tag{29}$$

The balance (28) equilibrates internal and external virtual powers P_{int} and P_{ext} for the quasi-static process under consideration, where P_{int} includes energetic and dissipative parts. Insertion of the functionals and application of the Gauss' theorem give the demand

$$\begin{aligned} 0 \in &\int_{\mathcal{B}} \{[\delta_{\boldsymbol{u}}\psi+\delta_{\dot{\boldsymbol{u}}}\phi-\overline{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{u}}+[\delta_{\boldsymbol{\eta}}\psi+\delta_{\dot{\boldsymbol{\eta}}}\phi-\tilde{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{\eta}}\}\,dV+\int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} [(\partial_{\nabla_s\boldsymbol{u}}\psi+\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi)\cdot\boldsymbol{n}-\overline{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{u}}\,dA \\ &+\int_{\partial\mathcal{B}_{\mathfrak{y}}} [(\partial_{\nabla\boldsymbol{\eta}}\psi+\partial_{\nabla\dot{\boldsymbol{\eta}}}\phi)\cdot\boldsymbol{n}-\tilde{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{\eta}}\,dA \end{aligned} \tag{30}$$

for all $\dot{\boldsymbol{u}} \in \mathcal{W}_u^0$ and $\dot{\boldsymbol{\eta}} \in \mathcal{W}_{\boldsymbol{\eta}}^0$. This results in the coupled micro- and macro-balance equations

$$\delta_{\boldsymbol{u}}\psi+\delta_{\dot{\boldsymbol{u}}}\phi=\overline{\boldsymbol{\gamma}}, \quad \delta_{\boldsymbol{\eta}}\psi+\delta_{\dot{\boldsymbol{\eta}}}\phi \ni \tilde{\boldsymbol{\gamma}} \tag{31}$$

in the domain $\mathcal{B}$ along with the *Neumann-type boundary conditions* for the macro- and microscopic tractions on the boundary of the gradient-type continuum

$$[\partial_{\nabla_s\boldsymbol{u}}\psi+\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi]\cdot\boldsymbol{n}=\overline{\boldsymbol{t}}_N \text{ on } \partial\mathcal{B}_{\boldsymbol{\sigma}} \quad \text{and} \quad [\partial_{\nabla\boldsymbol{\eta}}\psi+\partial_{\nabla\dot{\boldsymbol{\eta}}}\phi]\cdot\boldsymbol{n}=\tilde{\boldsymbol{t}}_N \text{ on } \partial\mathcal{B}_{\mathfrak{y}}. \tag{32}$$

The two coupled field equations (31) consist of the *macroscopic stress equilibrium* condition

$$-\mathrm{div}[\partial_{\nabla_s\boldsymbol{u}}\psi+\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi]=\overline{\boldsymbol{\gamma}} \tag{33}$$

and the *microscopic balance equation*

$$[\partial_{\boldsymbol{\eta}}\psi+\partial_{\dot{\boldsymbol{\eta}}}\phi]-\mathrm{div}[\partial_{\nabla\boldsymbol{\eta}}\psi+\partial_{\nabla\dot{\boldsymbol{\eta}}}\phi] \ni \tilde{\boldsymbol{\gamma}} \tag{34}$$

in the domain $\mathcal{B}$. The last equation determines the evolution of the micro-motion field $\boldsymbol{\eta}$. This summarizes the basic ingredients of gradient-type standard dissipative solids in the multi-field context in terms of the *two fields* $\boldsymbol{u}$ and $\boldsymbol{\eta}$ introduced in (1) and (4). Note the formal duality of macro- and micro-balances (33) and (34), which is an outcome of the constitutive assumptions (15) for the energy storage and the dissipation potential. It generalizes formulations outlined in Maugin (1990) and Maugin and Muschik (1994a,b), in particular with regard to the extended set of variables in the dissipation function (15). Observe that the standard concept of local internal variables is obtained for $\tilde{\boldsymbol{\gamma}}=\boldsymbol{0}$ and vanishing divergence term in (34), i.e. for the special case when the constitutive functions for ψ and ϕ in (15) do not contain gradient terms of $\boldsymbol{\eta}$.

2.4. Coupled three-field balances of gradient-type solids

We now introduce microstructural variables *dual* to the micro-motion $\boldsymbol{\eta}$ defined in (4). To this end, we define a representation of the dissipation

$$\mathcal{D}=\int_{\mathcal{B}} \boldsymbol{\mathfrak{b}}\cdot\dot{\boldsymbol{c}}\,dV \geq 0 \tag{35}$$

based on the inner product of the *dissipative force array*

$$\mathfrak{b} := \{\mathfrak{s}, \mathfrak{p}, \mathfrak{g}\} \tag{36}$$

and the rate $\dot{\mathfrak{c}}$ of the constitutive state defined in (14). $\mathfrak{b}$ and $\mathfrak{c}$ are *dual variables* in the sense

$$\mathfrak{b} \cdot \dot{\mathfrak{c}} = \mathfrak{s} \cdot \nabla_s \dot{\boldsymbol{u}} + \mathfrak{p} \cdot \dot{\mathfrak{q}} + \mathfrak{g} \cdot \nabla \dot{\mathfrak{q}} \geq 0, \tag{37}$$

i.e. the stress $\mathfrak{s} \in \mathcal{R}^{d(d+1)/2}$ is the dissipative driving force dual to the macroscopic strain $\nabla_s \boldsymbol{u}$, the force $\mathfrak{p} \in \mathcal{R}^{\delta}$ is dual to the micro-motion $\mathfrak{q}$ and $\mathfrak{g} \in \mathcal{R}^{\delta d}$ is the force dual to the gradient $\nabla \mathfrak{q}$ of the micro-motion. The *dissipative forces*

$$\mathfrak{b} : \begin{cases} \mathcal{B} \times \mathcal{T} \to \mathcal{R}^{d(d+1)/2+\delta+\delta d}, \\ (\boldsymbol{x}, t) \mapsto \mathfrak{b}(\boldsymbol{x}, t) \end{cases} \tag{38}$$

are considered in a *mixed setting* as a third variable field on the solid domain $\mathcal{B}$. With this field at hand, we define a dual dissipation function ϕ^* based on a Legendre transformation

$$\phi^*(\mathfrak{b}; \mathfrak{c}) = \sup_{\dot{\mathfrak{c}}} [\mathfrak{b} \cdot \dot{\mathfrak{c}} - \phi(\dot{\mathfrak{c}}; \mathfrak{c})] \tag{39}$$

at a given constitutive state $\mathfrak{c}$. Note that the necessary equation of this variational problem

$$\mathfrak{b} \in \partial_{\dot{\mathfrak{c}}} \phi(\dot{\mathfrak{c}}; \mathfrak{c}) \tag{40}$$

defines the dissipative forces $\mathfrak{b}$ in terms of the evolution $\dot{\mathfrak{c}}$ of the constitutive state via the dissipation function ϕ. The dual counterpart of the variational problem (39) reads

$$\phi(\dot{\mathfrak{c}}; \mathfrak{c}) = \sup_{\mathfrak{b}} [\mathfrak{b} \cdot \dot{\mathfrak{c}} - \phi^*(\mathfrak{b}; \mathfrak{c})] \tag{41}$$

and has the necessary equation

$$\dot{\mathfrak{c}} \in \partial_{\mathfrak{b}} \phi^*(\mathfrak{b}; \mathfrak{c}) \tag{42}$$

dual to (40), which relates the evolution $\dot{\mathfrak{c}}$ of the constitutive state to the dissipative forces $\mathfrak{b}$. The use of the dual dissipation function ϕ^* induces the following modification of Eqs. (32)–(34), which determine the boundary-value problem of gradient-type dissipative solids. The *Neumann-type boundary conditions*

$$[\partial_{\nabla_s \boldsymbol{u}} \psi + \mathfrak{s}] \cdot \boldsymbol{n} = \bar{\boldsymbol{t}}_N \text{ on } \partial\mathcal{B}_{\boldsymbol{\sigma}} \quad \text{and} \quad [\partial_{\nabla \mathfrak{q}} \psi + \mathfrak{g}] \cdot \boldsymbol{n} = \tilde{\boldsymbol{t}}_N \text{ on } \partial\mathcal{B}_{\mathfrak{h}} \tag{43}$$

accompany the *macroscopic stress equilibrium* condition

$$-\operatorname{div}[\partial_{\nabla_s \boldsymbol{u}} \psi + \mathfrak{s}] = \bar{\boldsymbol{\gamma}}, \tag{44}$$

the *microscopic balance equation*

$$[\partial_{\mathfrak{q}} \psi + \mathfrak{p}] - \operatorname{div}[\partial_{\nabla \mathfrak{q}} \psi + \mathfrak{g}] \ni \tilde{\gamma} \tag{45}$$

and the (inverse) definition of the dissipative driving forces via the three *evolution equations*

$$\nabla_s \dot{\boldsymbol{u}} \in \partial_{\mathfrak{s}} \phi^*, \quad \dot{\mathfrak{q}} \in \partial_{\mathfrak{p}} \phi^*, \quad \nabla \dot{\mathfrak{q}} \in \partial_{\mathfrak{g}} \phi^* \tag{46}$$

in the domain $\mathcal{B}$. This summarizes the basic ingredients of gradient-type standard dissipative solids in the multi-field context in terms of the *three fields* $\boldsymbol{u}$, $\mathfrak{q}$, and $\mathfrak{b} := \{\mathfrak{s}, \mathfrak{p}, \mathfrak{g}\}$ introduced in (1), (4) and (38).

2.5. Coupled balance equations in terms of threshold functions

2.5.1. Rate-independent formulation in terms of threshold function

In practical engineering applications, rate-independent dissipation functions are often modeled by the so-called *concept of maximum dissipation*. A terminology which can be traced back to plasticity theory, see for example Hill (1950), Martin (1975), and Han and Reddy (1999). Here, the dissipation function is defined by the constrained maximum problem

$$\phi(\dot{\mathfrak{c}}; \mathfrak{c}) = \sup_{\mathfrak{b} \in \mathbb{E}} \mathfrak{b} \cdot \dot{\mathfrak{c}}, \tag{47}$$

where $\mathbb{E}$ models a *reversible domain* in the space of the dissipative forces $\mathfrak{b}$

$$\mathbb{E} := \{\mathfrak{b} \in \mathcal{R}^{d(d+1)/2+\delta+\delta d} | f(\mathfrak{b}; \mathfrak{c}) \leq c\} \tag{48}$$

in terms of a *threshold or yield function* $f : \mathcal{R}^{d(d+1)/2+\delta+\delta d} \to \mathcal{R}$, which is positive $f(\mathfrak{b}; \mathfrak{c}) \geq 0$, normalized $f(\mathbf{0}; \mathfrak{c}) = 0$, convex

$$\alpha f(\mathfrak{b}_1; \mathfrak{c}) + (1-\alpha) f(\mathfrak{b}_2; \mathfrak{c}) > f(\alpha \mathfrak{b}_1 + (1-\alpha)\mathfrak{b}; \mathfrak{c}) \tag{49}$$

with $\alpha \in [0,1]$ and homogeneous of the order one

$$f(v\mathfrak{b}; \mathfrak{c}) = v f(\mathfrak{b}; \mathfrak{c}) \tag{50}$$

for $v > 0$. The *threshold value* $c > 0$ bounds in combination with a particular choice of the function f the dissipative force $\mathfrak{b}$. In a *heterogeneous* solid, the threshold c may depend on $\boldsymbol{x} \in \mathcal{B}$. The constrained maximum problem (47) can be solved by a

Lagrange method

$$\phi(\dot{\mathfrak{c}};\mathfrak{c}) = \sup_{\mathfrak{b},\lambda\geq 0}[\mathfrak{b}\cdot\dot{\mathfrak{c}} - \lambda(f(\mathfrak{b};\mathfrak{c})-c)], \tag{51}$$

yielding as necessary condition the specific form of (42)

$$\dot{\mathfrak{c}} = \lambda\partial_{\mathfrak{b}} f(\mathfrak{b};\mathfrak{c}), \tag{52}$$

which relates the evolution $\dot{\mathfrak{c}}$ of the constitutive state to the dissipative forces $\mathfrak{b}$ along with the loading–unloading conditions

$$\lambda\geq 0, \quad f(\mathfrak{b};\mathfrak{c})\leq c, \quad \lambda(f(\mathfrak{b};\mathfrak{c})-c)=0. \tag{53}$$

The latter determine the non-smooth dissipative response by the threshold function f, which is in this type of modeling the basic constitutive function besides the free energy function ψ. Hence, in Eqs. (43)–(46) of the *three-field setting*, we replace the three *evolution equations* (46) by the specific rate-independent form

$$\nabla_s\dot{\boldsymbol{u}} = \lambda\partial_{\mathfrak{s}} f, \quad \dot{\mathfrak{q}} = \lambda\partial_{\mathfrak{p}} f, \quad \nabla\dot{\mathfrak{q}} = \lambda\partial_{\mathfrak{g}} f \tag{54}$$

accompanied by the above loading condition (53). Note that insertion of (52) into (35) identifies, based on the property $\mathfrak{b}\cdot\partial_{\mathfrak{b}} f = f$ obtained from (50) along with the condition $f{=}c$ for loading, the dissipation

$$\mathcal{D} = \int_{\mathcal{B}} c\lambda\, dV \geq 0 \tag{55}$$

of this rate-independent framework.

2.5.2. Rate-dependent formulation in terms of threshold function

A rate-dependent class of dissipation functions with reversible range $\mathbb{E}$ governed by the above introduced threshold function f is obtained by an approximate penalty-type solution of the maximum problem (47)

$$\phi(\dot{\mathfrak{c}};\mathfrak{c}) = \sup_{\mathfrak{b}}\left[\mathfrak{b}\cdot\dot{\mathfrak{c}} - \frac{c}{\eta(m+1)}\langle f(\mathfrak{b};\mathfrak{c})/c-1\rangle^{m+1}\right], \tag{56}$$

where the constants $\eta>0$ and $m>0$ are interpreted as material parameters associated with the viscosity of the dissipative process. $\langle x\rangle = \frac{1}{2}(x+|x|)$ is the ramp function, expressed by the McAuley bracket. The necessary condition of (56) provides the nonlinear evolution equation

$$\dot{\mathfrak{c}} = \frac{1}{\eta}\langle f(\mathfrak{b};\mathfrak{c})/c-1\rangle^{m}\partial_{\mathfrak{b}} f(\mathfrak{b};\mathfrak{c}) \tag{57}$$

in terms of a dimensionless, scalar-valued *over-force* $\langle f(\mathfrak{b};\mathfrak{c})/c-1\rangle$. The structure of this evolution equation is borrowed from Perzyna-type visco-plasticity, see Perzyna (1966). The *smooth* evolution equation may be directly obtained from (42) based on the dual dissipation function

$$\phi^*(\mathfrak{b};\mathfrak{c}) = \frac{c}{\eta(m+1)}\langle f(\mathfrak{b};\mathfrak{c})/c-1\rangle^{m+1}, \tag{58}$$

which follows immediately from (56), if the penalty-type variational principle is interpreted as a Legendre transformation. Hence, in Eqs. (43)–(46) of the *three-field setting*, we replace the three *evolution equations* (46) by the specific rate-independent form

$$\nabla_s\dot{\boldsymbol{u}} = \lambda\partial_{\mathfrak{s}} f, \quad \dot{\mathfrak{q}} = \lambda\partial_{\mathfrak{p}} f, \quad \nabla\dot{\mathfrak{q}} = \lambda\partial_{\mathfrak{g}} f \tag{59}$$

accompanied by the constitutive definition

$$\lambda := \frac{1}{\eta}\langle f/c-1\rangle^{m} \geq 0 \tag{60}$$

for the rate-dependent loading. Note that insertion of (57) into (35) identifies, based on the property $\mathfrak{b}\cdot\partial_{\mathfrak{b}} f = f$ obtained from (50), the dissipation

$$\mathcal{D} = \int_{\mathcal{B}} f\lambda\, dV \geq 0 \tag{61}$$

of this rate-dependent framework. For $\eta\to 0$ we obtain in the limit the rate-independent form (52) combined with (53). Due to this limit of the smooth viscous over-force formulation and the well-posed setting of the rate-dependent power type expression, this formulation is of particular interest for numerical implementations.

3. Continuous incremental variational principles

The above outlined field equations for the coupled micro- and macro-mechanical response can be obtained by the variation of incremental potentials. This underlines the canonical structure of the proposed constitutive setting. To this end, we define *rate-type variational principles*, whose Euler equations are identical with the balance equations obtained in the

above Sections 2.3–2.5 from the principle for virtual power. We focus in this section on the *continuous setting* of the variational principles, and consider in the subsequent Section 4 their time- and space-discrete counterparts. The key aspect is the introduction of suitable *incremental potentials* based on the functionals introduced above.

3.1. The canonical two-field minimization principle

Based on the energy and the dissipation potential functionals E and D introduced in (10) and the external work functional P_{ext} introduced in (25), we define the *rate-type potential*

$$\underbrace{\Pi(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}})}_{\text{potential}} := \underbrace{\frac{d}{dt}E(\boldsymbol{u},\boldsymbol{\eta})}_{\text{energy}} + \underbrace{D(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};\boldsymbol{u},\boldsymbol{\eta})}_{\text{dissipation}} - \underbrace{P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t)}_{\text{work}} \tag{62}$$

at the given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$ at time t. Taking into account (17), the rate potential assumes the explicit form

$$\Pi = \int_{\mathcal{B}} \{[\delta_{\boldsymbol{u}}\psi - \overline{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{u}} + [\delta_{\boldsymbol{\eta}}\psi - \tilde{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{\eta}} + \phi\}\, dV + \int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} [(\partial_{\nabla_s\boldsymbol{u}}\psi)\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{u}}\, dA + \int_{\partial\mathcal{B}_{\boldsymbol{\eta}}} [(\partial_{\nabla\boldsymbol{\eta}}\psi)\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{\eta}}\, dA. \tag{63}$$

Note that the only nonlinear entry occurs through the dissipation function ϕ. All other terms are linear in the rates $\{\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}}\}$ of the macro- and micro-motion fields. We assume that the rates of the macro- and micro-deformation fields at a given state are governed by the variational principle

$$\{\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}}\} = \text{Arg}\Big\{\inf_{\dot{\boldsymbol{u}}}\inf_{\dot{\boldsymbol{\eta}}}\ \Pi(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}})\Big\}. \tag{64}$$

Hence, the constitutive setting of gradient-type, standard dissipative solids has an underlying incremental minimum structure. Note that the minimization structure of this variational principle is essentially governed by the convexity of the dissipation potential function ϕ. Taking the variation of the rate potential (63), we end up with an expression similar to (30) for all virtual rates $\delta_{\dot{\boldsymbol{u}}} \in \mathcal{W}_u^0$ and $\delta_{\dot{\boldsymbol{\eta}}} \in \mathcal{W}_{\boldsymbol{\eta}}^0$ of the macro- and micro-motion which satisfy the homogeneous form (29) of the Dirichlet-type boundary conditions. As a consequence, we find that Eqs. (43)–(46) are the Euler equations of the rate-type two-field principle (64).

3.2. The extended three-field saddle point principle

An extended incremental variational that contains the dissipative driving force is obtained by expressing the dissipation function ϕ by its dual ϕ^* via the Legendre transformation (41). To this end, we introduce the modified dissipation potential functional

$$D^*(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b}) := \int_{\mathcal{B}} \{\mathfrak{b}\cdot\dot{\mathfrak{c}} - \phi^*(\mathfrak{b};\mathfrak{c})\}\, dV \tag{65}$$

with the constitutive state $\mathfrak{c}$ defined in (14). We then define the extended three-field potential

$$\underbrace{\Pi^*(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b})}_{\text{potential}} := \underbrace{\frac{d}{dt}E(\boldsymbol{u},\boldsymbol{\eta})}_{\text{energy}} + \underbrace{D^*(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b})}_{\text{dissipation}} - \underbrace{P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t)}_{\text{work}} \tag{66}$$

at a given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$. Note that the only modification of (62) affects the dissipation, which is now expressed in terms of the dissipative forces $\mathfrak{b}$ defined in (36) and the rate of the constitutive state $\mathfrak{c}$ defined in (14). Using (17), the potential takes the explicit form

$$\Pi^* = \int_{\mathcal{B}} \{[\delta_{\boldsymbol{u}}\psi - \overline{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{u}} + [\delta_{\boldsymbol{\eta}}\psi - \tilde{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{\eta}} + \mathfrak{b}\cdot\dot{\mathfrak{c}} - \phi^*\}\, dV + \int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} [(\partial_{\nabla_s\boldsymbol{u}}\psi)\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{u}}\, dA + \int_{\partial\mathcal{B}_{\boldsymbol{\eta}}} [(\partial_{\nabla\boldsymbol{\eta}}\psi)\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{\eta}}\, dA, \tag{67}$$

a functional of the rates $\dot{\boldsymbol{u}}$, $\dot{\boldsymbol{\eta}}$ of the macro- and micro-motion and the dissipative driving forces $\dot{\mathfrak{b}}$. We then propose the extended three-field variational principle

$$\{\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b}\} = \text{Arg}\Big\{\inf_{\dot{\boldsymbol{u}}}\inf_{\dot{\boldsymbol{\eta}}}\sup_{\mathfrak{b}}\Pi^*(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b})\Big\}, \tag{68}$$

which defines at the given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$ at time t the rates of the macro- and micro-motion fields along with the dissipative driving force. Taking the variation of the potential (67), we find that Eqs. (43)–(46) are the Euler equations of the saddle point principle (68).

3.3. A rate-independent four-field principle with threshold

In order to obtain a characteristic variational principle for rate-independent dissipative processes with threshold function, we replace the dissipation potential function ϕ in (63) by the representation (51) in terms of the dissipative driving force,

inducing the modified dissipation potential functional

$$D^*_\lambda(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b},\lambda) := \int_{\mathcal{B}} \{\mathfrak{b}\cdot\dot{\mathfrak{c}} - \lambda(f(\mathfrak{b};\mathfrak{c}) - c)\}\, dV \tag{69}$$

in terms of the Lagrange multiplier field λ. We then consider the extended potential

$$\underbrace{\Pi^*_\lambda(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b},\lambda)}_{\text{potential}} := \underbrace{\frac{d}{dt}E(\boldsymbol{u},\boldsymbol{\eta})}_{\text{energy}} + \underbrace{D^*_\lambda(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b},\lambda)}_{\text{dissipation}} - \underbrace{P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t)}_{\text{work}} \tag{70}$$

at given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$ at load level t. With (17), the potential takes the form

$$\Pi^*_\lambda = \int_{\mathcal{B}} \{[\delta_{\boldsymbol{u}}\psi - \overline{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{u}} + [\delta_{\boldsymbol{\eta}}\psi - \tilde{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{\eta}} + \mathfrak{b}\cdot\dot{\mathfrak{c}} - \lambda(f-c)\}\, dV + \int_{\partial\mathcal{B}_\sigma} [(\partial_{\nabla_s\boldsymbol{u}}\psi)\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{u}}\, dA + \int_{\partial\mathcal{B}_\mathfrak{h}} [(\partial_{\nabla\boldsymbol{\eta}}\psi)\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{\eta}}\, dA, \tag{71}$$

a functional of the rates $\dot{\boldsymbol{u}}$, $\dot{\boldsymbol{\eta}}$ of the macro- and micro-motion, the dissipative driving forces $\dot{\mathfrak{b}}$ and the Lagrange multiplier λ. We then consider the extended four-field variational principle

$$\{\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b},\lambda\} = \text{Arg}\left\{\inf_{\dot{\boldsymbol{u}}}\inf_{\dot{\boldsymbol{\eta}}}\sup_{\mathfrak{b}}\sup_{\lambda\geq 0}\Pi^*_\lambda(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b},\lambda)\right\}, \tag{72}$$

which defines the rates of the macro- and micro-motion fields along with the dissipative driving force and the Lagrange parameter. Taking the variation of the potential (71), we find that Eqs. (43)–(45) and (53)–(54) are the Euler equations of the saddle point principle (72).

3.4. A rate-dependent three-field principle with threshold

Finally, we may construct a specific rate-dependent three-field principle with threshold function, by replacing the dissipation function ϕ in (63) by the representation (56), yielding the specific dissipation potential functional

$$D^*_\eta(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b}) = \int_{\mathcal{B}} \left\{\mathfrak{b}\cdot\dot{\mathfrak{c}} - \frac{c}{\eta(m+1)}\langle f(\mathfrak{b};\mathfrak{c})/c - 1\rangle^{m+1}\right\} dV. \tag{73}$$

We then consider the potential

$$\underbrace{\Pi^*_\eta(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b})}_{\text{potential}} := \underbrace{\frac{d}{dt}E(\boldsymbol{u},\boldsymbol{\eta})}_{\text{energy}} + \underbrace{D^*_\eta(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}},\mathfrak{b})}_{\text{dissipation}} - \underbrace{P_{ext}(\dot{\boldsymbol{u}},\dot{\boldsymbol{\eta}};t)}_{\text{work}} \tag{74}$$

at a given state $\{\boldsymbol{u},\boldsymbol{\eta}\}$ and time t, which may be considered as a specification of the potential Π^* defined in (66). It takes the explicit form

$$\begin{aligned}\Pi^*_\eta = &\int_{\mathcal{B}} \{[\delta_{\boldsymbol{u}}\psi - \overline{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{u}} + [\delta_{\boldsymbol{\eta}}\psi - \tilde{\boldsymbol{\gamma}}]\cdot\dot{\boldsymbol{\eta}} + \mathfrak{b}\cdot\dot{\mathfrak{c}} - \frac{c}{\eta(m+1)}\langle f/c - 1\rangle^{m+1}\}\, dV \\ &+ \int_{\partial\mathcal{B}_\sigma} [(\partial_{\nabla_s\boldsymbol{u}}\psi)\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{u}}\, dA + \int_{\partial\mathcal{B}_\mathfrak{h}} [(\partial_{\nabla\boldsymbol{\eta}}\psi)\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\dot{\boldsymbol{\eta}}\, dA.\end{aligned} \tag{75}$$

The three-field variational principle (68) applied to this specific potential defines the rates of the macro- and micro-motion fields along with the dissipative driving force. Taking the variation of the potential Π^*_η, we end up with Eqs. (43)–(45) and (59)–(60) as the Euler equations of the saddle point principle (68) for $\Pi^* = \Pi^*_\eta$.

4. Time-discrete incremental variational principles

4.1. Time-discrete field variables in incremental setting

The above outlined variational structure is of great importance with regard to the time-discrete setting of gradient-type dissipative solids. To show this, we consider solutions of the field variables at the discrete times $0, t_1, t_2, \ldots, t_n, t_{n+1}, \ldots, T$ of the process interval $[0,T]$. In order to advance the solution within a typical time step, we focus on the finite time increment $[t_n, t_{n+1}]$, where

$$\tau_{n+1} := t_{n+1} - t_n > 0 \tag{76}$$

denotes the step length. In the subsequent treatment, all field variables at time t_n are assumed to be *known*. The goal then is to determine the fields at time t_{n+1} based on variational principles valid for the time increment under consideration. In order to obtain a compact notation, we drop in what follows the subscript $n+1$ and consider all variables without subscript to be evaluated at time t_{n+1}. In particular, we write $\boldsymbol{u}(\boldsymbol{x}) := \boldsymbol{u}(\boldsymbol{x},t_{n+1})$ and $\boldsymbol{\eta}(\boldsymbol{x}) := \boldsymbol{\eta}(\boldsymbol{x},t_{n+1})$ for the displacement and order parameter fields at the current time t_{n+1} and $\boldsymbol{u}_n(\boldsymbol{x}) := \boldsymbol{u}(\boldsymbol{x},t_n)$ and $\boldsymbol{\eta}_n(\boldsymbol{x}) := \boldsymbol{\eta}(\boldsymbol{x},t_n)$ for the fields at time t_n. Then

$$\mathfrak{u} := \{\boldsymbol{u},\boldsymbol{\eta}\} \tag{77}$$

assembles the primary variables at the current time t_{n+1} and

$$\mathfrak{c} := \{\nabla_s \boldsymbol{u}, \mathfrak{q}, \nabla\mathfrak{q}\} \quad \text{and} \quad \mathfrak{c}_n := \{\nabla_s \boldsymbol{u}_n, \mathfrak{q}_n, \nabla\mathfrak{q}_n\} \tag{78}$$

denotes the constitutive states (14) at time t_{n+1} and time t_n, respectively. The rate of the constitutive state is considered to be constant in the time increment (76) under consideration and defined by the *algorithmic* expression

$$\dot{\mathfrak{c}} := (\mathfrak{c} - \mathfrak{c}_n)/\tau. \tag{79}$$

Note carefully that due to the given fields at time t_n, this rate is a linear function of state $\mathfrak{c}$ at the current time t_{n+1}.[3] Furthermore, setting $\mathfrak{s}(\boldsymbol{x}) := \mathfrak{s}(\boldsymbol{x}, t_{n+1})$, $\mathfrak{p}(\boldsymbol{x}) := \mathfrak{p}(\boldsymbol{x}, t_{n+1})$ and $\mathfrak{g}(\boldsymbol{x}) := \mathfrak{g}(\boldsymbol{x}, t_{n+1})$, we write in what follows

$$\mathfrak{b} := \{\mathfrak{s}, \mathfrak{p}, \mathfrak{g}\} \tag{80}$$

for the current, time-discrete dissipative force array (36). Finally, $\lambda(\boldsymbol{x}) := \lambda(\boldsymbol{x}, t_{n+1}) \geq 0$ denotes in what follows the Lagrangian multiplier at time t_{n+1}.

4.2. Incremental energy, dissipation and load functionals

The construction of incremental variational principles, which determine the macro- and micro-motion $\boldsymbol{u}$ and $\mathfrak{q}$ at the current time t_{n+1}, depends critically on the *incremental* energy storage, dissipation and external work done in a finite time step $[t_n, t_{n+1}]$.

4.2.1. Incremental energy

Associated with the time interval (76), we define the increment of the energy stored in the solid due to the coupled macro–micro-motion by

$$E^\tau(\boldsymbol{u}, \mathfrak{q}; \boldsymbol{u}_n, \mathfrak{q}_n) := \int_{t_n}^{t_{n+1}} \dot{E}\, dt = \int_{\mathcal{B}} \{\psi(\mathfrak{c}) - \psi(\mathfrak{c}_n)\}\, dV \tag{81}$$

at given state $\{\boldsymbol{u}_n, \mathfrak{q}_n\}$, where E is the energy functional defined in (10). Taking into account the constitutive assumption (15), we consider the above incremental energy as a functional of the field variables (77) at the current time t_{n+1}. It is governed by the free energy function ψ.

4.2.2. Incremental dissipation potential

Furthermore, we define associated with the time interval (76) an expression for an incremental dissipation potential in the solid due to the coupled macro–micro-motion

$$D^\tau := \int_{t_n}^{t_{n+1}} \phi\, dt, \tag{82}$$

where ϕ is the dissipation potential defined in (10). As mentioned above, this is the physical dissipation only for the rate-independent case where the dissipation function coincides with the dissipation. Taking into account the above definition (79) for the rate of the constitutive state, we consider the incremental dissipation as a functional of the field variables (77) at the current time t_{n+1}, defined by the *algorithmic* expression

$$D^\tau(\boldsymbol{u}, \mathfrak{q}; \boldsymbol{u}_n, \mathfrak{q}_n) = \int_{\mathcal{B}} \tau\phi([\mathfrak{c} - \mathfrak{c}_n]/\tau; \mathfrak{c}_n)\, dV \tag{83}$$

at given state $\{\boldsymbol{u}_n, \mathfrak{q}_n\}$. The above canonical dissipation functional is governed by the dissipation function ϕ. The insertion of the Legendre transformation outlined in (41) gives an extended dissipation functional

$$D^{\tau *}(\boldsymbol{u}, \mathfrak{q}, \mathfrak{b}; \boldsymbol{u}_n, \mathfrak{q}_n) = \int_{\mathcal{B}} \{\mathfrak{b} \cdot [\mathfrak{c} - \mathfrak{c}_n] - \tau\phi^*(\mathfrak{b}; \mathfrak{c}_n)\}\, dV. \tag{84}$$

This extended dissipation functional is a function of an extended set of variables, including the dissipative forces at the time t_{n+1} defined in (80). Setting $\phi^* = \lambda(f - c)$ in terms of the multiplier λ and the threshold function f, we obtain a third incremental dissipation functional

$$D^{\tau *}_\lambda(\boldsymbol{u}, \mathfrak{q}, \mathfrak{b}, \lambda; \boldsymbol{u}_n, \mathfrak{q}_n) = \int_{\mathcal{B}} \{\mathfrak{b} \cdot [\mathfrak{c} - \mathfrak{c}_n] - \tau\lambda[f(\mathfrak{b}; \mathfrak{c}_n) - c]\}\, dV, \tag{85}$$

which depends in addition on the multiplier field λ at the current time t_{n+1}. Recall that $c > 0$ is a constant threshold parameter. A fourth incremental dissipation functional is obtained by insertion of the specific dual dissipation function ϕ^*

[3] *Remark on primary variables.* As a consequence of the finite-step-sized algorithmic representation of rates such as (79), the subsequent incremental variational principles determine the *discrete state variables* at the current time t_{n+1}. This makes a formal difference to the continuous setting outlined in Section 3, where the rates are the primary variables. As shown below, the algorithmic definition (79) results in variational implicit Euler integrators of the evolution equations.

defined in (58) into (84), yielding

$$D_{\eta}^{\tau *}(\boldsymbol{u},\mathfrak{q},\mathfrak{b};\boldsymbol{u}_n,\mathfrak{q}_n)=\int_{\mathcal{B}}\left\{\mathfrak{b}\cdot[\mathfrak{c}-\mathfrak{c}_n]-\frac{\tau c}{\eta(m+1)}\langle f(\mathfrak{b};\mathfrak{c}_n)/c-1\rangle^{m+1}\right\}dV. \tag{86}$$

Here, $\eta>0$ is a viscosity parameter and $m>1$ a power exponent. Note carefully that the penalty-type dissipation functional (86) can be considered as the viscous *regularization* of the Lagrange-type dissipation functional (85), where the inverse viscosity $1/\eta$ plays the role of a penalty parameter.

4.2.3. Incremental load

Associated with the time interval (76), we define the increment of the work due to the external actions on the multi-field problem by

$$P_{ext}^{\tau}:=\int_{t_n}^{t_{n+1}}P_{ext}\,dt, \tag{87}$$

where P_{ext} is the total power of external loading defined in (25). Assuming a constant velocity in the time increment under consideration, we consider the incremental work as a functional of the macro- and micro-motion $\boldsymbol{u}$ and $\mathfrak{q}$ at the current time t_{n+1}, defined by the *algorithmic* expression

$$P_{ext}^{\tau}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n,t)=\int_{\mathcal{B}}\{\overline{\boldsymbol{\gamma}}\cdot(\boldsymbol{u}-\boldsymbol{u}_n)+\tilde{\boldsymbol{\gamma}}\cdot(\mathfrak{q}-\mathfrak{q}_n)\}dV+\int_{\partial\mathcal{B}_{\sigma}}\overline{\boldsymbol{t}}_N\cdot(\boldsymbol{u}-\boldsymbol{u}_n)dA+\int_{\partial\mathcal{B}_{\mathfrak{q}}}\tilde{\boldsymbol{t}}_N\cdot(\mathfrak{q}-\mathfrak{q}_n)dA \tag{88}$$

at given state $\{\boldsymbol{u}_n,\mathfrak{q}_n\}$. The functional is obtained by time integration of the macro- and micro-contributions (26). Here, $\overline{\boldsymbol{\gamma}}$, $\tilde{\boldsymbol{\gamma}}$, $\overline{\boldsymbol{t}}_N$ and $\tilde{\boldsymbol{t}}_N$ are *prescribed* body force and traction fields evaluated at the current time t_{n+1}.

4.3. The canonical two-field minimization principle

4.3.1. Time-discrete formulation

A canonical incremental variational principle of gradient-type dissipative solids may be formulated in terms of the functional

$$\underbrace{\Pi^{\tau}(\boldsymbol{u},\mathfrak{q})}_{potential}:=\underbrace{E^{\tau}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n)}_{energy}+\underbrace{D^{\tau}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n)}_{dissipation}-\underbrace{P_{ext}^{\tau}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n,t)}_{work} \tag{89}$$

with the incremental energy functional (81), the incremental dissipation functional (83) and the incremental work functional (88). With the compact notation of the objective state vectors (78) at hand, we may write the variational functional

$$\Pi^{\tau}=\int_{\mathcal{B}}\{\pi^{\tau}(\mathfrak{c};\mathfrak{c}_n)-\overline{\boldsymbol{\gamma}}\cdot(\boldsymbol{u}-\boldsymbol{u}_n)-\tilde{\boldsymbol{\gamma}}\cdot(\mathfrak{q}-\mathfrak{q}_n)\}\,dV-\int_{\partial\mathcal{B}_{\sigma}}\overline{\boldsymbol{t}}_N\cdot(\boldsymbol{u}-\boldsymbol{u}_n)\,dA-\int_{\partial\mathcal{B}_{\mathfrak{q}}}\tilde{\boldsymbol{t}}_N\cdot(\mathfrak{q}-\mathfrak{q}_n)\,dA, \tag{90}$$

where we call π^{τ} the *incremental internal work density*. It has the representation

$$\pi^{\tau}(\mathfrak{c};\mathfrak{c}_n)=\psi(\mathfrak{c})-\psi_n+\tau\phi([\mathfrak{c}-\mathfrak{c}_n]/\tau;\mathfrak{c}_n) \tag{91}$$

in terms of the free energy function ψ and dissipation potential functions ϕ, respectively. Then, the finite-step-sized incremental minimization principle

$$\{\boldsymbol{u},\mathfrak{q}\}=\mathrm{Arg}\left\{\inf_{\boldsymbol{u}}\inf_{\mathfrak{q}}\Pi^{\tau}(\boldsymbol{u},\mathfrak{q})\right\} \tag{92}$$

determines the displacement and the order parameter fields $\boldsymbol{u}$ and $\mathfrak{q}$ at the current time t_{n+1} as the *minimum* of the incremental functional Π^{τ}. The variation of the functional (90) gives the necessary condition $0\in\delta\Pi^{\tau}$ with

$$\begin{aligned}\delta\Pi^{\tau}=&\int_{\mathcal{B}}\{[\delta_{\boldsymbol{u}}\psi-\overline{\boldsymbol{\gamma}}]\cdot\delta\boldsymbol{u}+[\delta_{\mathfrak{q}}\psi+\delta_{\dot{\mathfrak{q}}}\phi-\tilde{\boldsymbol{\gamma}}]\cdot\delta\mathfrak{q}\}\,dV+\int_{\partial\mathcal{B}_{\sigma}}[(\partial_{\nabla\boldsymbol{u}}\psi+\partial_{\nabla\dot{\boldsymbol{u}}}\phi)\cdot\boldsymbol{n}-\overline{\boldsymbol{t}}_N]\cdot\delta\boldsymbol{u}\,dA\\&+\int_{\partial\mathcal{B}_{\mathfrak{q}}}[(\partial_{\nabla\mathfrak{q}}\psi+\partial_{\nabla\dot{\mathfrak{q}}}\phi)\cdot\boldsymbol{n}-\tilde{\boldsymbol{t}}_N]\cdot\delta\mathfrak{q}\,dA\end{aligned} \tag{93}$$

and the admissible variations $\delta\boldsymbol{u}\in\mathcal{W}_{\boldsymbol{u}}^0$ and $\delta\mathfrak{q}\in\mathcal{W}_{\mathfrak{q}}^0$. The Euler equations of this minimization principle (92) are Eqs. (32)–(34), evaluated at the discrete time t_{n+1}. Here, the rate $\dot{\mathfrak{q}}$ is understood to be defined for the current time increment by the algorithmic expressions (79). Note that the above statement can be interpreted as a *virtual work balance* of internal and external actions at the discrete time t_{n+1}, where the internal work decomposes additively into energetic and dissipative parts.

4.3.2. Finite element discretization

We now consider the spatial discretization of the coupled problem by a finite element method. Let $\mathfrak{T}^h$ denote a finite element triangulation of the solid domain $\mathcal{B}$. The index h indicates a typical mesh size based on E^h finite element domains $\mathcal{B}_e^h\in\mathfrak{T}^h$ and N^h global nodal points. Associated with the triangulation $\mathfrak{T}^h$, we write the finite element interpolations of the

macro- and micro-motions and the constitutive state vector in the compact form

$$\boldsymbol{u}^h = \overline{\boldsymbol{N}}(\boldsymbol{x})\boldsymbol{d}, \quad \boldsymbol{\mathfrak{y}}^h = \tilde{\boldsymbol{N}}(\boldsymbol{x})\boldsymbol{d}, \quad \boldsymbol{\mathfrak{c}}^h = \boldsymbol{B}(\boldsymbol{x})\boldsymbol{d} \tag{94}$$

in terms of the *global nodal state vector* $\boldsymbol{d} \in \mathcal{R}^{(d+\delta)N^h}$, which contains the macro- and micro-motions $\boldsymbol{\mathfrak{u}}$ defined in (77) at a typical nodal point of the finite element mesh. $\overline{\boldsymbol{N}}$, $\tilde{\boldsymbol{N}}$, and $\boldsymbol{B}$ are symbolic representations of the global matrices of shape functions for the coupled problem. Clearly, these global arrays are never formulated explicitly, but represent symbolically the interpolations on all finite element domains $\mathcal{B}_e^h \in \mathfrak{T}^h$. Note that the global nodal state vector $\boldsymbol{d}$ is formed from the element state vectors $\boldsymbol{d}^e$ by a standard finite element assembling procedure.[4]

The shape matrices $\overline{\boldsymbol{N}}$, $\tilde{\boldsymbol{N}}$, and $\boldsymbol{B}$ introduced above govern the algebraic expressions of the incremental work, energy and dissipation functionals. With the discretization of the generalized displacement and the constitutive state fields (94), we write the spatial discretization of the incremental two-field functional (90)

$$\Pi^h(\boldsymbol{d}) = \int_{\mathcal{B}} \{\pi^\tau(\boldsymbol{B}\boldsymbol{d}; \boldsymbol{B}\boldsymbol{d}_n) - \overline{\boldsymbol{\gamma}} \cdot \overline{\boldsymbol{N}}(\boldsymbol{d}-\boldsymbol{d}_n) - \tilde{\boldsymbol{\gamma}} \cdot \tilde{\boldsymbol{N}}(\boldsymbol{d}-\boldsymbol{d}_n)\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{t}}_N \cdot \overline{\boldsymbol{N}}(\boldsymbol{d}-\boldsymbol{d}_n)\, dA - \int_{\partial\mathcal{B}_{\mathfrak{y}}} \tilde{\boldsymbol{t}}_N \cdot \tilde{\boldsymbol{N}}(\boldsymbol{d}-\boldsymbol{d}_n)\, dA. \tag{97}$$

Then, the finite-step-sized discrete minimization principle

$$\boldsymbol{d} = \mathrm{Arg}\left\{ \inf_{\boldsymbol{d}} \Pi^h(\boldsymbol{d}) \right\} \tag{98}$$

determines the nodal state vector $\boldsymbol{d}$ of the finite element mesh at the current time t_{n+1}. The necessary condition of the discrete variational problem (98) reads

$$\boldsymbol{0} \in \Pi^h_{,\boldsymbol{d}} = \int_{\mathcal{B}} \{\boldsymbol{B}^T[\partial_{\mathfrak{c}}\pi^\tau] - \overline{\boldsymbol{N}}^T\overline{\boldsymbol{\gamma}} - \tilde{\boldsymbol{N}}^T\tilde{\boldsymbol{\gamma}}\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{N}}^T\overline{\boldsymbol{t}}_N\, dA - \int_{\partial\mathcal{B}_{\mathfrak{y}}} \tilde{\boldsymbol{N}}^T\tilde{\boldsymbol{t}}_N\, dA \tag{99}$$

and provides a nonlinear algebraic system for the determination of the nodal state $\boldsymbol{d}$. For smooth problems, a standard Newton-type iteration of the nonlinear algebraic system (99) updates the state vector by the algorithm

$$\boldsymbol{d} \Leftarrow \boldsymbol{d} - [\Pi^h_{,\boldsymbol{d}\boldsymbol{d}}]^{-1}[\Pi^h_{,\boldsymbol{d}}] \tag{100}$$

in terms of the monolithic tangent matrix of the coupled problem

$$\Pi^h_{,\boldsymbol{d}\boldsymbol{d}} := \int_{\mathcal{B}} \boldsymbol{B}^T[\partial^2_{\mathfrak{c}\mathfrak{c}}\pi^\tau]\boldsymbol{B}\, dV. \tag{101}$$

Observe the *symmetry of the tangent matrix* induced by the incremental variational structure of the coupled two-field problem. The update (100) is performed until convergence is achieved in the sense $|\Pi^h_{,\boldsymbol{d}}| < tol$. Observe that the finite element residual and tangent are governed by the *generalized stress and tangent arrays*

$$\boldsymbol{S}^h := \partial_{\mathfrak{c}}\pi^\tau(\boldsymbol{\mathfrak{c}}^h; \boldsymbol{\mathfrak{c}}^h_n) \quad \text{and} \quad \mathbb{C}^h := \partial^2_{\mathfrak{c}\mathfrak{c}}\pi^\tau(\boldsymbol{\mathfrak{c}}^h; \boldsymbol{\mathfrak{c}}^h_n), \tag{102}$$

i.e. the first and second derivatives of the incremental internal work density π^τ defined in (91) by the discretized constitutive state vector $\boldsymbol{\mathfrak{c}}^h$ at current time t_{n+1}. These arrays are a critical ingredient of the proposed variational formulation and make the notation extremely compact.

4.4. The extended three-field saddle point principle

4.4.1. Time-discrete formulation

An extended incremental variational principle for gradient-type dissipative solids is based on the modified functional

$$\underbrace{\Pi^{*\tau}(\boldsymbol{u},\boldsymbol{\mathfrak{y}},\boldsymbol{\mathfrak{b}})}_{\text{potential}} := \underbrace{E^\tau(\boldsymbol{u},\boldsymbol{\mathfrak{y}};\boldsymbol{u}_n,\boldsymbol{\mathfrak{y}}_n)}_{\text{energy}} + \underbrace{D^{*\tau}(\boldsymbol{u},\boldsymbol{\mathfrak{y}},\boldsymbol{\mathfrak{b}};\boldsymbol{u}_n,\boldsymbol{\mathfrak{y}}_n)}_{\text{dissipation}} - \underbrace{P^\tau_{ext}(\boldsymbol{u},\boldsymbol{\mathfrak{y}};\boldsymbol{u}_n,\boldsymbol{\mathfrak{y}}_n,t)}_{\text{work}}, \tag{103}$$

where we have used the extended dissipation potential functional (84) in terms of the dual dissipation potential function ϕ^*. Introducing the *extended* variable vector

$$\boldsymbol{\mathfrak{u}}^* := \{\boldsymbol{u},\boldsymbol{\mathfrak{y}},\boldsymbol{\mathfrak{b}}\} \in \mathcal{R}^{d+\delta+[d(d+1)/2+\delta+\delta d]} \tag{104}$$

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[4] *Shapes for two-field model problem.* For two-dimensional problems $d = 2$ with a scalar micro-variable $\delta = 1$, the nodal state vector in (94) at the node I is

$$\boldsymbol{d}_I = [u_1, u_2, \mathfrak{y}]^T_I. \tag{95}$$

The constitutive state vector (78) reads $\boldsymbol{\mathfrak{c}} = [u_{1,1}, u_{2,2}, u_{1,2}+u_{2,1}, \mathfrak{y}, \mathfrak{y}_{,1}, \mathfrak{y}_{,2}]$. Then, associated with node I of a standard finite element e, the finite element interpolation matrices in (94) have the form

$$\overline{\boldsymbol{N}}^e_I = \begin{bmatrix} N & 0 & 0 \\ 0 & N & 0 \end{bmatrix}_I, \quad \tilde{\boldsymbol{N}}^e_I = [0 \quad 0 \quad N]_I, \quad \boldsymbol{B}^e_I = \begin{bmatrix} N_{,1} & 0 & N_{,2} & 0 & 0 & 0 \\ 0 & N_{,2} & N_{,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & M & M_{,1} & M_{,2} \end{bmatrix}^T_I \tag{96}$$

in terms of the shape functions N_I, M_I at note I and their derivatives. For identical interpolations of micro- and macro-motions, we set $M_I = N_I$.

and the *extended constitutive state vector*

$$\mathfrak{c}^* := \{\mathfrak{c},\mathfrak{b}\}^T \in \mathcal{R}^{2[d(d+1)/2+\delta+\delta d]}, \tag{105}$$

that contains both the constitutive state vector (78) and the dissipative driving force (80), we may write the variational functional (103)

$$\Pi^{*\tau} = \int_{\mathcal{B}} \{\pi^{*\tau}(\mathfrak{c}^*;\mathfrak{c}^*_n) - \overline{\boldsymbol{\gamma}}\cdot(\boldsymbol{u}-\boldsymbol{u}_n) - \tilde{\boldsymbol{\gamma}}\cdot(\mathfrak{q}-\mathfrak{q}_n)\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{t}}_N\cdot(\boldsymbol{u}-\boldsymbol{u}_n)\, dA - \int_{\partial\mathcal{B}_\mathfrak{h}} \tilde{\boldsymbol{t}}_N\cdot(\mathfrak{q}-\mathfrak{q}_n)\, dA, \tag{106}$$

where we call $\pi^{*\tau}$ the *extended incremental work density*. It has the representation

$$\pi^{*\tau}(\mathfrak{c}^*;\mathfrak{c}^*_n) = \psi(\mathfrak{c}) - \psi_n + \mathfrak{b}\cdot[\mathfrak{c}-\mathfrak{c}_n] - \tau\phi^*(\mathfrak{b};\mathfrak{c}_n) \tag{107}$$

in terms of the free energy function ψ and dual dissipation potential ϕ^*, respectively. The finite-step-sized incremental saddle point principle

$$\{\boldsymbol{u},\mathfrak{q},\mathfrak{b}\} = \text{Arg}\Big\{\inf_{\boldsymbol{u}}\inf_{\mathfrak{q}}\sup_{\mathfrak{b}} \Pi^{*\tau}(\boldsymbol{u},\mathfrak{q},\mathfrak{b})\Big\} \tag{108}$$

determines the macro- and micro-motions $\boldsymbol{u}$ and $\mathfrak{q}$ as well as the dissipative forces $\mathfrak{b}$ at the current time t_{n+1} as a *saddle point* of the incremental functional $\Pi^{\tau*}$. The necessary condition of the above principle reads $0 \in \delta\Pi^{*\tau}$ with

$$\begin{aligned}\delta\Pi^{*\tau} := &\int_{\mathcal{B}} ([-\text{div}[\partial_{\nabla_s\boldsymbol{u}}\psi+\mathfrak{s}]-\overline{\boldsymbol{\gamma}}]\cdot\delta\boldsymbol{u} + [\mathfrak{c}-\mathfrak{c}_n-\tau\partial_\mathfrak{b}\phi^*]\cdot\delta\mathfrak{b})\, dV + \int_{\mathcal{B}} [(\partial_\mathfrak{q}\psi+\mathfrak{p}) - \text{div}(\partial_{\nabla_\mathfrak{q}}\psi+\mathfrak{g}) - \tilde{\boldsymbol{\gamma}}]\cdot\delta\mathfrak{q}\, dV \\ &+ \int_{\partial\mathcal{B}_\sigma} [(\partial_{\nabla_s\boldsymbol{u}}\psi+\mathfrak{s})\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\delta\boldsymbol{u}\, dA + \int_{\partial\mathcal{B}_\mathfrak{h}} [(\partial_{\nabla_\mathfrak{q}}\psi+\mathfrak{g})\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\delta\mathfrak{q}\, dA\end{aligned} \tag{109}$$

and the admissible variations $\delta\boldsymbol{u} \in \mathcal{W}^0_{\boldsymbol{u}}$, $\delta\mathfrak{q} \in \mathcal{W}^0_\mathfrak{q}$ and $\delta\mathfrak{p}$ of the current macro- and micro-motions and dissipative forces. The Euler equations of the principle (108) are Eqs. (43)–(46), evaluated at the discrete time t_{n+1}. The above statement can again be interpreted as a *virtual work balance* similar to (28), but now supplemented by weak statements of the incremental update equations which define the dissipative forces.

4.4.2. Finite element discretization

In analogy to (94), we introduce for the finite element triangulation $\mathfrak{T}^h$ interpolations of the macro- and micro-motions and the *extended* generalized state vector (105)

$$\boldsymbol{u}^h = \overline{\boldsymbol{N}}^*(\boldsymbol{x})\boldsymbol{d}^*, \quad \mathfrak{q}^h = \tilde{\boldsymbol{N}}^*(\boldsymbol{x})\boldsymbol{d}^*, \quad \mathfrak{c}^{*h} = \boldsymbol{B}^*(\boldsymbol{x})\boldsymbol{d}^* \tag{110}$$

in terms of the *extended* global nodal state vector $\boldsymbol{d}^*$, which contains the macro- and micro-motions *and* driving forces $\mathfrak{u}^*$ as defined in (104) at a typical nodal point of the finite element mesh. $\overline{\boldsymbol{N}}^*$, $\tilde{\boldsymbol{N}}^*$, and $\boldsymbol{B}^*$ are symbolic representations of the global matrices of shape functions for the coupled problem.[5] Then, the spatial discretization of the incremental two-field functional (106) takes the form

$$\Pi^{*h}(\boldsymbol{d}^*) = \int_{\mathcal{B}} \{\pi^{*\tau}(\boldsymbol{B}^*\boldsymbol{d}^*;\boldsymbol{B}^*\boldsymbol{d}^*_n) dV - \overline{\boldsymbol{\gamma}}\cdot\overline{\boldsymbol{N}}^*(\boldsymbol{d}^*-\boldsymbol{d}^*_n) - \tilde{\boldsymbol{\gamma}}\cdot\tilde{\boldsymbol{N}}^*(\boldsymbol{d}^*-\boldsymbol{d}^*_n)\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{t}}_N\cdot\overline{\boldsymbol{N}}^*(\boldsymbol{d}^*-\boldsymbol{d}^*_n) dA - \int_{\partial\mathcal{B}_\mathfrak{h}} \tilde{\boldsymbol{t}}_N\cdot\tilde{\boldsymbol{N}}^*(\boldsymbol{d}^*-\boldsymbol{d}^*_n)\, dA \tag{113}$$

in full analogy to (97). Then, the finite-step-sized discrete saddle point principle

$$\boldsymbol{d}^* = \text{Arg}\Big\{\underset{\boldsymbol{d}^*}{\text{stat}}\ \Pi^{*h}(\boldsymbol{d}^*)\Big\} \tag{114}$$

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[5] *Shapes for three-field model problem.* For two-dimensional problems $d = 2$ with a scalar micro-variable $\delta = 1$ and a simple dual dissipation function $\phi^*(\mathfrak{p})$ depending only on the force $\mathfrak{p}$, i.e. with simple form $\mathfrak{b} = \{\mathfrak{p}\}$ of (36), the extended nodal state vector in (104) at the node I is

$$\boldsymbol{d}^*_I = [u_1, u_2, \mathfrak{q}, \mathfrak{p}]^T_I. \tag{111}$$

The *extended* constitutive state vector (105) reads $\mathfrak{c}^* = [u_{1,1}, u_{2,2}, u_{1,2}+u_{2,1}, \mathfrak{q}, \mathfrak{q}_{,1}, \mathfrak{q}_{,2}, \mathfrak{p}]$. Associated with node I of a standard finite element e, the interpolation matrix for the constitutive state reads

$$\boldsymbol{B}^{*e}_I = \begin{bmatrix} N_{,1} & 0 & N_{,2} & 0 & 0 & 0 & 0 \\ 0 & N_{,2} & N_{,1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & M & M_{,1} & M_{,2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & G \end{bmatrix}^T_I \tag{112}$$

in terms of the shape functions N_I, M_I, G_I at node I and their derivatives. For identical interpolations of displacements, order parameters, and driving forces, we set $G_I = M_I = N_I$.

determines the extended nodal state $\boldsymbol{d}^*$ of the finite element mesh at the current time t_{n+1}. The necessary condition of the discrete variational problem (98) reads

$$\mathbf{0} \in \Pi^{*h}_{,\boldsymbol{d}^*} = \int_{\mathcal{B}} \{\boldsymbol{B}^{*T}[\partial_{\mathfrak{e}^*}\pi^{*\tau}] - \overline{\boldsymbol{N}}^{*T}\overline{\boldsymbol{\gamma}} - \tilde{\boldsymbol{N}}^{*T}\tilde{\boldsymbol{\gamma}}\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{N}}^{*T}\overline{\boldsymbol{t}}_N\, dA - \int_{\partial\mathcal{B}_\mathfrak{y}} \tilde{\boldsymbol{N}}^{*T}\tilde{\boldsymbol{t}}_N\, dA \tag{115}$$

and provides a nonlinear algebraic system for the determination of the state $\boldsymbol{d}^*$. For smooth problems, a standard Newton-type iteration of the nonlinear algebraic system (115) updates the nodal state by the algorithm

$$\boldsymbol{d}^* \Leftarrow \boldsymbol{d}^* - [\Pi^{*h}_{,\boldsymbol{d}^*\boldsymbol{d}^*}]^{-1}[\Pi^{*h}_{,\boldsymbol{d}^*}] \tag{116}$$

in terms of the monolithic tangent matrix of the coupled problem

$$\Pi^{*h}_{,\boldsymbol{d}^*\boldsymbol{d}^*} := \int_{\mathcal{B}} \boldsymbol{B}^{*T}[\partial^2_{\mathfrak{e}^*\mathfrak{e}^*}\pi^{*\tau}]\boldsymbol{B}^*\, dV. \tag{117}$$

Observe the *symmetry of the tangent matrix* induced by the incremental variational structure of the coupled two-field problem. The iterative update (116) is performed until convergence is achieved in the sense $|\Pi^{*h}_{,\boldsymbol{d}^*}| < tol$. The finite element residual and tangent are governed by the *extended generalized stress and tangent arrays*

$$\boldsymbol{S}^{*h} := \partial_{\mathfrak{e}^*}\pi^{*\tau}(\mathfrak{e}^{*h};\mathfrak{e}^{*h}_n) \quad \text{and} \quad \mathbb{C}^{*h} := \partial^2_{\mathfrak{e}^*\mathfrak{e}^*}\pi^{*\tau}(\mathfrak{e}^{*h};\mathfrak{e}^{*h}_n) \tag{118}$$

as the first and second derivatives of the incremental internal work density $\pi^{*\tau}$ defined in (107) by the discretized constitutive state vector $\mathfrak{e}^{*h}$ at current time t_{n+1}. These compact arrays are an important consequence of the proposed variational formulation.

4.5. The rate-independent four-field principle with threshold

4.5.1. Time-discrete formulation

An alternative extended incremental variational principle of gradient-type dissipative solids for rate-independent response with threshold function is based on the functional

$$\underbrace{\Pi^{*\tau}_\lambda(\boldsymbol{u},\mathfrak{q},\mathfrak{b},\lambda)}_{potential} := \underbrace{E^\tau(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n)}_{energy} + \underbrace{D^{*\tau}_\lambda(\boldsymbol{u},\mathfrak{q},\mathfrak{b},\lambda;\boldsymbol{u}_n,\mathfrak{q}_n)}_{dissipation} - \underbrace{P^\tau_{ext}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n,t)}_{work} \tag{119}$$

with the Lagrange-type incremental dissipation functional (85) in terms of the threshold function f. Introducing an extended variable vector

$$\mathfrak{u}^*_\lambda := \{\boldsymbol{u},\mathfrak{q},\mathfrak{b},\lambda\} \in \mathcal{R}^{d+\delta+[d(d+1)/2+\delta+\delta d]+1} \tag{120}$$

and the *extended constitutive state vector*

$$\mathfrak{e}^*_\lambda := [\mathfrak{e},\mathfrak{b},\lambda]^T \in \mathcal{R}^{2[d(d+1)/2+\delta+\delta d]+1}, \tag{121}$$

which contain in addition to (104) and (105) the Lagrangian multiplier field λ at time t_{n+1}, we may write the variational functional (119)

$$\Pi^{*\tau}_\lambda = \int_{\mathcal{B}} \{\pi^{*\tau}_\lambda(\mathfrak{e}^*_\lambda;\mathfrak{e}^*_{\lambda n}) - \overline{\boldsymbol{\gamma}}\cdot(\boldsymbol{u}-\boldsymbol{u}_n) - \tilde{\boldsymbol{\gamma}}\cdot(\mathfrak{q}-\mathfrak{q}_n)\}\, dV - \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{t}}_N\cdot(\boldsymbol{u}-\boldsymbol{u}_n)\, dA - \int_{\partial\mathcal{B}_\mathfrak{y}} \tilde{\boldsymbol{t}}_N\cdot(\mathfrak{q}-\mathfrak{q}_n)\, dA, \tag{122}$$

where we call $\pi^{*\tau}_\lambda$ the *extended* incremental internal work density. It has the representation

$$\pi^{*\tau}_\lambda(\mathfrak{e}^*_\lambda;\mathfrak{e}^*_{\lambda n}) = \psi(\mathfrak{e}) - \psi_n + \mathfrak{b}\cdot[\mathfrak{e}-\mathfrak{e}_n] - \tau\lambda[f(\mathfrak{b};\mathfrak{e}_n) - c] \tag{123}$$

in terms of the free energy function ψ and the threshold function f, respectively. The finite-step-sized incremental stationary principle

$$\{\boldsymbol{u},\mathfrak{q},\mathfrak{b},\lambda\} = \mathrm{Arg}\left\{ \inf_{\boldsymbol{u}} \inf_{\mathfrak{q}} \sup_{\mathfrak{b}} \sup_{\lambda\geq 0} \Pi^{*\tau}_\lambda(\boldsymbol{u},\mathfrak{q},\mathfrak{b},\lambda) \right\} \tag{124}$$

determines besides the macro- and micro-motion fields $\boldsymbol{u}$ and $\mathfrak{q}$, the dissipative force fields $\mathfrak{b}$, and the Lagrangian multiplier field $\lambda \geq 0$ at the current time t_{n+1} as a *saddle point* of the incremental functional $\Pi^{*\tau}_\lambda$. The necessary condition of the above principle reads $0 \in \delta\Pi^{*\tau}_\lambda$ with

$$\begin{aligned}\delta\Pi^{*\tau}_\lambda := &\int_{\mathcal{B}} ([-\mathrm{div}(\partial_{\nabla_s\boldsymbol{u}}\psi + \mathfrak{s}) - \overline{\boldsymbol{\gamma}}]\cdot\delta\boldsymbol{u} + [\mathfrak{e}-\mathfrak{e}_n - \tau\lambda\partial_\mathfrak{b} f]\cdot\delta\mathfrak{b})\, dV + \int_{\mathcal{B}} (-\tau[f-c]\delta\lambda + [(\partial_\mathfrak{q}\psi + \mathfrak{p}) - \mathrm{div}(\partial_{\nabla\mathfrak{q}}\psi + \mathfrak{g}) - \tilde{\boldsymbol{\gamma}}]\cdot\delta\mathfrak{q})\, dV \\ &+ \int_{\partial\mathcal{B}_\sigma} [(\partial_{\nabla_s\boldsymbol{u}}\psi + \mathfrak{s})\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\delta\boldsymbol{u}\, dA + \int_{\partial\mathcal{B}_\mathfrak{y}} [(\partial_{\nabla\mathfrak{q}}\psi + \mathfrak{g})\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\delta\mathfrak{q}\, dA\end{aligned} \tag{125}$$

with admissible variations $\delta\boldsymbol{u} \in \mathcal{W}^0_{\boldsymbol{u}}$, $\delta\mathfrak{q} \in \mathcal{W}^0_{\mathfrak{q}}$, $\delta\mathfrak{p}$, and $\delta\lambda \geq 0$ of the current displacements, order parameters, dissipative forces, and the Lagrange parameter. The Euler equations of this variational principle are Eqs. (43)–(45) and (53)–(54), evaluated at the discrete time t_{n+1}. The statement is a *balance of virtual internal and external work*, supplemented by weak

statements of the incremental update equations which define the dissipative forces and the threshold-function-based loading condition.

4.5.2. Finite element discretization

In analogy to (110), we introduce for the finite element triangulation $\mathfrak{T}^h$ interpolations of the macro- and micro-motions and the *extended* constitutive state vector (121)

$$\boldsymbol{u} = \overline{\boldsymbol{N}}^*_\lambda(\boldsymbol{x})\boldsymbol{d}^*_\lambda, \quad \mathfrak{q} = \tilde{\boldsymbol{N}}^*_\lambda(\boldsymbol{x})\boldsymbol{d}^*_\lambda, \quad \mathfrak{e}^{*h}_\lambda = \boldsymbol{B}^*_\lambda(\boldsymbol{x})\boldsymbol{d}^*_\lambda \tag{126}$$

in terms of the *extended* generalized nodal displacement vector $\boldsymbol{d}^*_\lambda$, which contains the micro- and macro-motions, the dissipative forces *and* the Lagrange parameter as defined in (120) at a typical nodal point of the finite element mesh. $\overline{\boldsymbol{N}}^*_\lambda$, $\tilde{\boldsymbol{N}}^*_\lambda$ and $\boldsymbol{B}^*_\lambda$ are symbolic representations of the global matrices of shape functions for the coupled problem.[6] Then, the spatial discretization of the incremental two-field functional (106) takes the form

$$\Pi^{*h}_\lambda(\boldsymbol{d}^*_\lambda) = \int_{\mathcal{B}} \{\pi^{*\tau}_\lambda(\boldsymbol{B}^*_\lambda\boldsymbol{d}^*_\lambda; \boldsymbol{B}^*_\lambda\boldsymbol{d}^*_{\lambda n})dV - \overline{\boldsymbol{\gamma}}\cdot\overline{\boldsymbol{N}}^*_\lambda(\boldsymbol{d}^*_\lambda - \boldsymbol{d}^*_{\lambda n}) - \tilde{\boldsymbol{\gamma}}\cdot\tilde{\boldsymbol{N}}^*_\lambda(\boldsymbol{d}^*_\lambda - \boldsymbol{d}^*_{\lambda n})\}dV - \int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} \overline{\boldsymbol{t}}_N\cdot\overline{\boldsymbol{N}}^*_\lambda(\boldsymbol{d}^*_\lambda - \boldsymbol{d}^*_{\lambda n})dA - \int_{\partial\mathcal{B}_{\mathfrak{h}}} \tilde{\boldsymbol{t}}_N\cdot\tilde{\boldsymbol{N}}^*_\lambda(\boldsymbol{d}^*_\lambda - \boldsymbol{d}^*_{\lambda n})dA \tag{129}$$

in full analogy to (97). Then, the finite-step-sized discrete stationary principle

$$\boldsymbol{d}^*_\lambda = \mathrm{Arg}\left\{ \underset{\boldsymbol{d}^*_\lambda}{\mathrm{stat}}\ \Pi^{*h}_\lambda(\boldsymbol{d}^*_\lambda) \right\} \tag{130}$$

determines the nodal state $\boldsymbol{d}^*_\lambda$ of the finite element mesh at the current time t_{n+1}. The necessary condition of the discrete variational problem (130) reads

$$\boldsymbol{0} \in \Pi^{*h}_{\lambda,\boldsymbol{d}^*_\lambda} = \int_{\mathcal{B}} \{\boldsymbol{B}^{*T}_\lambda[\partial_{\mathfrak{e}^*_\lambda}\pi^{*\tau}_\lambda] - \overline{\boldsymbol{N}}^{*T}_\lambda\overline{\boldsymbol{\gamma}} - \tilde{\boldsymbol{N}}^{*T}_\lambda\tilde{\boldsymbol{\gamma}}\}\, dV - \int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} \overline{\boldsymbol{N}}^{*T}_\lambda\overline{\boldsymbol{t}}_N\, dA - \int_{\partial\mathcal{B}_{\mathfrak{h}}} \tilde{\boldsymbol{N}}^{*T}_\lambda\tilde{\boldsymbol{t}}_N\, dA \tag{131}$$

and provides a nonlinear algebraic system for the determination of the state $\boldsymbol{d}^*_\lambda$. The *non-smooth* character (53) of the rate-independent dissipative response is treated by an *active set strategy*, which generalizes treatments of gradient plasticity by Liebe and Steinmann (2001) to the variational-based setting of standard dissipative solids. Let λ_I be the nodal value of the Lagrange parameter at the node I of the finite element mesh and r_I the residual of the associated equation of the algebraic equation (131), thus

$$\lambda_I \in \boldsymbol{d}^*_\lambda \quad \text{and} \quad r_I \coloneqq \Pi^{*h}_{\lambda,\lambda_I}. \tag{132}$$

We introduce for the finite element discretization loading–unloading conditions of the form (53) at each node $I=1,\ldots,N^h$ of the finite element mesh

$$\lambda_I \geq 0, \quad r_I \leq 0, \quad \lambda_I r_I = 0. \tag{133}$$

This defines an *active set of nodes* $\mathcal{A}$ and associated finite element equations that has to be solved for active nodal Lagrange parameters $\lambda_I > 0$. In the finite step sized algorithmic setting, we define this active set by the *trial value* of the residual defined in (132)

$$\mathcal{A} \coloneqq \{I \in (1\ldots N^h) | r^{\mathrm{trial}}_I > 0\} \tag{134}$$

at the beginning of the incremental solution process. For non-active nodes, the nodal Lagrange parameter is set to zero

$$\lambda_I = 0 \quad \text{for } I \in (1,\ldots,N^h)\backslash\mathcal{A}. \tag{135}$$

[6] *Shapes for four-field model problem.* For two-dimensional problems $d = 2$ with a scalar micro-variable $\delta = 1$ and a simple dual dissipation function $\phi^*(\mathfrak{p})$ depending only on the force $\mathfrak{p}$, i.e. with simple form $\mathfrak{b} = \{\mathfrak{p}\}$ of (36), the extended global nodal state vector in (120) at the node I is

$$\boldsymbol{d}^*_{\lambda I} = [u_1, u_2, \mathfrak{q}, \mathfrak{p}, \lambda]^T_I. \tag{127}$$

The *extended* constitutive state vector (121) reads $\mathfrak{e}^* = [u_{1,1}, u_{2,2}, u_{1,2}+u_{2,1}, \mathfrak{q}, \mathfrak{q}_{,1}, \mathfrak{q}_{,2}, \mathfrak{p}, \lambda]$. Associated with node I of a standard finite element e, the interpolation matrix for the constitutive state reads

$$\boldsymbol{B}^{*e}_{\lambda I} = \begin{bmatrix} N_{,1} & 0 & N_{,2} & 0 & 0 & 0 & 0 & 0 \\ 0 & N_{,2} & N_{,1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & M & M_{,1} & M_{,2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & G & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & H \end{bmatrix}^T_I \tag{128}$$

in terms of the shape functions N_I, M_I, G_I, H_I at note I and their derivatives. For identical interpolations of displacements, order parameters, driving forces, and Lagrange parameter, we set $G_I = M_I = N_I = H_I$.

The active Lagrange parameters at the active node $I \in \mathcal{A}$ together with the other nodal degrees define a *reduced* global nodal state vector $\boldsymbol{d}^*_{\mathcal{A}}$, which is obtained for frozen active set (134) from the Newton updates of the reduced algebraic system (131)

$$\boldsymbol{d}^*_{\mathcal{A}} \Leftarrow \boldsymbol{d}^*_{\mathcal{A}} - [\Pi^{*h}_{\lambda,\boldsymbol{d}^*_{\mathcal{A}}\boldsymbol{d}^*_{\mathcal{A}}}]^{-1}[\Pi^{*h}_{\lambda,\boldsymbol{d}^*_{\mathcal{A}}}] \quad \text{with } \boldsymbol{d}^*_{\mathcal{A}} \subset \boldsymbol{d}^*_{\lambda} \tag{136}$$

in terms of the monolithic tangent matrix of the coupled problem

$$\Pi^{*h}_{\lambda,\boldsymbol{d}^*_{\mathcal{A}}\boldsymbol{d}^*_{\mathcal{A}}} := \int_{\mathcal{B}} \boldsymbol{B}^{*T}_{\mathcal{A}} [\partial^2_{\mathfrak{e}^*_\lambda \mathfrak{e}^*_\lambda} \pi^{*\tau}_\lambda] \boldsymbol{B}^*_{\mathcal{A}} \, dV. \tag{137}$$

Here, $\boldsymbol{B}^*_{\mathcal{A}}$ is obtained from $\boldsymbol{B}^*_\lambda$ defined in (126) by deleting the columns associated with the Lagrange parameters for non-active nodes. Observe the *symmetry of the tangent matrix* induced by the incremental variational structure of the coupled two-field problem. The update (136) is performed until convergence is achieved in the sense $|\Pi^{*h}_{\lambda,\boldsymbol{d}^*_{\mathcal{A}}}| < tol$. Observe that the finite element residual and tangent are governed by the *generalized stress and tangent arrays*

$$\boldsymbol{S}^{*h}_\lambda := \partial_{\mathfrak{e}^*_\lambda} \pi^{*\tau}_\lambda(\mathfrak{e}^{*h}_\lambda; \mathfrak{e}^{*h}_{\lambda n}) \quad \text{and} \quad \mathbb{C}^{*h}_\lambda := \partial^2_{\mathfrak{e}^*_\lambda \mathfrak{e}^*_\lambda} \pi^{\tau}_\lambda(\mathfrak{e}^{*h}_\lambda; \mathfrak{e}^{*h}_{\lambda n}) \tag{138}$$

as the first and second derivatives of the incremental internal work density $\pi^{*\tau}_\lambda$ defined in (123) by the discretized constitutive state vector $\mathfrak{e}^{*h}_\lambda$ at current time t_{n+1}. These arrays are a critical ingredient of the proposed variational formulation and make the notation extremely compact.

4.6. The rate-dependent three-field principle with threshold

An extended incremental variational principle of gradient-type dissipative solids for rate-dependent response with threshold function is based on the specific representation of the functional (103)

$$\underbrace{\Pi^{*\tau}(\boldsymbol{u},\mathfrak{q},\mathfrak{b})}_{\text{potential}} := \underbrace{E^\tau(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n)}_{\text{energy}} + \underbrace{D^{*\tau}_\eta(\boldsymbol{u},\mathfrak{q},\mathfrak{b};\boldsymbol{u}_n,\mathfrak{q}_n)}_{\text{dissipation}} - \underbrace{P^\tau_{ext}(\boldsymbol{u},\mathfrak{q};\boldsymbol{u}_n,\mathfrak{q}_n,t)}_{\text{work}} \tag{139}$$

in terms of the penalty-type incremental dissipation functional $D^{\tau*}_\eta$ introduced in (86). In this formulation, the extended incremental internal work density (107) has the specific representation

$$\pi^{*\tau}(\mathfrak{e}^*;\mathfrak{e}^*_n) = \psi(\mathfrak{e}) - \psi_n + \mathfrak{b}\cdot[\mathfrak{e}-\mathfrak{e}_n] - \frac{\tau c}{\eta(m+1)} \langle f(\mathfrak{b};\mathfrak{e}_n)/c - 1 \rangle^{m+1} \tag{140}$$

in terms of the free energy function ψ and the threshold function f, respectively. Then the variation of the principle (108) reads $0 \in \delta\Pi^{*\tau}$ with

$$\begin{aligned}\delta\Pi^{*\tau} := &\int_{\mathcal{B}} ([-\mathrm{div}[\partial_{\nabla_s \boldsymbol{u}}\psi + \mathfrak{s}] - \overline{\mathfrak{y}}]\cdot\delta\boldsymbol{u} + [\mathfrak{e}-\mathfrak{e}_n - \frac{\tau}{\eta}\langle f/c-1\rangle^m \partial_{\mathfrak{b}} f]\cdot\delta\mathfrak{b})\, dV + \int_{\mathcal{B}} [(\partial_{\mathfrak{q}}\psi + \mathfrak{p}) - \mathrm{div}(\partial_{\nabla_{\mathfrak{q}}}\psi + \mathfrak{g}) - \tilde{\mathfrak{y}}]\cdot\delta\mathfrak{q}\, dV \\ &+ \int_{\partial\mathcal{B}_{\boldsymbol{\sigma}}} [(\partial_{\nabla_s \boldsymbol{u}}\psi + \mathfrak{s})\cdot\boldsymbol{n} - \overline{\boldsymbol{t}}_N]\cdot\delta\boldsymbol{u}\, dA + \int_{\partial\mathcal{B}_{\mathfrak{h}}} [(\partial_{\nabla_{\mathfrak{q}}}\psi + \mathfrak{g})\cdot\boldsymbol{n} - \tilde{\boldsymbol{t}}_N]\cdot\delta\mathfrak{q}\, dA\end{aligned} \tag{141}$$

and the admissible variations $\delta\boldsymbol{u} \in \mathcal{W}^0_{\boldsymbol{u}}$, $\delta\mathfrak{q} \in \mathcal{W}^0_{\mathfrak{q}}$ and $\delta\mathfrak{b}$. Hence, the Euler equations of the variational principle (108) are algorithmic forms of Eqs. (43)–(45) and (59) with (60), evaluated at the discrete time t_{n+1}. Such a formulation is particularly convenient due to the smooth nature of the viscous dissipation function. The finite element formulation is based on the representations (110)–(118).

5. Representative model problems

In this section, we outline a spectrum of model problems that demonstrates the range of applications of the proposed variational framework. A critical goal is to point out the key importance of the *incremental potentials per unit volume*, which completely determine the coupled field equations as the Euler equations of the proposed variational principles. We set $\tilde{\boldsymbol{\gamma}} = \boldsymbol{0}$ in all subsequent examples.

5.1. The Kelvin-type viscoelastic solid

The simplest gradient-type dissipative model is the Kelvin-type viscoelastic solid, which is fully governed by the macro-motion $\boldsymbol{u}(\boldsymbol{x},t)$. Hence, the objective constitutive state (14) reduces to the strain tensor

$$\mathfrak{e} := \{\nabla_s \boldsymbol{u}\} \tag{142}$$

and the energy and dissipation potential functions (15) have the structure

$$\psi(\mathfrak{e}) = \psi^e(\nabla_s \boldsymbol{u}) \quad \text{and} \quad \phi(\dot{\mathfrak{e}};\mathfrak{e}) = \phi^\nu(\nabla_s \dot{\boldsymbol{u}}). \tag{143}$$

Simple quadratic functions of isotropic, linear viscoelasticity are $\psi^e = \frac{1}{2}|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}^e}$ and $\phi^\nu = \frac{1}{2}|\nabla_s \dot{\boldsymbol{u}}|^2_{\mathbb{E}^\nu}$ with the elastic and viscous moduli $\mathbb{E}^\alpha := \lambda^\alpha \boldsymbol{1}\otimes\boldsymbol{1} + 2\mu^\alpha \mathbb{I}$ for $\alpha = e,\nu$, respectively. The dissipation potential is a smooth function of the macroscopic strain

rate. The *incremental potential* (91) for this model problem reads

$$\pi^\tau(\mathfrak{c};\mathfrak{c}_n)=\frac{1}{2}|\nabla_s\boldsymbol{u}|^2_{\mathbb{E}^e}-\psi^e_n+\frac{1}{2\tau}|\nabla_s[\boldsymbol{u}-\boldsymbol{u}_n]|^2_{\mathbb{E}^v}. \tag{144}$$

The finite-step-sized incremental minimum principle (92) gives the Euler equation

$$-\mathrm{div}[\mathbb{E}^e:\nabla_s\boldsymbol{u}+\mathbb{E}^v:\nabla_s[\boldsymbol{u}-\boldsymbol{u}_n]/\tau]=\overline{\boldsymbol{\gamma}}, \tag{145}$$

which is a time-discrete form of the macroscopic balance (33). The Kelvin solid constitutes an additive decomposition of the macro-stresses $\boldsymbol{\sigma}$ into energetic and dissipative parts $\boldsymbol{\sigma}^e:=\partial_{\nabla_s\boldsymbol{u}}\psi^e$ and $\boldsymbol{\sigma}^v:=\partial_{\nabla_s\dot{\boldsymbol{u}}}\phi^v$, respectively. It is a typical example for a dependence of the incremental dissipation potential on the macro-motion $\boldsymbol{u}$.

5.2. Ginzburg–Landau-type phase-field evolution

A further very simple gradient-type dissipative model is the rigid solid undergoing phase transformations. Here, the so-called Ginzburg–Landau theory characterizes important features of two-phase-systems in material science, see Gurtin (1996) for a review. It is fully governed by a micro-motion $v(\boldsymbol{x},t)$, denoted as the phase field, which interpolates between the two phases. The objective constitutive state (14)

$$\mathfrak{c}:=\{v,\nabla v\} \tag{146}$$

contains the phase field and its gradient. The energy and dissipation potential functions (15) may have the particular form

$$\psi(\mathfrak{c})=\psi^s(v)+\frac{\kappa}{2}|\nabla v|^2\quad\text{and}\quad\phi(\dot{\mathfrak{c}};\mathfrak{c})=\frac{\eta}{2}\dot{v}^2. \tag{147}$$

$\psi^s(v)$ is a coarse grain free energy describing a double-well potential whose wells define the two phases. A simple example is the non-convex function $\psi^s=hv^2[1-v]^2$ with two minima at $v=0$ and 1 corresponding to the two phases. The gradient-type energetic term governs the diffuse phase-interface. The smooth dissipation function determines the evolution of the phase field. The *incremental potential* (91) for this model problem reads

$$\pi^\tau(\mathfrak{c};\mathfrak{c}_n)=hv^2[1-v]^2+\frac{\kappa}{2}|\nabla v|^2-\psi_n+\frac{\eta}{2\tau}[v-v_n]^2. \tag{148}$$

The finite-step-sized incremental minimum principle (92) gives the Euler equation

$$-\kappa\Delta v+h(2v-6v^2+4v^3)+\eta[v-v_n]/\tau=0, \tag{149}$$

which is a time-discrete form of the microscopic balance (34). With the variational derivative $\delta_v\psi$ of the energy function, this equation takes the standard form

$$[v-v_n]/\tau=-\frac{1}{\eta}\delta_v\psi \tag{150}$$

of an incremental Ginzburg–Landau-type phase field evolution.

5.3. Gradient-type damage with energetic threshold

Gradient damage models described in a homogenized macroscopic sense the degradation of stiffness due to the development of micro-cracks or micro-voids, see e.g. Maugin (1990), Peerlings et al. (1996), Frémond and Nedjar (1996), Mielke and Roubicek (2006), and references cited therein. This is in the simplest case of isotropic damage mechanics achieved by the introduction of a dimensionless scalar micro-field

$$d(\boldsymbol{x},t)=\frac{1}{A}\int_{\Gamma(t)}d\Gamma\in[0,1] \tag{151}$$

that relates at a macroscopic position $\boldsymbol{x}\in\mathcal{B}$ an arbitrarily orientated, evolving micro-crack surface $\Gamma(t)$ to a representative reference surface A in which the crack surface is embedded. The micro-field grows in time $\dot{d}(\boldsymbol{x},t)\geq 0$ from an unbroken initial state $d(\boldsymbol{x},0)=0$ to a broken state $d(\boldsymbol{x},t)=1$. This is a physically well motivated feature of damage mechanics which expresses the irreversibility of the micro-cracking. The objective constitutive state (14)

$$\mathfrak{c}:=\{\nabla_s\boldsymbol{u},d,\nabla d\} \tag{152}$$

contains the strains, the damage variable and its gradient. A simple model of isotropic damage may be based on the energy storage function

$$\psi(\mathfrak{c})=g(d)\psi^e(\nabla_s\boldsymbol{u})+\frac{\kappa}{2}|\nabla d|^2, \tag{153}$$

where $\psi^e=\frac{1}{2}|\nabla_s\boldsymbol{u}|^2_{\mathbb{E}}$ with $\mathbb{E}:=\lambda\boldsymbol{1}\otimes\boldsymbol{1}+2\mu\mathbb{I}$ is an isotropic nominal energy function and $g=(1-d)^2$ a degradation function. The second term in (153) contains with $\kappa=\mu l^2$ the length-scale-dependent contribution, which is assumed to be energetic in nature. In what follows, we consider different approaches to a threshold type response, where damage accumulation takes place if strain energy at a point of the solid reaches a certain energetic threshold c.

5.3.1. A rate-independent two-field setting

The most simple form of a dissipation function for a rate-independent evolution of damage is

$$\phi(\dot{\mathbf{c}};\mathbf{c}) = c\dot{d} + I_+(\dot{d}). \tag{154}$$

$I_+(x)$ with subdifferential $\partial_x I_+$ is the indicator function of the set $\mathcal{R}_+$ of positive real numbers, defined by

$$I_+(x) = \begin{cases} 0 & \text{for } x>0 \\ \infty & \text{otherwise} \end{cases} \quad \text{and} \quad \partial_x I_+(x) = \begin{cases} 0 & \text{for } x>0, \\ \mathcal{R}_+ & \text{for } x=0, \\ \emptyset & \text{otherwise,} \end{cases} \tag{155}$$

which ensures locally the growth of damage. With the functions (153) and (154) at hand, the *incremental potential* (91) for this model problem reads

$$\pi^\tau(\mathbf{c};\mathbf{c}_n) = \frac{1}{2}(1-d)^2|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}} + \frac{\kappa}{2}|\nabla d|^2 - \psi_n + c(d-d_n) + I_+(d-d_n). \tag{156}$$

It is non-smooth due to the indicator function I_+. The finite-step-sized incremental minimum principle (92) gives the Euler equations of the two-field problem

$$\left.\begin{aligned} &\mathrm{Div}[(1-d)^2\mathbb{E} : \nabla_s \boldsymbol{u}] = \mathbf{0}, \\ &-\kappa\Delta d - (1-d)|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}} + [c + \partial_{\dot{d}} I_+(\dot{d})] \ni 0, \end{aligned}\right\} \tag{157}$$

which are time-discrete forms of the balance equations (33) and (34). Eq. $(157)_1$ is the macro-equilibrium for a degrading stress. The non-smooth micro-balance equation $(157)_2$ determines the damage field d in terms of the degraded strain energy $(1-d)|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}}$.

5.3.2. A rate-independent four-field setting

The dissipative force array introduced in (36) takes as model the simple form

$$\mathfrak{b} := \{\mathfrak{p}\}, \tag{158}$$

where $\mathfrak{p}$ is the force dual to d. A reversible domain $\mathbb{E}$ in the space of this dissipative force has the form (48) in terms of the simple threshold function

$$f(\mathfrak{b};\mathbf{c}) = \mathfrak{p}. \tag{159}$$

Then, writing the extended constitutive state vector (121) for the model problem

$$\mathbf{c}^*_\lambda := \{\nabla_s \boldsymbol{u}, d, \nabla d, \mathfrak{p}, \lambda\}, \tag{160}$$

we get with functions (153) and (159) the *extended incremental potential* (123) for the model problem

$$\pi^{*\tau}_\lambda(\mathbf{c}^*_\lambda;\mathbf{c}^*_{\lambda n}) = \frac{1}{2}(1-d)^2|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}} + \frac{\kappa}{2}|\nabla d|^2 - \psi_n + \mathfrak{p}[d-d_n] - \tau\lambda[\mathfrak{p}-c]. \tag{161}$$

The finite-step-sized incremental stationary principle (124) gives the Euler equations

$$\left.\begin{aligned} &\mathrm{Div}[(1-d)^2\mathbb{E} : \nabla_s \boldsymbol{u}] = \overline{\boldsymbol{\gamma}}, \\ &-\kappa\Delta d - (1-d)|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}} + \mathfrak{p} = 0, \\ &d - d_n - \tau\lambda = 0, \\ &\tau\lambda \geq 0, \mathfrak{p} \leq c, \tau\lambda(\mathfrak{p}-c) = 0, \end{aligned}\right\} \tag{162}$$

which are time-discrete forms of the balance equations (44), (45), (53), (54). This set of equations can be reduced by eliminating the Lagrange multiplier field $\tau\lambda = d - d_n$ by $(162)_3$ and the dissipative force field $\mathfrak{p} = -\delta_d\psi$ by the variational derivative $(162)_2$ of the free energy function, yielding the compact representation

$$d \geq d_n, \quad -\delta_d\psi \leq c, \quad (d-d_n)(-\delta_d\psi - c) = 0 \tag{163}$$

of Eqs. $(162)_{2-4}$, which govern the incremental evolution of the damage field.

5.3.2.1. A rate-dependent three-field setting. A time regularization of the incremental potential (161) is based on the specific form of the extended constitutive state vector (105)

$$\mathbf{c}^* := \{\nabla_s \boldsymbol{u}, d, \nabla d, \mathfrak{p}\}. \tag{164}$$

Then, functions (153) and (159) give a specific form of the *incremental potential* (140)

$$\pi^{*\tau}(\mathbf{c}^*;\mathbf{c}^*_n) = \frac{1}{2}(1-d)^2|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}} + \frac{\kappa}{2}|\nabla d|^2 - \psi_n + \mathfrak{p}[d-d_n] - \frac{\tau c}{2\eta}\langle\, \mathfrak{p}/c - 1\,\rangle^2. \tag{165}$$

The finite-step-sized incremental stationary principle (108) gives the Euler equations

$$\left.\begin{array}{l} \mathrm{Div}[(1-d)^2\,\mathbb{E}:\nabla_s \boldsymbol{u}]=\overline{\gamma}, \\ -\kappa\Delta d-(1-d)|\nabla_s \boldsymbol{u}|^2_{\mathbb{E}}+\mathfrak{p}=0, \\ d-d_n-\tau\langle\,\mathfrak{p}/c-1\,\rangle/\eta=0, \end{array}\right\} \tag{166}$$

which are time-discrete forms of the balance equations (44)–(46). Elimination of the dissipative force $\mathfrak{p}=-\delta_d\psi$ by the variational derivative $(166)_2$ of the free energy function gives the compact representation

$$[d-d_n]/\tau=\frac{1}{\eta}\langle-\delta_d\psi/c-1\rangle \tag{167}$$

of Eqs. $(166)_{2-3}$, which govern the evolution of the damage field. Due to its smooth character, this time-regularized setting of a threshold-based damage evolution is highly attractive for numerical implementation.

5.4. A model of gradient-type crystal plasticity

Models of gradient single crystal plasticity are outlined in Fleck and Hutchinson (1997), Gurtin (2000, 2002), Menzel and Steinmann (2000), Svendsen (2002), Evers et al. (2004), see also the references cited therein. The basic kinematic relationship in small-strain crystal plasticity is the additive decomposition of the macroscopic displacement gradient into elastic and plastic parts

$$\nabla\boldsymbol{u}=\boldsymbol{h}^e+\boldsymbol{h}^p \quad \text{with } \boldsymbol{h}^p:=\sum_{\alpha=1}^{n}\gamma^\alpha \boldsymbol{s}^\alpha\otimes\boldsymbol{m}^\alpha. \tag{168}$$

The plastic part $\boldsymbol{h}^p$ is solely defined in terms of the plastic slip γ^α on the systems $\alpha=1,\dots,n$, which occur in prescribed directions associated with the crystallographic orientations. These unit vectors $\{\boldsymbol{s}^\alpha,\boldsymbol{m}^\alpha\}$ determine the slip direction and the slip plane normal, respectively. The symmetric part of $\boldsymbol{h}^e$ is the *elastic distortion* of the crystal lattice

$$\boldsymbol{\varepsilon}^e:=\nabla_s\boldsymbol{u}-\sum_{\alpha=1}^{n}\gamma^\alpha[\boldsymbol{s}^\alpha\otimes\boldsymbol{m}^\alpha]_s, \tag{169}$$

depending on the macro-strain and the plastic slip. Micro-lattice distortions due to statistically distributed dislocations (SSDs) may be described on the phenomenological level by the *accumulated slip*

$$\gamma^{\alpha+}:=\int_0^{\gamma^\alpha}|d\gamma^\alpha| \quad \text{for } \alpha=1,\dots,m, \tag{170}$$

whose evolution $\dot\gamma^{\alpha+}=|\dot\gamma^\alpha|$ is in a trivial manner related to the plastic slip.[7] Further micro-distortions are related to geometric necessary dislocations (GNDs) which are needed to realize inhomogeneous plastic deformations. These distortions can be estimated on the phenomenological level by an incompatibility measure of the plastic distortion field. It is characterized by a closed Burgers circle $\mathcal{C}\subset\mathcal{B}$ with area $\mathcal{A}(\mathcal{C})\subset\mathcal{B}$ by

$$\boldsymbol{b}_{\mathcal{C}}:=\oint_{\mathcal{C}}\boldsymbol{h}^p\cdot\boldsymbol{t}\,d\boldsymbol{s}=\int_{\mathcal{A}(\mathcal{C})}\mathrm{curl}^T\,\boldsymbol{h}^p\cdot\boldsymbol{n}\,dA \tag{171}$$

in terms of the second-order tensor

$$\mathrm{curl}\,\boldsymbol{h}^p:=\sum_{\alpha=1}^{n}(\nabla\gamma^\alpha\times\boldsymbol{m}^\alpha)\otimes\boldsymbol{s}^\alpha, \tag{172}$$

denoted in Nye (1953) and Kröner (1960) as the *dislocation density tensor*. Clearly, we have $\mathrm{curl}\,\boldsymbol{h}^p=\boldsymbol{0}$ for a homogeneous plastic deformation of the body $\mathcal{B}$. The above introduced physically meaningful constitutive state variables $\{\boldsymbol{\varepsilon}^e,\gamma^{1+},\dots,\gamma^{n+},\mathrm{curl}\,\boldsymbol{h}^p\}$ are functions of the specific constitutive state (14)

$$\mathfrak{e}:=\{\nabla_s\boldsymbol{u},\gamma^1,\dots,\gamma^n,\nabla\gamma^1,\dots,\nabla\gamma^n\}. \tag{173}$$

The energy storage function is assumed to have contributions due to (i) elastic distortions of the macroscopically deforming lattice, (ii) elastic micro-distortions of the lattice due to statistically stored dislocations (SSDs), and (iii) elastic micro-distortions of the lattice due to geometrically stored dislocations (GNDs). We consider the simple decoupled representation

$$\psi(\mathfrak{e})=\psi^e(\boldsymbol{\varepsilon}^e)+\psi^p_{SSD}(\gamma^{1+},\dots,\gamma^{n+})+\psi^p_{GND}(\mathrm{curl}\,\boldsymbol{h}^p), \tag{174}$$

where the last contribution accounts for length-scale effects due to the dependence on the gradient of the plastic slip. Simple examples are $\psi^e=\frac{1}{2}|\boldsymbol{\varepsilon}^e|^2_{\mathbb{E}}$ with isotropic macro-elastic moduli $\mathbb{E}:=\lambda\boldsymbol{1}\otimes\boldsymbol{1}+2\mu\mathbb{I}$, $\psi^p_{SSD}=\frac{1}{2}\sum_{\alpha=1}^{n}h\gamma^{\alpha+2}$ with isotropic hardening modulus h and $\psi^p_{GND}=\frac{1}{2}\kappa|\mathrm{curl}\,\boldsymbol{h}^p|^2$, where $\kappa=\mu l^2$ contains an energetic length scale.

[7] The dependence of $\gamma^{\alpha+}$ on γ^α is understood to be valid in an incremental sense, i.e. $\gamma^{\alpha+}(\gamma^\alpha)=\gamma^{\alpha+}_n+|\gamma^\alpha-\gamma^\alpha_n|$ at finite increments.

5.4.1. A rate-independent four-field setting

The dissipative force array introduced in (36) takes as model the simple form

$$\mathfrak{b} := \{\mathfrak{p}^1 \dots \mathfrak{p}^n\}, \tag{175}$$

where $\mathfrak{p}^\alpha$ is the dissipative force dual to γ^α. A reversible domain $\mathbb{E}^\alpha$ for each slip system in the space of this dissipative force has the form (48) in terms of the simple threshold function

$$f^\alpha(\mathfrak{b};\mathfrak{c}) = |\mathfrak{p}^\alpha|. \tag{176}$$

Then, writing the extended constitutive state vector (121) for the model problem

$$\mathfrak{c}^*_\lambda := \{\nabla_s \boldsymbol{u}, \gamma^1 \dots \gamma^n, \nabla\gamma^1 \dots \nabla\gamma^n, \mathfrak{p}^1 \dots \mathfrak{p}^n, \lambda^1 \dots \lambda^n\}, \tag{177}$$

we obtain with functions (174) and (176) the *extended incremental potential* (123) for the model problem

$$\begin{aligned}\pi^{*\tau}_\lambda(\mathfrak{c}^*_\lambda;\mathfrak{c}^*_{\lambda n}) = {}& \frac{1}{2}|\nabla_s \boldsymbol{u} - \sum_{\alpha=1}^n \gamma^\alpha [\boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha]_s|^2_{\mathbb{E}} + \frac{1}{2}\kappa |\sum_{\alpha=1}^n (\nabla\gamma^\alpha \times \boldsymbol{m}^\alpha) \otimes \boldsymbol{s}^\alpha|^2 \\ & + \sum_{\alpha=1}^n \left\{ \frac{1}{2} h(\gamma_n^{\alpha+} + |\gamma^\alpha - \gamma_n^\alpha|)^2 + \mathfrak{p}^\alpha[\gamma^\alpha - \gamma_n^\alpha] - \tau\lambda^\alpha[|\mathfrak{p}^\alpha| - c] \right\} - \psi_n,\end{aligned} \tag{178}$$

where the threshold c plays the role of a critical resolved shear stress. The finite-step-sized incremental stationary principle (124) gives the Euler equations

$$\left.\begin{array}{l} \mathrm{Div}[\mathbb{E} : \boldsymbol{\varepsilon}^e] = \overline{\boldsymbol{\gamma}}, \\ -\kappa\, \mathrm{Div}[|\mathrm{curl}\, \boldsymbol{h}^p| \boldsymbol{m}^\alpha \times \boldsymbol{s}^\alpha] - \boldsymbol{s}^\alpha \cdot (\mathbb{E} : \boldsymbol{\varepsilon}^e) \cdot \boldsymbol{m}^\alpha + h\gamma^{\alpha+} \mathrm{sign}[\gamma^\alpha - \gamma_n^\alpha] + \mathfrak{p}^\alpha = 0, \\ \gamma^\alpha - \gamma_n^\alpha - \tau\lambda^\alpha\, \mathrm{sign}[\mathfrak{p}^\alpha] = 0, \\ \tau\lambda^\alpha \geq 0, \quad |\mathfrak{p}^\alpha| \leq c, \quad \tau\lambda^\alpha(|\mathfrak{p}^\alpha| - c) = 0 \end{array}\right\} \tag{179}$$

for $\alpha = 1, \dots, n$, where we inserted the definitions (169), (170), and (172). Note that the hardening mechanisms are *energetic* in nature and have *local* and *gradient-type* characteristics. The above equations are time-discrete forms of the balance equations (44), (45), (53), (54). It can be reduced by eliminating the Lagrange multiplier fields $\tau\lambda^\alpha = (\gamma^\alpha - \gamma_n^\alpha)\mathrm{sign}[\mathfrak{p}^\alpha]$ by $(179)_3$ and the dissipative force fields $\mathfrak{p}^\alpha = -\delta_{\gamma^\alpha}\psi$ by the variational derivative $(179)_2$ of the free energy function, yielding the compact representation

$$(\gamma^\alpha - \gamma_n^\alpha)\mathrm{sign}[-\delta_{\gamma^\alpha}\psi] \geq 0, \quad |-\delta_{\gamma^\alpha}\psi| \leq c, \quad (\gamma^\alpha - \gamma_n^\alpha)(|-\delta_{\gamma^\alpha}\psi| - c) = 0 \tag{180}$$

of Eqs. $(179)_{2-4}$ which govern the incremental evolution of the plastic slip.

5.4.1.1. A rate-dependent three-field setting. A time regularization of the incremental potential (178) is based on the specific form of the extended constitutive state vector (105)

$$\mathfrak{c}^* := \{\nabla_s \boldsymbol{u}, \gamma^1 \dots \gamma^n, \nabla\gamma^1 \dots \nabla\gamma^n, \mathfrak{p}^1 \dots \mathfrak{p}^n\}. \tag{181}$$

Then functions (174) and (176) give a specific form of the *incremental potential* (140)

$$\begin{aligned}\pi^{*\tau}(\mathfrak{c}^*;\mathfrak{c}^*_n) = {}& \frac{1}{2}|\nabla_s \boldsymbol{u} - \sum_{\alpha=1}^n \gamma^\alpha [\boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha]_s|^2_{\mathbb{E}} + \frac{1}{2}\kappa |\sum_{\alpha=1}^n (\nabla\gamma^\alpha \times \boldsymbol{m}^\alpha) \otimes \boldsymbol{s}^\alpha|^2 \\ & + \sum_{\alpha=1}^n \left\{ \frac{1}{2} h(\gamma_n^{\alpha+} + |\gamma^\alpha - \gamma_n^\alpha|)^2 + \mathfrak{p}^\alpha[\gamma^\alpha - \gamma_n^\alpha] - \frac{\tau c}{2\eta} \langle\, |\mathfrak{p}^\alpha|/c - 1 \,\rangle^2 - \psi_n. \right.\end{aligned} \tag{182}$$

The finite-step-sized incremental stationary principle (108) gives the Euler equations

$$\left.\begin{array}{l} \mathrm{Div}[\mathbb{E} : \boldsymbol{\varepsilon}^e] = \overline{\boldsymbol{\gamma}}, \\ -\kappa\, \mathrm{Div}[|\mathrm{curl}\, \boldsymbol{h}^p| \boldsymbol{m}^\alpha \times \boldsymbol{s}^\alpha] - \boldsymbol{s}^\alpha \cdot (\mathbb{E} : \boldsymbol{\varepsilon}^e) \cdot \boldsymbol{m}^\alpha + h\gamma^{\alpha+} \mathrm{sign}[\gamma^\alpha - \gamma_n^\alpha] + \mathfrak{p}^\alpha = 0, \\ \gamma^\alpha - \gamma_n^\alpha - \tau \langle\, \mathfrak{p}^\alpha/c - 1 \,\rangle \mathrm{sign}[\mathfrak{p}^\alpha]/\eta = 0, \end{array}\right\} \tag{183}$$

which are time-discrete forms of the balance equations (44)–(46). Elimination of the dissipative force $\mathfrak{p}^\alpha = -\delta_{\gamma^\alpha}\psi$ by the variational derivative $(183)_2$ of the free energy function gives the compact representation

$$[\gamma^\alpha - \gamma_n^\alpha]/\tau = \frac{1}{\eta} \langle\, |-\delta_{\gamma^\alpha}\psi|/c - 1 \,\rangle \mathrm{sign}[-\delta_{\gamma^\alpha}\psi] \tag{184}$$

of Eqs. $(183)_{2-3}$ which govern the evolution of the plastic slip. Due to its smooth character, this time-regularized setting of a threshold-based plastic slip is highly attractive for numerical implementation.

5.5. Gradient-type extension of von Mises plasticity

Purely phenomenological formulations of gradient plasticity are outlined for example in Aifantis (1987), Maugin (1990), Mühlhaus and Aifantis (1991), Gurtin (2003), Gudmundson (2004), Francfort and Mielke (2006), and Fleck and Willis (2009a,b), see also the references cited therein. We consider a model that extends in a simple format the standard von Mises theory. The formulation bases on the additive decomposition of the macroscopic strain into elastic and plastic parts, yielding the definition $\nabla_s \boldsymbol{u} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$, where $\boldsymbol{\varepsilon}^p$ is the plastic strain tensor. Taking into account a phenomenological hardening/softening variable α, the constitutive state (14) reads for the model problem

$$\mathfrak{c} := \{\nabla_s \boldsymbol{u}, \boldsymbol{\varepsilon}^p, \alpha, \nabla\alpha\}. \tag{185}$$

A simple ansatz for the objective energy function (15) may have the structure

$$\psi(\mathfrak{c}) = \frac{1}{2}|\nabla_s \boldsymbol{u} - \boldsymbol{\varepsilon}^p|^2_{\mathbb{E}} + \frac{h}{2}\alpha^2 + \frac{\kappa}{2}|\nabla\alpha|^2 \tag{186}$$

with isotropic macro-elastic moduli $\mathbb{E} := \lambda \mathbf{1}\otimes\mathbf{1} + 2\mu\mathbb{I}$. Note that, for simplicity of the representation, the gradient term that includes a length scale via $\kappa = \mu l^2$ is assumed to affect only the scalar hardening variable α.

5.5.1. A rate-independent four-field setting

The dissipative force array introduced in (36) contains the subsequently used variables

$$\mathfrak{b} := \{\boldsymbol{\sigma}, \beta\}, \tag{187}$$

where $\boldsymbol{\sigma}$ and β are the dissipative forces dual to $\boldsymbol{\varepsilon}^p$ and α, respectively. An elastic domain $\mathbb{E}$ in the space of this dissipative force has the form (48) in terms of the threshold function

$$f(\mathfrak{b};\mathfrak{c}) = |\mathrm{dev}[\boldsymbol{\sigma}]| + \beta. \tag{188}$$

Writing the extended constitutive state vector (121) for the model problem

$$\mathfrak{c}^*_\lambda := \{\nabla_s \boldsymbol{u}, \boldsymbol{\varepsilon}^p, \alpha, \nabla\alpha, \boldsymbol{\sigma}, \beta, \lambda\}, \tag{189}$$

we obtain with functions (186) and (188) the *extended incremental potential* (123) for the model problem

$$\pi^{*\tau}_\lambda(\mathfrak{c}^*_\lambda; \mathfrak{c}^*_{\lambda n}) = \frac{1}{2}|\nabla_s \boldsymbol{u} - \boldsymbol{\varepsilon}^p|^2_{\mathbb{E}} + \frac{h}{2}\alpha^2 + \frac{\kappa}{2}|\nabla\alpha|^2 - \psi_n + \boldsymbol{\sigma} : [\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}^p_n] + \beta : [\alpha - \alpha_n] - \tau\lambda\{|\mathrm{dev}[\boldsymbol{\sigma}]| + \beta - c\}, \tag{190}$$

where the threshold c is related to a one-dimensional yield stress. The finite-step-sized incremental stationary principle (124) gives the Euler equations

$$\left.\begin{array}{l} \mathrm{div}[\mathbb{E} : (\nabla_s \boldsymbol{u} - \boldsymbol{\varepsilon}^p)] = \overline{\boldsymbol{\gamma}}, \\ \mathbb{E} : (\nabla_s \boldsymbol{u} - \boldsymbol{\varepsilon}^p) - \boldsymbol{\sigma} = \mathbf{0}, \\ -\kappa\Delta\alpha + h\alpha + \beta = 0, \\ \boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}^p_n - \tau\lambda\,\mathrm{dev}[\boldsymbol{\sigma}]/|\mathrm{dev}[\boldsymbol{\sigma}]| = \mathbf{0}, \\ \alpha - \alpha_n - \tau\lambda = 0, \\ \tau\lambda \geq 0, f \leq c, \tau\lambda(f - c) = 0. \end{array}\right\} \tag{191}$$

The above equations are time-discrete forms of the balance equations (44), (45), (53), (54). The identification of the Lagrange parameter via $(191)_4$ gives $\tau\lambda = |\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}^p_n|$ and characterizes with $(191)_5$ the variable α as the equivalent plastic strain. Hence, when setting

$$\alpha = \alpha_n + |\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}^p_n| \quad \text{and} \quad \chi := |\mathrm{dev}[\boldsymbol{\sigma}]| - [c + h\alpha - \kappa\Delta\alpha], \tag{192}$$

we may recast $(191)_6$ into the form

$$\alpha \geq \alpha_n, \quad \chi \leq 0, \quad (\alpha - \alpha_n)\chi = 0. \tag{193}$$

Thus we have a strain-gradient plasticity model of the Aifantis type, where the Laplace term $\kappa\Delta\alpha$ influences the yield resistance.

5.5.1.1. A rate-dependent three-field setting. A time regularization of the incremental potential (190) is based on the specific form of the extended constitutive state vector (105)

$$\mathfrak{c}^* := \{\nabla_s \boldsymbol{u}, \boldsymbol{\varepsilon}^p, \alpha, \nabla\alpha, \boldsymbol{\sigma}, \beta\}. \tag{194}$$

Then functions (186) and (188) give a specific form of the *incremental potential* (140)

$$\pi^{*\tau}(\mathfrak{e}^*;\mathfrak{e}_n^*)=\frac{1}{2}|\nabla_s\boldsymbol{u}-\boldsymbol{\varepsilon}^p|^2_{\mathbb{E}}+\frac{h}{2}\alpha^2+\frac{\kappa}{2}|\nabla\alpha|^2-\psi_n+\boldsymbol{\sigma}:[\boldsymbol{\varepsilon}^p-\boldsymbol{\varepsilon}_n^p]+\beta:[\alpha-\alpha_n]-\frac{\tau c}{2\eta}\langle(|\mathrm{dev}[\boldsymbol{\sigma}]|+\beta)/c-1\rangle^2. \tag{195}$$

The finite-step-sized incremental stationary principle (108) gives the Euler equations

$$\left.\begin{array}{l}\mathrm{div}[\mathbb{E}:(\nabla_s\boldsymbol{u}-\boldsymbol{\varepsilon}^p)]=\overline{\boldsymbol{\gamma}},\\ \mathbb{E}:(\nabla_s\boldsymbol{u}-\boldsymbol{\varepsilon}^p)-\boldsymbol{\sigma}=\boldsymbol{0},\\ -\kappa\Delta\alpha+h\alpha+\beta=0,\\ \boldsymbol{\varepsilon}^p-\boldsymbol{\varepsilon}_n^p-(\tau/\eta)\langle f/c-1\rangle\,\mathrm{dev}[\boldsymbol{\sigma}]/|\mathrm{dev}[\boldsymbol{\sigma}]|=\boldsymbol{0},\\ \alpha-\alpha_n-(\tau/\eta)\langle f/c-1\rangle=0,\end{array}\right\} \tag{196}$$

which are time-discrete forms of the balance equations (44)–(46). The evolution equation $(196)_5$ for the equivalent plastic strain can be recast into the format

$$[\alpha-\alpha_n]/\tau=\frac{1}{\eta}\langle(|\mathrm{dev}[\boldsymbol{\sigma}]|-h\alpha+\kappa\Delta\alpha)/c-1\rangle, \tag{197}$$

which shows again the dependence of the hardening on $\kappa\Delta\alpha$. Due to its smooth character, this time-regularized setting of gradient plasticity is highly attractive for numerical implementation.

5.6. Remarks on micromorphic gradient-type solids

We finally remark that the micromorphic approach to a systematic construction of gradient-type dissipative solids proposed by Forest (2009) can be viewed as a special application of the framework outlined in Sections 2–4 above. The key idea of a systematic construction of micromorphic gradient-type models is (i) *a split* of the microstructural variables

$$\mathfrak{q}=\{\tilde{\mathfrak{q}},\overline{\mathfrak{q}}\} \tag{198}$$

into *associated local and micromorphic variables* $\tilde{\mathfrak{q}}$ and $\overline{\mathfrak{q}}$, respectively, where the latter account for gradient effects. These pair of variables is then connected by (ii) *a penalty-type link* in the stored energy function, for example in the quadratic format

$$\psi(\nabla_s\boldsymbol{u},\tilde{\mathfrak{q}},\overline{\mathfrak{q}},\nabla\overline{\mathfrak{q}})=\psi_{loc}(\nabla_s\boldsymbol{u},\tilde{\mathfrak{q}})+\frac{\varepsilon}{2}|\tilde{\mathfrak{q}}-\overline{\mathfrak{q}}|^2+\frac{\kappa}{2}|\nabla\overline{\mathfrak{q}}|^2. \tag{199}$$

Clearly, for the limit $\varepsilon\to\infty$ the micromorphic variable converges to the local variable $\overline{\mathfrak{q}}\to\tilde{\mathfrak{q}}$ and the model reduces to the formulations considered in Sections 2–4 above. The method provides a simple guide for gradient-type extensions of given local constitutive models for dissipative solids. However, though very general due to the intrinsic kinematic ingredients, it has the disadvantage of an extended set of physically equivalent variables. This is demonstrated for the damage model outlined in Section 5.3. A micromorphic counterpart to Eqs. (152)–(157) is based on an extension of the constitutive state (152)

$$\mathfrak{e}:=\{\nabla_s\boldsymbol{u},\tilde{d},\overline{d},\nabla\overline{d}\}, \tag{200}$$

that contains beside the local damage variable $\tilde{d}$ the micromorphic variable $\overline{d}$. The energy storage function (153) appears in the modified form

$$\psi(\mathfrak{e})=g(\tilde{d})\psi^e(\nabla_s\boldsymbol{u})+\frac{\varepsilon}{2}(\tilde{d}-\overline{d})^2+\frac{\kappa}{2}|\nabla\overline{d}|^2, \tag{201}$$

where the penalty parameter ε must be considered as an *additional* material parameter. Using the dissipation potential function (154)

$$\phi(\dot{\mathfrak{e}};\mathfrak{e})=c\dot{\tilde{d}}+I_+(\dot{\tilde{d}}) \tag{202}$$

in terms of the rate of the local damage variable $\tilde{d}$, the *incremental potential* (91) reads for this model problem

$$\pi^\tau(\mathfrak{e};\mathfrak{e}_n)=\frac{1}{2}(1-\tilde{d})^2|\nabla_s\boldsymbol{u}|^2_{\mathbb{E}}+\frac{\varepsilon}{2}(\tilde{d}-\overline{d})^2+\frac{\kappa}{2}|\nabla\overline{d}|^2-\psi_n+c(\tilde{d}-\tilde{d}_n)+I_+(\tilde{d}-\tilde{d}_n). \tag{203}$$

Then, the finite-step-sized incremental minimum principle (92) gives the Euler equations of the two-field problem

$$\left.\begin{array}{l}\mathrm{Div}[(1-\tilde{d})^2\mathbb{E}:\nabla_s\boldsymbol{u}]=\overline{\boldsymbol{\gamma}},\\ -(1-\tilde{d})|\nabla_s\boldsymbol{u}|^2_{\mathbb{E}}+[c+\partial_{\dot{\tilde{d}}}I_+(\dot{\tilde{d}})]+\varepsilon(\tilde{d}-\overline{d})\ni 0,\\ -\kappa\Delta\overline{d}-\varepsilon(\tilde{d}-\overline{d})=0.\end{array}\right\}. \tag{204}$$

Thus we have due to the *enlargement* of the amount of microstructural variables (198) the additional equation $(204)_3$, which may be recast into the form

$$\overline{d}-l^2\Delta\overline{d}=\tilde{d}\quad\text{with } l:=\sqrt{\kappa/\varepsilon}. \tag{205}$$

This modified Helmholtz equation appears also in the so-called implicit gradient theory of damage proposed by Peerlings et al. (1996, 2004), however in a slightly different context.

6. Conclusion

A unified framework for dissipative solids was outlined that accounts for micro-structural-based size effects. We developed incremental minimization and saddle point principles for a class of gradient-type dissipative materials which incorporate micro-structural or order parameter fields, whose gradients enter the energy storage and dissipation functions. In contrast to classical local continuum approaches to inelastic solids based on locally evolving internal variables, these global micro-structural fields are governed by additional balance equations including micro-structural boundary conditions. They describe changes of the substructure of the material which evolve relatively to the material as a whole. Such models incorporate non-local effects based on length scales, which reflect properties of the material micro-structure. The proposed unified framework covers first-order gradient-type standard dissipative solids. Particular emphasis was put on alternative multi-field representations, where both the microstructural variable itself and its dual driving force are present. These three-field settings are very convenient for practical implementation of models with threshold- or yield functions formulated in the space of the driving forces. It was shown that the coupled macro- and micro-balances are the Euler equations of the proposed minimization and saddle point principles. The inherent symmetry of the multi-field formulations is considered as an important feature with regard to their numerical implementation. The unified character of the framework was demonstrated by a specification of incremental potentials for a spectrum of model problems, which addressed phase field models and formulations of gradient damage and gradient plasticity. These applications underlined the generality of the proposed variational framework.

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