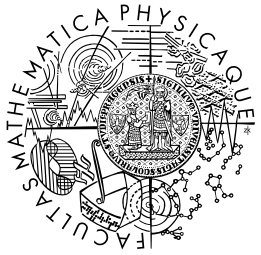

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Variational Methods in Thermomechanics of Solids

Mathematical Institute of Charles University

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Sněhuláčkovi a Bivojovi.

Title: Variational Methods in Thermomechanics of Solids

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Abstract: The thesis is devoted to study of continuum mechanics and thermodynamics and the related mathematical analysis. It consists of four self-contained chapters dealing with different aspects. The first chapter focuses on peridynamics, a non-local theory of continuum mechanics, and its relation to conventional local theory of Cauchy-Green elasticity. Similar comparisons has been used for proving consistency and for determining some of the material coefficients in peridynamics, provided the material parameters in the local theory are known. In this chapter the formula for the non-local force-flux is computed in terms of the peridynamic interaction, relating the fundamental concepts of these two theories and establishing hence a new connection, not present in the previous works. The second and third chapters are both devoted to Rate-Independent Systems (RIS) and their applications to continuum mechanics. RIS represents a suitable approximation when the internal, viscous, and thermal effects can be neglected. RIS has been proven to be useful in modeling hysteresis, phase transitions in solids, elastoplasticity, damage, or fracture in both small and large strain regimes. In the second chapter the existence of solutions to an evolutionary rate-independent model of Shape Memory Alloys (SMAs) is proven. The model considers non-convex energies, and is hence suitable for predicting the mechanical response at large strains. Compared to the previous works we weaken the assumptions on the energy functional, using the notion of gradient polyconvexity (GPC), and hence broaden the range of materials that can be modeled. The third chapter generalizes the concept of local solutions, originally introduced for problems at small strain. As opposed to energetic solutions, they do not force too early jumps and are hence more favorable for predicting damage or fracture. The existence of here defined separately global solutions is proven under hypotheses common in large strain mechanics; energy may be non-convex, depend on the Eulerian gradient of the internal variable, blow up for extreme compression, and the deformations are injective everywhere in the domain. The last chapter of the thesis is devoted to fundamentals of continuum mechanics and thermodynamics. It tries to provide a partial answer to the question how the theory should be constructed, taking models of anisotropic visco-elastic fluids as an accompanying example. It shows it is not necessary to abandon the variational principles (least action or Hamiltonian mechanics), because they lead to reversible and non-dissipative systems; instead they can be successfully modified, yielding then an evolution that dissipates energy and is compatible with the laws of thermodynamics; a particular example of such a generalization being the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC).

Keywords: Continuum mechanics and thermodynamics, Rate-independent systems, Large strain, Damage, Shape Memory Alloys, Gradient polyconvexity, Peridynamics, Stress, Flux, GENERIC, Anisotropic visco-elasto-plasticity

Contents

Introduction

This thesis summarizes the results obtained during my doctoral studies, all of them concerning with continuum mechanics and thermodynamics and the related mathematical analysis. The content is based mostly on the following publications

- P. Pelech. The peridynamic stress tensors and the non-local to local passage. *ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik*, 99(6):e201800010, 2019.
- M. Kružík, P. Pelech, and A. Schlömerkemper. Gradient polyconvexity in evolutionary models of shape-memory alloys. *Journal of Optimization Theory and Applications*, 184:5–20, 01 2020.
- E. Davoli, M. Kružík, and P. Pelech. Separately global solutions to rate-independent processes in large-strain inelasticity. *In preparation*, 2020.

Each chapter is self-contained, but all the results are discussed together in the conclusion.

Peridynamics

The first chapter, based on the paper Pelech [2019], is devoted to peridynamics, a non-local theory of continuum mechanics where points interact with each other over a finite distance; see Silling [2000]. It is customary to assume that two distinct points do not interact if the distance between them in the reference configuration is more than a specific length $\delta > 0$ called *horizon*, which represents a simple material length-scale. This is in a contrast to the classical Cauchy-Green elasticity, where the stress (or traction) vector carries the force interaction of points strictly adjacent to an infinitesimal surface which separates them; see e.g. Cauchy [1828], Love [1892], Truesdell and Noll [2004], Ciarlet [1988] or Gurtin et al. [2010]. It is exactly the relation of these two different descriptions of the same natural phenomena to which the first part of the thesis is devoted to.

Although the method presented here is not the only one that can be found in the literature, see e.g. Emmrich and Weckner [2007] or Bellido et al. [2015] for a different ones, it is the one which appeared in the pioneering paper Silling [2000] and was later developed in Silling and Lehoucq [2008]. These approaches define respectively a notion of traction or stress tensor, expressed in terms of the non-local peridynamic interaction, and compares them with their analogues from the local theory. Based on this comparison one can then determine some of the material coefficients in peridynamics, provided the material parameters in the standard theory of local elasticity are known. The peridynamics stress tensor has been also used in Silling and Lehoucq [2008] to prove consistency of peridynamics with the standard theory when the horizon tends to zero.

Even though the definition of the peridynamic stress tensor introduced in Silling and Lehoucq [2008] is crystal clear and definitely serves the stated purposes, it rather comes out of the blue; any justification, starting from the concepts that are fundamental in peridynamics, is missing. Moreover, the criteria described

there, which the peridynamic stress tensor has to satisfy, leave its choice non-unique. Finally, in the classical theory of elasticity the Cauchy stress tensor has to be symmetric, while the question of symmetry of the peridynamic stress tensor remained open.

The main objective of the work is to derive an analogue of traction in peridynamics, that would justify the definition of the peridynamic stress tensor (and hence solves the non-uniqueness issue). Moreover, this tensor should comply with the symmetry requirement, and help to understand deeper the notion of stress in peridynamics.

Peridynamics has been my research topic for many years, it has already started in my master studies. In this thesis, I significantly deepen and extend some ideas that previously appeared there. The results were already published in an impact journal; see Pelech [2019]. New results obtained during my doctoral studies are highlighted at the end of the introduction to the first chapter.

Rate-Independent System in Continuum Mechanics

The second and third chapters are both devoted to Rate-Independent Systems (RIS) and their applications to continuum mechanics. RIS are characterized by their lack of any internal time length scale - rescaling of the input of the system in time leads to the very same rescaling of its solution. In continuum mechanics, rate-independent models represent a suitable approximation when the external conditions change slowly enough so that the system can always reach its equilibrium. This applies if inertial, viscous, and thermal effects are neglected. Rate independent systems have proven to be useful in modeling hysteresis, phase transitions in solids, elastoplasticity, damage, or fracture in small and large strain regimes. The rate-independence of the system leads to a loss of temporal regularity and for non-convex energies the solutions may develop jumps. The strong formulation of the problem is therefore ill-defined and a suitable reformulation not involving time derivatives of the solution is necessary; however, the weak formulation is not unique as there exist various definitions and solutions, for example energetic, local, Balanced Viscosity (BV) or vanishing viscosity to mention a few. As mentioned in Roubíček [2015]: 'the concept of [...] solution is a vital part of the modeling procedure.' The reader is referred to Mielke and Roubíček [2015] for a thorough overview of various results and applications to continuum mechanics.

The second chapter is based on the paper Kružík et al. [2020], and focuses on applications of Rate-Independent Processes (RIP) to phase transformations in solids, particularly in Shape Memory Alloys (SMAs), and mathematical analysis of the models. SMAs belong to so-called intelligent (or active) materials exhibiting remarkable stress/strain/temperature hysteresis and find therefore numerous applications in engineering and human science. In particular, SMAs are able to recover their original shape after being heated up, which is referred to as the shape-memory effect. Moreover, when mechanically loaded, they deform reversibly to very high strains, this effect being called superelasticity. The outstanding properties of SMAs are due to their atomic structure which poses multiple stable phases, co-existing in a diffusionless solid-to-solid interface. The occurrence of a phase interfaces is caused by non-convexity of the energy, which

in continuum models of SMAs depends on the deformation gradient. The lack of convexity in these models corresponds to the loss of lower semi-continuity of the energy functional. This in turn leads to the nonexistence of energy minimizers, indicated by faster and faster spatial oscillations of the deformation gradient, resulting in formation of microstructure described, for example, by a gradient Young measure; see Kružík [1998], Bhattacharya [2003], Pitteri and Zanzotto [2003], Roubíček [2005], Kružík et al. [2005], Benešová [2011].

Models aiming at describing these oscillations at finite scale need to consider an additional energy contribution penalizing the phase interfaces; in other words they need to make the energy functional lower semi-continuous to achieve existence of minimizers. The interfacial energy penalizes jumps in the first deformation gradient and contains also a contribution depending on the second gradient of deformation [1] and satisfies a suitable coercivity assumptions [2]; see Blanc et al. [2002], Beck and Robins [2007], Rosakis [2014, 2016] for atomic derivations. While an explicit formula for a one dimensional case was obtained in Mora-Corral [2009], for a given interatomic potential, the structure of the formula in higher dimensions remains unclear. The reader is referred to Ball and Mora-Corral [2009], Dondl and Bhattacharya [2010], Ball and Crooks [2011], Šilhavý [2011], Grandi et al. [2019] for static models and to Mielke and Roubíček [2015] for an overview of rate-independent evolutionary models, especially of energetic solutions which represents a useful approximation when the precise energy landscape is not known. Both the static and evolutionary models have energies coercive in a p norm of the second gradient.

Although the coercivity in the second gradient is completely natural, it is not the only option assuring the existence of minimizers. In Benešová et al. [2018], the notion of Gradient PolyConvexity (GPC) was introduced. It generalizes the Ball's polyconvexity by considering only gradients of nonlinear minors in which the energy is convex. The generalization consists in showing that the minimizing deformations do not necessarily have integrable second weak derivatives.

The goal of the second chapter is to prove the existence of energetic solutions to rate-independent evolutionary models of SMAs in which the energy is described by means of a gradient polyconvex functional, and hence generalizing the static model from Benešová et al. [2018] to an evolutionary case, while encompassing more materials than in Mielke and Roubíček [2015] by weakening the assumptions on the energy functional.

The third chapter is based on the manuscript Davoli et al. [2020] and is concerned with finding a suitable concept of solution to RIP arising in large strain mechanics of solids and with developing the corresponding existence theory. While for energetic solutions existence or uniqueness is known under quite general assumptions, they often 'jump too early' when compared to physical experiments. On the other hand, the BV solutions 'jump as late as possible', but they require strong assumptions on data and also their numerical treatment is rather

[1] Materials whose energy does not depend solely on the first deformation gradient are called non-simple; c.f. Truesdell and Noll [2004].

[2] Interestingly, the microstructures obtained by letting the interfacial energy contribution converge to zero and those given by a direct relaxation of the non-convex energy functional may differ, the former being a proper subclass of the latter; see Della Porta [2019].

challenging. A different notion of solution, more accessible by the contemporary tools of mathematical and numerical analysis, is represented by local solutions, originally introduced by Toader and Zanini [2009]. Its applications to delamination and bulk damage are presented and thoroughly discussed in Roubíček [2015], while the computational aspects are addressed in Knees and Negri [2017]. However, both these papers are by their assumptions on the energy functional inevitably restricted to applications at small strains.

The aim of the third chapter is therefore to modify the concept of local solutions and make it more suitable for problems in large-strain mechanics, and to extend the existence results also to these cases, broadening hence considerably the range of possible applications.

GENERIC

The last chapter of the thesis is devoted to fundamentals of continuum mechanics and thermodynamics. It tries to provide a partial answer to the question how the theory should be constructed, taking models of anisotropic visco-elastic fluids as an accompanying example. Concerning the modeling of anisotropic continua, it builds on the paper by Rajagopal and Srinivasa [2001]. The approach presented there extends the framework of natural configuration, which was originally suggested in Rajagopal and Srinivasa [2000a] as a general methodology for deriving models of *isotropic* visco-elasto-plastic materials in the realm of continuum mechanics and thermodynamics of simple materials; see Truesdell and Noll [2004], Gurtin et al. [2010] and also Málek and Průša [2016], Šípka [2020] for an overview reflecting the recent development of the thermodynamic framework of natural configuration. The extension to anisotropic fluids is done by augmenting the set of state variables by an additional vector field describing the material anisotropy (only transverse isotropy is considered for simplicity); however, the evolution is rather reduced to the isotropic case by an additional assumption that the vector remains constant in the natural configuration.

Concerning the main purpose of the chapter, GENERIC plays the role of an alternative approach to the development of continuum thermodynamics. The acronym stands for General Equation for Non-Equilibrium Reversible-Irreversible Coupling and was first used in Grmela and Öttinger [1997], Öttinger and Grmela [1997], but the theory has a longer history; see also the overview in the monographs Öttinger [2005], Pavelka et al. [2018a]. Although the GENERIC framework has been used successfully for deriving continuum models of complex materials from microscopic description, e.g. by means of statistical mechanics, the use of the framework is not limited to it; a purely phenomenological approach is also possible. A general method based on differential geometry was described in [Öttinger, 2005, App. B.4], but here rather a simpler and more basic route of Edwards and Beris [1991], Pavelka et al. [2020] is followed since it avoids the explicit use of the machinery of differential geometry, Lie groups, and Lie algebras and hence is accessible to a broader audience. In both of these works, however, only isotropic continua are considered.

The first goal of this chapter is therefore straightforward, to remove the kinematic constraint imposed on the evolution of the anisotropy vector and the restrictions on energy coming from the theory of simple materials, because it will

allow for modeling of a broader class of materials, whose energy storage and dissipative mechanisms are truly general. The second goal, the more important one, is to show and explain an alternative formulation of continuum mechanics, which is not restricted by the Cauchy straitjacket of surface forces and their little sibling, the heat and entropy fluxes. A formulation, in which the set of variables, energy storage, and dissipative mechanisms determine the evolution completely. A formulation, within a sufficiently abstract framework, where a purely phenomenological description is possible, but at the same time, the framework's generality makes a multiscale derivation and various limit passages (either formal or informal) feasible.

1. Peridynamics

Peridynamics is a non-local model in continuum mechanics introduced in Silling [2000] and elaborated later in Silling et al. [2007] (see also Silling and Lehoucq [2010] or Emmrich et al. [2013] for survey of most important results). The non-locality is reflected in the fact that points at a finite distance exert a force upon each other. This force interaction is described by a *pairwise force function* $\mathbf{f} : \Omega\times\Omega\times[0,T] \to \mathbb{R}^3$, where $\Omega \subset \mathbb{R}^3$ denotes the body in the reference configuration and $[0,T]$, with $T > 0$, is the time interval of interest. If, however, the points are in the reference configuration more distant than a characteristic length called *horizon*, it is customary to assume that they do not interact. This is stated in the assumption that

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = \mathbf{0} \quad \text{whenever} \quad |\mathbf{x}' - \mathbf{x}| \geq \delta,$$

where $\delta > 0$ denotes the horizon length (or just the horizon for simplicity). The meaning of horizon is that it represents an internal material length scale (see e.g. Bobaru and Hu [2012], Silling and Lehoucq [2008] and Silling and Lehoucq [2010] for further explanation and examples). The force $F(A, B, t)$ which one part of the body $A \subset \Omega$ exerts on another part $B \subset \Omega$ at time t is a summation of all point interactions

$$F(A, B, t) = \int_B \int_A \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\, \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}. \tag{1.1}$$

Hence even disjoint parts $A, B \subset \Omega$ may interact with each other. From this formula it is also obvious that the dimension of $\mathbf{f}$ is force per volume squared. The equation of motion in peridynamics then takes the form

$$\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \int_\Omega \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\, \mathrm{d}\mathbf{x}' + \mathbf{b}(\mathbf{x}, t), \quad \text{for all } (\mathbf{x}, t) \in \Omega \times [0, T],$$

where $\ddot{\mathbf{y}}$ is the second time derivative of the deformation $\mathbf{y} : \Omega \times [0,T] \to \mathbb{R}^3$, $\rho_0 : \Omega \to (0, +\infty)$ the density in the reference configuration, and $\mathbf{b} : \Omega \times [0,T] \to \mathbb{R}^3$ the density of external forces with respect to the volume in the reference configuration. The specific form of $\mathbf{f}$ is a matter of a constitutive theory and it usually involves the deformation field in a non-local way.

This is in contrast to standard local theories of simple materials (cf. Gurtin et al. [2010] or Ciarlet [1988]) where two *adjacent* parts of the deformed body interacts through a common surface. The interaction is described by the Cauchy stress vector $\mathbf{t}^{\mathbf{y}} : \mathbf{y}(\Omega) \times \mathbb{S}^2 \times [0,T] \to \mathbb{R}^3$ which depends on the position in the deformed configuration, the surface normal vector at that point ($\mathbb{S}^2$ denotes the unit sphere in $\mathbb{R}^3$), and time. This vector represents the surface density of that force interaction. Hence the force between two adjacent spatial regions $A^{\mathbf{y}} \subset \mathbf{y}(\Omega)$ and $B^{\mathbf{y}} \subset \mathbf{y}(\Omega)$ at time t is expressed by the surface integral

$$F(A^{\mathbf{y}}, B^{\mathbf{y}}, t) = \int_{\partial A^{\mathbf{y}} \cap \partial B^{\mathbf{y}}} \mathbf{t}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}}, t)\, \mathrm{d}S(\mathbf{s}^{\mathbf{y}}), \tag{1.2}$$

where $\mathbf{n}^{\mathbf{y}}$ denotes the outer normal at the point $\mathbf{s}^{\mathbf{y}}$. By the Cauchy theorem there exists the Cauchy stress tensor $\mathbf{T}^{\mathbf{y}} : \mathbf{y}(\Omega) \times [0,T] \to \mathbb{R}^{3\times3}$ such that

$$\mathbf{t}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}}, t) = \mathbf{T}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, t)\mathbf{n}^{\mathbf{y}} \tag{1.3}$$

for all $(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}}, t) \in \mathbf{y}(\Omega) \times \mathbb{S}^2 \times [0,T]$, i.e. the dependence on the unit normal is linear. The Gauss theorem then implies that

$$\int_{A^{\mathbf{y}}} \operatorname{div}^{\mathbf{y}} \mathbf{T}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}, t)\, \mathrm{d}\mathbf{x}^{\mathbf{y}} = \int_{\partial A^{\mathbf{y}}} \mathbf{T}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, t)\mathbf{n}^{\mathbf{y}}\, \mathrm{d}S(\mathbf{s}^{\mathbf{y}})$$

for any $t \in [0,T]$ and $A^{\mathbf{y}} \subset \mathbf{y}(\Omega)$ smooth enough, where $\operatorname{div}^{\mathbf{y}}$ means the divergence with respect to the spatial variables in the deformed configuration. Therefore, using (1.3) and (1.2), the divergence of the Cauchy tensor expresses the volume density of internal forces with respect to the volume in the deformed configuration. The first Piola Kirchhoff stress tensor $\mathbf{T} : \Omega \times [0,T] \to \mathbb{R}^{3\times 3}$ is defined as the Piola transform of the Cauchy tensor

$$\mathbf{T}(\mathbf{x}, t) = (\det \nabla \mathbf{y}(\mathbf{x}, t))\mathbf{T}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}, t)(\nabla \mathbf{y}(\mathbf{x}, t))^{-\top}, \quad \mathbf{x}^{\mathbf{y}} = \mathbf{y}(\mathbf{x}). \tag{1.4}$$

Thanks to the properties of this transform, the following equality holds

$$\int_A \operatorname{div} \mathbf{T}(\mathbf{x}, t)\, \mathrm{d}\mathbf{x} = \int_{A^{\mathbf{y}}} \operatorname{div}^{\mathbf{y}} \mathbf{T}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}, t)\, \mathrm{d}\mathbf{x}^{\mathbf{y}}$$

for any $t \in [0,T]$, where $A \subset \Omega$, $A^{\mathbf{y}} = \mathbf{y}(A)$, and 'div' stands for spatial divergence in the reference configuration. The divergence of the first Piola-Kirchhoff stress tensor then expresses the density of internal forces with respect to the volume in the reference configuration. Hence the equation of motion in the reference configuration takes the form

$$\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \operatorname{div} \mathbf{T}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t), \quad \text{for all } (\mathbf{x}, t) \in \Omega \times [0,T].$$

The divergence of any stress tensor provides knowledge only of the total force flux through closed surfaces which is, however, not sufficient for building the whole theory. For incorporation of the boundary conditions or formulation of the balance of angular momentum the whole tensor is needed. It can be shown that this balance is equivalent to the symmetry of the Cauchy stress tensor, i.e.

$$\mathbf{T}^{\mathbf{y}} = \mathbf{T}^{\mathbf{y}\top}.$$

A corresponding condition for the first Piola-Kirchhoff tensor can be derived from (1.4).

The question whether such different concepts of interaction can be related to each other was addressed already in the pioneering work Silling [2000]. Because of its importance in relation to measurable quantities, the *areal force density* τ was defined there. For a given point $\mathbf{s} \in \Omega$, a direction unit vector $\mathbf{n}$ in the reference configuration and a time $t \in [0,T]$ its definition reads

$$\tau(\mathbf{s}, \mathbf{n}, t) = \int_{\mathcal{L}(\mathbf{s},\mathbf{n})} \int_{\Omega^+(\mathbf{s},\mathbf{n})} \mathbf{f}(\mathbf{x}', \hat{\mathbf{x}}, t)\, \mathrm{d}\mathbf{x}' \mathrm{d}l(\hat{\mathbf{x}}),$$

where

$$\begin{aligned} \Omega^+(\mathbf{s}, \mathbf{n}) &= \{\mathbf{x}' \in \Omega : (\mathbf{x}' - \mathbf{s}) \cdot \mathbf{n} \geq 0\}, \\ \mathcal{L}(\mathbf{s}, \mathbf{n}) &= \{\hat{\mathbf{x}} \in \Omega : \exists s \geq 0 \text{ s.t. } \hat{\mathbf{x}} = \mathbf{s} - s\mathbf{n}\}, \end{aligned}$$

and '$\mathrm{d}l$' represents a length element. According to Silling [2000], this quantity is about as close as one can come to the concept of traction, which plays a central

role in conventional theory. On the other hand, as it was also pointed there, this definition of τ is most useful in the case of a homogeneous deformation (i.e. a deformation whose gradient is a constant matrix). Moreover, its linear dependence on $\mathbf{n}$ is not obvious, and it provides no explicit formula for the first Piola-Kirchhoff tensor in terms of the pairwise force function $\mathbf{f}$. This issue was somehow overcome later in Silling and Lehoucq [2008] where the *peridynamic stress tensor* ν was defined as

$$\nu(\mathbf{x},t) = \frac{1}{2}\int\limits_{\mathbb{S}^2}\int\limits_0^{+\infty}\int\limits_0^{+\infty}(\alpha+\beta)^2\mathbf{f}(\mathbf{x}+\alpha\mathbf{m},\mathbf{x}-\beta\mathbf{m},t)\otimes\mathbf{m}\,\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}S(\mathbf{m}), \qquad (1.5)$$

though no connection to areal force density was provided. Note that through the function $\mathbf{f}$ the dependence of ν on the deformation is non-local. The spatial divergence of this tensor is equal to the density of internal forces in the reference configuration, i.e.

$$\operatorname{div}\nu(\mathbf{x},t) = \int_\Omega \mathbf{f}(\mathbf{x}',\mathbf{x},t)\,\mathrm{d}\mathbf{x}', \quad (\mathbf{x},t)\in\Omega\times[0,T],$$

and so the equation of motion in peridynamics can be rewritten to the form

$$\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \operatorname{div}\nu(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t), \quad \text{for all } (\mathbf{x},t)\in\Omega\times[0,T]$$

which is formally similar to the equation of motion in conventional theory. This fact was subsequently used in Silling and Lehoucq [2008] where the convergence of peridynamics to the conventional theory is investigated for the horizon tending to zero. After performing an appropriate scaling, the measure of the non-locality is represented by a dimensionless parameter $s\to 0$ and the scaled peridynamic stress tensor is denoted by $\nu_s(\mathbf{x},t)$. It is shown that, for a sufficiently smooth fixed deformation and constitutive relation,

$$\lim_{s\to 0_+}\nu_s(\mathbf{x},t) = \nu_0(\mathbf{x},t), \quad (\mathbf{x},t)\in\Omega\times[0,T].$$

The tensor $\nu_0(\mathbf{x},t)$ is called the *collapsed peridynamic tensor* and it depends on the deformation only through the deformation gradient at a point.

If one is interested in the convergence of the equation of motion alone, then the description provided by $\operatorname{div}\nu(\mathbf{x},t)$ and $\operatorname{div}\nu_0(\mathbf{x},t)$ is sufficient. Nevertheless, for identifying the limiting model in standard elasticity the knowledge of the whole limiting first Piola-Kirchhoff stress tensor $\mathbf{T}_0$ is necessary. Since the $\operatorname{div}\nu$ expresses the volume density of internal forces, its limit $\operatorname{div}\nu_0$ express the density of internal forces in the limiting model and therefore it must hold

$$\operatorname{div}\mathbf{T}_0 = \operatorname{div}\nu_0.$$

This requirement, however, determines the tensor $\mathbf{T}_0$ only up to an additive solenoidal tensor field. Hence a closer connection between these two stress tensors is needed.

This also applies to the peridynamic tensor ν which is suggested in Silling and Lehoucq [2008] as an analogue of the first Piola-Kirchhoff stress tensor $\mathbf{T}$. This suggestion is also based only on the divergence of ν which is, for reason mentioned above, not sufficient for the identification of the whole tensor. In fact,

any such an identification of ν and $\mathbf{T}$ is problematic. One reason is connected to the balance of angular momentum. If one considers a sufficiently regular deformation, then the inverse Piola transform of ν (which would be an analogue of the Cauchy tensor) is *not* symmetric in general. Even though the balance of angular momentum in peridynamics is satisfied and only materials with no internal structure (also called non-polar materials in Silling and Lehoucq [2010]) are considered; therefore the analogy between the peridynamic tensor and the first Piola-Kirchhoff tensor remains rather unclear.

As already stated in the introduction, the aim of this chapter is to derive a notion of stress in peridynamics in a consistent way. In particular this means to define another tensor $\mathbf{P}$ whose divergence would also satisfy

$$\operatorname{div} \mathbf{P}(\mathbf{x}, t) = \int_{\Omega} \mathbf{f}(\mathbf{x}', \mathbf{x}, t) \, \mathrm{d}\mathbf{x}',$$

i.e. it would express the volume density of internal forces. At the same time either its inverse Piola transform would be symmetric, or some explanation of its asymmetry would be provided. Last but not least, it would be directly related to the Cauchy stress *vector*. Only such a direct relation would make it a real analogue of the first Piola-Kirchhoff stress tensor $\mathbf{T}$, since from the Cauchy stress vector any other stress measures are derived. In this way the tensor $\mathbf{P}$ would also generalize the areal force density $\tau(\mathbf{s}, \mathbf{n}, t)$ which is useful only for homogeneous deformations and whose linear dependence on the vector $\mathbf{n}$ is unclear.

In addition, the tensor $\mathbf{P}$ can be used for investigating the limiting behavior of peridynamics for vanishing non-locality in the same spirit as the tensor ν was used. Thanks to its relation to the Cauchy stress vector, its limiting counterpart $\mathbf{P_0}$ may be identified with the first Piola-Kirchhoff stress tensor, and hence it may provide a full description of the limiting model in classical theory.

Although discontinuous deformations are possible in peridynamics, we restrict ourselves to sufficiently smooth deformations for which all objects from both theories are well defined. At the same time, the choice of optimal function spaces and control volumes is left for further investigation.

The structure of the chapter is as follows. In Section 1.1 we motivate our definition of peridynamic tensors $\mathbf{P^y}$ and $\mathbf{P}$; it mostly coincides with a part of the diploma thesis, but it is included for making the whole chapter consistent. In Section 1.2 we show some of their properties, compare them with the peridynamic tensor ν and compute the limit of $\mathbf{P}$ for horizon tending to zero; only the result about symmetry and Theorem 1.1 were contained in the diploma thesis, the counter-example and Theorem 1.3 are new. In the last section we derive a general formula of force flux in peridynamics which is then used for a comparison between Cauchy stress tensor $\mathbf{T^y}$ and peridynamic tensor $\mathbf{P^y}$; these last results were obtained completely during Ph.D.

1.1 Derivation of Peridynamic Stress Tensors

We shall define two peridynamic tensors, denoted by $\mathbf{P^y}$ and $\mathbf{P}$, which are an analogues of the Cauchy and the first Piola-Kirchhoff stress tensors respectively. The definition of the first tensor $\mathbf{P^y}$ is based on a heuristic derivation of an analogue of the Cauchy stress vector $\mathbf{t^y}$ in terms of the pairwise force function $\mathbf{f}$. The desired peridynamic tensor $\mathbf{P}$ is then defined as the Piola transform of $\mathbf{P^y}$.

In order to compute the vector $\mathbf{t}^{\mathbf{y}}$ we divide the deformed body by a plane into two pieces. The mutual force interaction between these parts is given by a double volume integral in (1.1). Using a suitable substitution we rewrite it as a surface integral over the dividing plane. The vector $\mathbf{t}^{\mathbf{y}}$ is set to be equal to the corresponding surface density. This way of deriving the formula for $\mathbf{t}^{\mathbf{y}}$ seems to be similar to the one used in Silling [2000] for obtaining the expression for the areal force density τ. The difference is that here all the computations are performed in the deformed configuration, where the force interactions really take place, and that the integration over the dividing surface is done in a different manner. The latter results in a formula for $\mathbf{t}^{\mathbf{y}}$ from which the form of the stress tensor $\mathbf{P}^{\mathbf{y}}$ is explicitly visible. The former makes the derivation meaningful even for non-homogeneous large deformations. Computing directly in the deformed configuration is also much more straightforward than in the reference one, since there one must deal with difficult geometrical nonlinearities caused by the deformation. One can therefore see more easily that the computed vector $\mathbf{t}^{\mathbf{y}}$ indeed corresponds to the rough primitive idea of traction.

Since we want to compute in the deformed configuration, we define the vector field $\mathbf{f}^{\mathbf{y}}$ as the corresponding density with respect to the volume in the deformed configuration, i.e.

$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})(\det \nabla \mathbf{y}(\mathbf{x}'))(\det \nabla \mathbf{y}(\mathbf{x})), \quad \mathbf{x}'^{\mathbf{y}} = \mathbf{y}(\mathbf{x}'),\ \mathbf{x}^{\mathbf{y}} = \mathbf{y}(\mathbf{x}) \tag{1.6}$$

and

$$\int_B \int_A \mathbf{f}(\mathbf{x}', \mathbf{x})\, \mathrm{d}\mathbf{x}' \mathrm{d}\mathbf{x} = \int_{B^{\mathbf{y}}} \int_{A^{\mathbf{y}}} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})\, \mathrm{d}\mathbf{x}'^{\mathbf{y}} \mathrm{d}\mathbf{x}^{\mathbf{y}}.$$

From now on, for the sake of brevity, the time argument will be suppressed. For later simplicity, we set

$$\begin{aligned} \mathbf{f}(\mathbf{x}', \mathbf{x}) &= \mathbf{0}, && \text{whenever } \mathbf{x}' \notin \Omega \text{ or } \mathbf{x} \notin \Omega, \\ \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}) &= \mathbf{0}, && \text{whenever } \mathbf{x}'^{\mathbf{y}} \notin \mathbf{y}(\Omega) \text{ or } \mathbf{x}^{\mathbf{y}} \notin \mathbf{y}(\Omega). \end{aligned} \tag{1.7}$$

Consider now an arbitrary plane $\mathcal{P}^{\mathbf{y}} \subset \mathbb{R}^3$ in the deformed configuration which has a normal vector $\mathbf{n}^{\mathbf{y}} \in \mathbb{S}^2$ and divides the body $\mathbf{y}(\Omega)$ into two pieces. Without loss of generality we may choose a Cartesian coordinate system $\mathbf{x}^{\mathbf{y}} = (x_1^y, x_2^y, x_3^y)$ such that $\mathbf{n}^{\mathbf{y}} = (1, 0, 0)$ and $(0, 0, 0) \in \mathcal{P}^{\mathbf{y}}$. The two parts of the deformed body are then given by

$$\mathbf{y}(\Omega)_+ = \{\mathbf{x}^{\mathbf{y}} \in \mathbf{y}(\Omega) : \mathbf{n}^{\mathbf{y}} \cdot \mathbf{x}^{\mathbf{y}} = x_1^y > 0\}, \tag{1.8}$$

$$\mathbf{y}(\Omega)_- = \{\mathbf{x}^{\mathbf{y}} \in \mathbf{y}(\Omega) : \mathbf{n}^{\mathbf{y}} \cdot \mathbf{x}^{\mathbf{y}} = x_1^y < 0\}. \tag{1.9}$$

The force which one part exerts on the other is then expressed as

$$F(\mathbf{y}(\Omega)_+, \mathbf{y}(\Omega)_-) = \int_{\mathbf{y}(\Omega)_-} \int_{\mathbf{y}(\Omega)_+} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})\, \mathrm{d}\mathbf{x}'^{\mathbf{y}} \mathrm{d}\mathbf{x}^{\mathbf{y}}.$$

The line segment $[\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}]$ given by the couple of interacting points intersects the dividing plane $\mathcal{P}^{\mathbf{y}}$ at a unique point $\mathbf{s}^{\mathbf{y}}$. The line segment $[\mathbf{s}^{\mathbf{y}}, \mathbf{x}'^{\mathbf{y}}]$ has the length α and points in the outer direction $\mathbf{m}$, i.e. $\mathbf{m} \cdot \mathbf{n}^{\mathbf{y}} > 0$ (see Fig. 1.1).

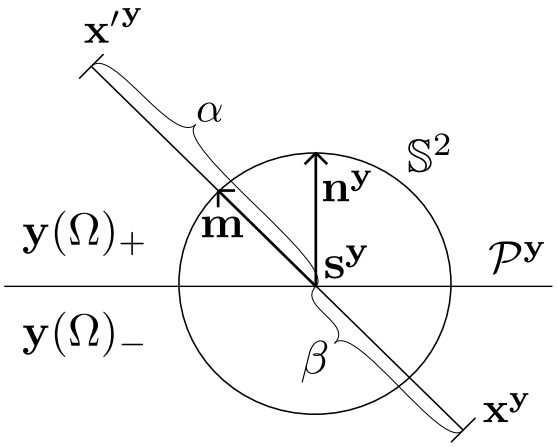

Figure 1.1: The force flux through the plane $\mathcal{P}^{\mathbf{y}}$

The line segment $[\mathbf{s}^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}]$ has the length β and points in the opposite direction. This gives rise to a substitution [1]

$$\mathbf{x}'^{\mathbf{y}} = \mathbf{s}^{\mathbf{y}} + \alpha\mathbf{m}, \quad \mathbf{x}^{\mathbf{y}} = \mathbf{s}^{\mathbf{y}} - \beta\mathbf{m}, \tag{1.10}$$

by which the integration over all interacting couples $[\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}] \in \mathbf{y}(\Omega)_+ \times \mathbf{y}(\Omega)_-$ can be rewritten as a surface integral over the contact plane $\mathcal{P}^{\mathbf{y}}$ of a corresponding surface density. This surface density is the sought vector $\mathbf{t}^{\mathbf{y}}$.

In order to perform the substitution properly we rewrite the double integral using the coordinates (note the different limits of integration for the coordinates $\mathrm{d}x_1'^y$ and $\mathrm{d}x_1^y$ which are due to (1.8) and (1.9) respectively)

$$F(\mathbf{y}(\Omega)_+, \mathbf{y}(\Omega)_-) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{0}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{0}^{+\infty} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})\,\mathrm{d}x_1'^y\,\mathrm{d}x_2'^y\,\mathrm{d}x_3'^y\,\mathrm{d}x_1^y\,\mathrm{d}x_2^y\,\mathrm{d}x_3^y,$$

where we use the abbreviation

$$\mathbf{x}'^{\mathbf{y}} = (x_1'^y, x_2'^y, x_3'^y), \quad \mathbf{x}^{\mathbf{y}} = (x_1^y, x_2^y, x_3^y).$$

Note that the equality (1.7) allows us to integrate up to infinity. The substitution in coordinates then takes the form

$$\begin{aligned} x_1'^y &= \alpha\cos\theta, & x_2'^y &= s_2^y + \alpha\sin\theta\cos\varphi, & x_3'^y &= s_3^y + \alpha\sin\theta\sin\varphi, \\ x_1^y &= -\beta\cos\theta, & x_2^y &= s_2^y - \beta\sin\theta\cos\varphi, & x_3^y &= s_3^y - \beta\sin\theta\sin\varphi, \end{aligned}$$

where

$$\theta \in (0, \frac{\pi}{2}), \quad \varphi \in (0, 2\pi), \quad \alpha, \beta \in (0, +\infty), \quad s_2^y, s_3^y, \in (-\infty, +\infty).$$

[1] This calculation presented here resembles to the one used already by Cauchy (see Cauchy [1828] or Love [1892]). Since we are nevertheless interested in large deformation in general and the horizon cannot be considered infinitesimal, we have to proceed differently.

The corresponding Jacobian is

$$J = \begin{vmatrix} -\alpha\sin\theta & 0 & \cos\theta & 0 & 0 & 0 \\ \alpha\cos\theta\cos\varphi & -\alpha\sin\theta\sin\varphi & \sin\theta\cos\varphi & 0 & 1 & 0 \\ \alpha\cos\theta\sin\varphi & \alpha\sin\theta\cos\varphi & \sin\theta\sin\varphi & 0 & 0 & 1 \\ \beta\sin\theta & 0 & 0 & -\cos\theta & 0 & 0 \\ -\beta\cos\theta\cos\varphi & \beta\sin\theta\sin\varphi & 0 & -\sin\theta\cos\varphi & 1 & 0 \\ -\beta\cos\theta\sin\varphi & -\beta\sin\theta\cos\varphi & 0 & -\sin\theta\sin\varphi & 0 & 1 \end{vmatrix}$$
$$= -(\alpha+\beta)^2\cos\theta\sin\theta.$$

The force is then equal to

$$F(\mathbf{y}(\Omega)_+, \mathbf{y}(\Omega)_-)$$
$$= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{0}^{+\infty}\int_{0}^{+\infty}\int_{0}^{2\pi}\int_{0}^{\frac{\pi}{2}} (\alpha+\beta)^2\,\mathbf{f}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}+\alpha\mathbf{m}, \mathbf{s}^{\mathbf{y}}-\beta\mathbf{m})\cos\theta\sin\theta$$
$$\mathrm{d}\theta\,\mathrm{d}\varphi\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}s_2^y\,\mathrm{d}s_3^y,$$

where

$$\mathbf{s}^{\mathbf{y}} = (0, s_2^y, s_3^y), \quad \mathbf{m} = (\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi).$$

Since $\mathbf{m}\cdot\mathbf{n}^{\mathbf{y}} = \cos\theta$ and $\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$ is the differential solid angle, the integral can be expressed in a coordinate-less form

$$F(\mathbf{y}(\Omega)_+, \mathbf{y}(\Omega)_-)$$
$$= \int_{\mathcal{P}^{\mathbf{y}}}\int_{\mathbb{S}^2_+}\int_{0}^{+\infty}\int_{0}^{+\infty} (\alpha+\beta)^2\,\mathbf{f}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}+\alpha\mathbf{m}, \mathbf{s}^{\mathbf{y}}-\beta\mathbf{m})(\mathbf{m}\cdot\mathbf{n}^{\mathbf{y}})\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}S(\mathbf{m})\,\mathrm{d}S(\mathbf{s}^{\mathbf{y}}),$$

where

$$\mathbb{S}^2_+ := \{\mathbf{m}\in\mathbb{S}^2 : \mathbf{m}\cdot\mathbf{n}^{\mathbf{y}} > 0\}.$$

It should be noted that the integration is not done over the common boundary of the parts $\mathcal{P}^{\mathbf{y}}\cap\mathbf{y}(\Omega)$, since some line segments connecting the pairs of interacting points may intersect the plane $\mathcal{P}^{\mathbf{y}}$ outside the deformed body $\mathbf{y}(\Omega)$. Yet we set

$$\mathbf{t}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}})$$
$$:= \int_{\mathbb{S}^2_+}\int_{0}^{+\infty}\int_{0}^{+\infty} (\alpha+\beta)^2\,\mathbf{f}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}+\alpha\mathbf{m}, \mathbf{s}^{\mathbf{y}}-\beta\mathbf{m})(\mathbf{m}\cdot\mathbf{n}^{\mathbf{y}})\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}S(\mathbf{m}), \quad (1.11)$$

but we can now already foresee some aspects of the nature of the non-local peridynamic interaction which are treated in greater detail in the Section 1.3. Thanks to the skew-symmetry of $\mathbf{f}^{\mathbf{y}}$ in its arguments and to the symmetry of the integrand in $\alpha\in(0,+\infty)$ and $\beta\in(0,+\infty)$, the integration over the opposite hemisphere $\mathbb{S}^2_-$ yields the same value and hence

$$\mathbf{t}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}})$$
$$= \frac{1}{2}\int_{\mathbb{S}^2}\int_{0}^{+\infty}\int_{0}^{+\infty} (\alpha+\beta)^2\,\mathbf{f}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}+\alpha\mathbf{m}, \mathbf{s}^{\mathbf{y}}-\beta\mathbf{m})(\mathbf{m}\cdot\mathbf{n}^{\mathbf{y}})\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}S(\mathbf{m}). \quad (1.12)$$

Based on this result we define the peridynamic stress tensor $\mathbf{P}^{\mathbf{y}}$ in the following way

$$\mathbf{P}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}) := \frac{1}{2}\int_{\mathbb{S}^2}\int_0^{+\infty}\int_0^{+\infty}(\alpha+\beta)^2\,\mathbf{f}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}+\alpha\mathbf{m},\mathbf{x}^{\mathbf{y}}-\beta\mathbf{m})\otimes\mathbf{m}\,\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}S(\mathbf{m}). \tag{1.13}$$

The peridynamic stress tensor $\mathbf{P}$ is defined via Piola transform as

$$\mathbf{P}(\mathbf{x}) := (\det\nabla\mathbf{y}(\mathbf{x}))\mathbf{P}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}})(\nabla\mathbf{y}(\mathbf{x}))^{-\top},\quad \mathbf{x}^{\mathbf{y}}=\mathbf{y}(\mathbf{x}).$$

Using the relation (1.6), the tensor can be expressed in terms of the pairwise force function $\mathbf{f}$ by

$$\begin{aligned}\mathbf{P}(\mathbf{x}) = \frac{\det\nabla\mathbf{y}(\mathbf{x})}{2}\int_{\mathbb{S}^2}\int_0^{+\infty}\int_0^{+\infty}&\chi_{\mathbf{y}(\Omega)}(\mathbf{y}(\mathbf{x})+\alpha\mathbf{m})\chi_{\mathbf{y}(\Omega)}(\mathbf{y}(\mathbf{x})-\beta\mathbf{m})\\ &\frac{(\alpha+\beta)^2\,\mathbf{f}(\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})+\alpha\mathbf{m}),\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})-\beta\mathbf{m}))}{(\det\nabla\mathbf{y}(\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})+\alpha\mathbf{m})))(\det\nabla\mathbf{y}(\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})-\beta\mathbf{m})))}\otimes(\nabla\mathbf{y}(\mathbf{x}))^{-1}\mathbf{m}\\ &\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}S(\mathbf{m}),\end{aligned}$$

where $\chi_{\mathbf{y}(\Omega)}$ is the characteristic function of Ω. The integrand is to be understood as zero whenever the preimage of $\mathbf{y}(\mathbf{x})+\alpha\mathbf{m}$ or $\mathbf{y}(\mathbf{x})-\beta\mathbf{m}$ is not well defined. This final formula is much more complicated than the one for peridynamic tensor ν, but it reflects the fact that although the constitutive theory in peridynamics is primarily being done in the reference configuration, the forces exert in the deformed one. This will be treated in a greater detail in next section (see Example 1.2 and the subsequent discussion).

1.2 Properties of Peridynamic Tensors

In this section we shall investigate the symmetry of $\mathbf{P}^{\mathbf{y}}$, compute the divergence of $\mathbf{P}$, and provide an example of the deformation for which the tensors $\mathbf{P}$ and ν differ.

The question of symmetry of the peridynamic tensor $\mathbf{P}^{\mathbf{y}}$ is quite straightforward in bond-based peridynamics (the earlier version of the theory proposed in Silling [2000]). Here the balance of angular momentum reduces to the requirement of parallelism of the exerting force

$$\mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}},\mathbf{x}^{\mathbf{y}})\ \|\ (\mathbf{x}'^{\mathbf{y}}-\mathbf{x}^{\mathbf{y}})$$

and it can be seen easily in (1.13) that the peridynamic tensor $\mathbf{P}^{\mathbf{y}}$ is indeed symmetric. In state-based peridynamics (the latest version appearing in Silling et al. [2007]), however, this does not seem to be such an easy task and the question still remains open. We conjecture that for non-polar materials the tensor $\mathbf{P}^{\mathbf{y}}$ might be also symmetric. We will nevertheless explain in the Section 1.3 why the possible asymmetry of $\mathbf{P}^{\mathbf{y}}$ actually does not have to contradict the balance of angular momentum, as it might seem at first sight. Yet we consider this partial result about symmetry of $\mathbf{P}^{\mathbf{y}}$ interesting and will take a profit from it.

Next we proceed with investigating the tensors' divergence. The divergence of $\mathbf{P}$ is computed using the knowledge of the divergence of $\mathbf{P}^{\mathbf{y}}$ and the properties of the Piola transform which implies

$$\operatorname{div}\mathbf{P}(\mathbf{x}) = (\det\nabla\mathbf{y}(\mathbf{x}))\operatorname{div}\mathbf{P}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}), \quad \mathbf{x}^{\mathbf{y}} = \mathbf{y}(\mathbf{x}). \tag{1.14}$$

The divergence of $\mathbf{P}^{\mathbf{y}}$ can be obtained using the theorem about the divergence of the peridynamic tensor ν, since these two tensors are formally identical, see (1.5) and (1.13). The only difference (but a crucial one for the mechanical interpretation as it can be seen from Example 1.2) is that the integration in the former is done in the deformed configuration whereas in the later in the reference one. Denoting

$$\mathcal{I} = \{(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}) \in \mathbb{R}^3 \times \mathbb{R}^3 : \mathbf{x}'^{\mathbf{y}} = \mathbf{x}^{\mathbf{y}}\},$$

the transcription of the mentioned theorem reads (c.f. [Silling and Lehoucq, 2008, Theorem 6]):

Theorem 1.1 (see Silling and Lehoucq [2008])**.** *Let a deformation $\mathbf{y} : \Omega \to \mathbb{R}^3$ be given, let $\mathbf{f}^{\mathbf{y}}$ be the corresponding pairwise force density, and let $\mathbf{P}^{\mathbf{y}}$ be given by* (1.13)*. If $\mathbf{f}^{\mathbf{y}}$ is continuously differentiable on $(\mathbb{R}^3 \setminus \partial\mathbf{y}(\Omega)) \times (\mathbb{R}^3 \setminus \partial\mathbf{y}(\Omega)) \setminus \mathcal{I}$ and if*

$$\mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}) = o(|\mathbf{x}'^{\mathbf{y}} - \mathbf{x}^{\mathbf{y}}|^{-2}) \quad \text{as } |\mathbf{x}'^{\mathbf{y}} - \mathbf{x}^{\mathbf{y}}| \to +\infty,$$

then

$$\operatorname{div}\mathbf{P}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}) = \int_{\mathbf{y}(\Omega)} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})\,\mathrm{d}\mathbf{x}'^{\mathbf{y}}, \quad \forall \mathbf{x}^{\mathbf{y}} \in \mathbb{R}^3.$$

The continuity of $\mathbf{f}^{\mathbf{y}}$ in $\mathbf{y}(\Omega)$ is determined both by the regularity of the deformation and by the smoothness of the constitutive relation (this means for instance that there cannot be a jump on the horizon neither a blow-up near $\mathcal{I}$); however, due to (1.7), there may be a discontinuity located on $\partial\mathbf{y}(\Omega) \times \partial\mathbf{y}(\Omega)$ which is therefore excluded. The condition of the decay at infinity is satisfied for any material with finite horizon.

This theorem together with (1.14), (1.6) and substitution formula implies the desired result

$$\begin{aligned}\operatorname{div}\mathbf{P}(\mathbf{x}) &= (\det\nabla\mathbf{y}(\mathbf{x}))\operatorname{div}\mathbf{P}^{\mathbf{y}}(\mathbf{x}^{\mathbf{y}}) = (\det\nabla\mathbf{y}(\mathbf{x}))\int_{\mathbf{y}(\Omega)} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})\,\mathrm{d}\mathbf{x}'^{\mathbf{y}} \\ &= \int_\Omega \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}})(\det\nabla\mathbf{y}(\mathbf{x}'))(\det\nabla\mathbf{y}(\mathbf{x}))\,\mathrm{d}\mathbf{x}' = \int_\Omega \mathbf{f}(\mathbf{x}', \mathbf{x})\,\mathrm{d}\mathbf{x}'. \end{aligned} \tag{1.15}$$

Although the tensors $\mathbf{P}$ and ν have the same divergence, they are not equal, as the following example shows.

Example 1.2. *Let us consider a non-homogeneous deformation $\mathbf{y} : \mathbb{R}^3 \to \mathbb{R}^3$ given by the formula*

$$\mathbf{y}(x_1, x_2, x_3) = (x_1, x_2 + x_3^3, x_3)$$

and a pairwise force function

$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \gamma(|\mathbf{x}' - \mathbf{x}|)(|\mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})|^2 - |\mathbf{x}' - \mathbf{x}|^2)(\mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x}))$$

which is a particular example of the class of materials introduced in [Silling, 2000, eq. (49)]. The so-called shielding function $\gamma : [0, +\infty) \to [0, +\infty)$ *is supposed to be sufficiently smooth and to vanish for* $|\mathbf{x}' - \mathbf{x}| \geq \delta$*, where* δ *is the horizon. Since*

$$\nabla \mathbf{y}(\mathbf{0}) = \mathbf{I},$$

the Piola transform is also identity and hence $\mathbf{P}(\mathbf{0}) = \mathbf{P}^{\mathbf{y}}(\mathbf{0})$*. This implies that* $\mathbf{P}(\mathbf{0})$ *is symmetric and therefore it is sufficient to show the non-symmetry of* $\nu(0)$*. To show this we compute* $\nu_{12}(0)$ *and* $\nu_{21}(0)$ *which will turn out to be different. The integral over* $\mathbb{S}^2$ *in* (1.5) *can be rewritten using spherical coordinates*

$$\begin{aligned} &\mathbf{m} = (\cos\theta, \cos\varphi \sin\theta, \sin\varphi \sin\theta), \quad \mathrm{d}S(\mathbf{m}) = \sin\theta \, \mathrm{d}\theta \mathrm{d}\varphi, \\ &\theta \in (0, \pi), \quad \varphi \in (0, 2\pi) \end{aligned}$$

and then a straightforward calculation shows that

$$\nu_{12}(0) = \frac{4\pi}{35} \int_0^{+\infty} \int_0^{+\infty} (\alpha + \beta)^4 (\alpha^3 + \beta^3) \gamma(\alpha + \beta) \, \mathrm{d}\alpha \mathrm{d}\beta$$

and

$$\nu_{21}(0) = \nu_{12}(0) + \frac{2\pi}{11} \int_0^{+\infty} \int_0^{+\infty} (\alpha + \beta)^2 (\alpha^3 + \beta^3)^3 \gamma(\alpha + \beta) \, \mathrm{d}\alpha \mathrm{d}\beta.$$

Hence, for an appropriate choice of the function γ*, indeed* $\nu_{12}(0) \neq \nu_{21}(0)$*.*

The reason why the tensor

$$\nu^{\mathbf{y}}(\mathbf{x}) = \frac{1}{2 \det \nabla \mathbf{y}(\mathbf{x})} \int_{\mathbb{S}^2} \int_0^{+\infty} \int_0^{+\infty} (\alpha + \beta)^2 \mathbf{f}(\mathbf{x} + \alpha\mathbf{m}, \mathbf{x} - \beta\mathbf{m}, t) \otimes \nabla \mathbf{y}(\mathbf{x}) \mathbf{m} \, \mathrm{d}\alpha \mathrm{d}\beta \mathrm{d}S(\mathbf{m})$$

(the inverse Piola transform of $\nu(\mathbf{x})$) is not symmetric at the origin ,while the tensor $\mathbf{P}^{\mathbf{y}}$ is, lies in the fact that the original tensor ν is computed in the reference configuration, taking into account only local transformation of geometry described by $\nabla \mathbf{y}$. Since peridynamics is a non-local theory the transformation within the whole horizon has to be incorporated (which is done in the definition of $\mathbf{P}^{\mathbf{y}}$). For a non-homogeneous deformation, such as the one in the example, it happens for $\mathbf{x}' = \alpha\mathbf{m}$ and $\mathbf{x} = -\beta\mathbf{m}$ that

$$\mathbf{x}' - \mathbf{x} \parallel \mathbf{m} \quad \text{, whilst} \quad \mathbf{f}(\mathbf{x}', \mathbf{x}) \nparallel \nabla \mathbf{y}(\mathbf{0}) \mathbf{m} = \mathbf{m}$$

for almost every $\mathbf{m} \in \mathbb{S}^2$ (see Fig. 1.2 for illustration). This means that $\mathbf{m}$ is not the direction under which the points $\mathbf{x}'$ and $\mathbf{x}$ exert force upon each other

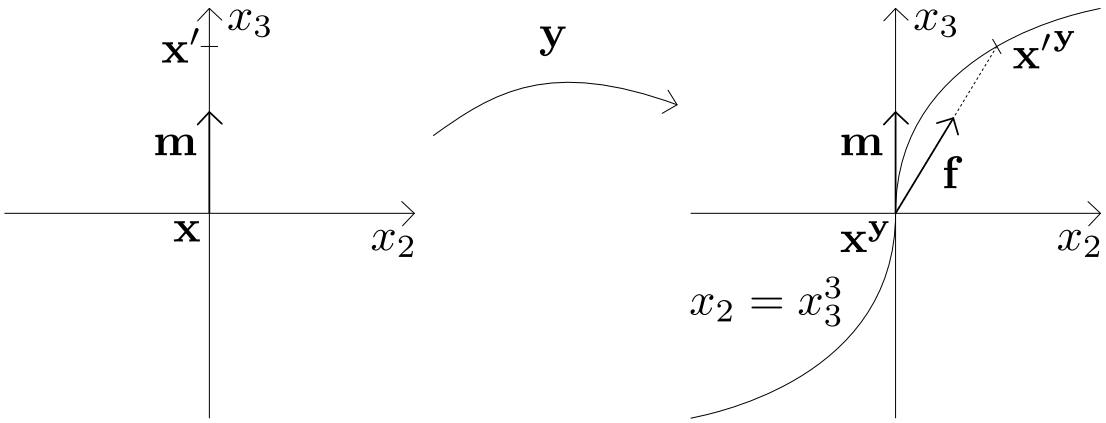

Figure 1.2: The geometric inconsistency in the definition of the tensor ν

in the deformed configuration and hence $\nu(0)$ does not describe the force-flux properly. This geometric inconsistency makes therefore the mechanical interpretation of ν presented in [Silling and Lehoucq, 2008, sec. 6] problematic.

We end up this section by an investigation of the limiting behavior of the peridynamic tensor $\mathbf{P}$ for horizon tending to zero. To do so, we have to specify first what the pairwise force function $\mathbf{f}$ depends on. For the sake of clarity, we restrict ourselves to a simpler constitutive relation of bond-based peridynamics, thought the following steps may be easily generalized also for simple materials in state-based peridynamics, following the proof in Silling and Lehoucq [2008] for the original peridynamic tensor ν. Let

$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \hat{\mathbf{f}}(\mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x}), \mathbf{x}' - \mathbf{x}, \mathbf{x}),$$

where $\hat{\mathbf{f}} : \mathbb{R}^3 \times \mathbb{R}^3 \times \Omega \to \mathbb{R}^3$ is such that

$$\hat{\mathbf{f}}(\cdot, \tilde{\mathbf{x}}, \cdot) \equiv 0 \quad \text{whenever } |\tilde{\mathbf{x}}| \geq \delta$$

and δ is some fixed horizon. After performing the scaling in the same spirit as in Silling and Lehoucq [2008] we obtain a family of peridynamic tensors

$$\begin{aligned}\mathbf{P}_s(\mathbf{x}) := \frac{\det \nabla \mathbf{y}(\mathbf{x})}{2} \int_{\mathbb{S}^2} \int_0^{+\infty} \int_0^{+\infty} \\ (\alpha+\beta)^2 \chi_{\mathbf{y}(\Omega)}(\mathbf{y}(\mathbf{x}) + s\alpha\mathbf{m}) \chi_{\mathbf{y}(\Omega)}(\mathbf{y}(\mathbf{x}) - s\beta\mathbf{m}) \\ \frac{\hat{\mathbf{f}}((\alpha+\beta)\mathbf{m}, \frac{\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})+s\alpha\mathbf{m}) - \mathbf{y}^{-1}(\mathbf{y}(\mathbf{x})-s\beta\mathbf{m})}{s}, \mathbf{y}^{-1}(\mathbf{y}(\mathbf{x}) - s\beta\mathbf{m}))}{(\det \nabla \mathbf{y}(\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x}) + s\alpha\mathbf{m})))(\det \nabla \mathbf{y}(\mathbf{y}^{-1}(\mathbf{y}(\mathbf{x}) - s\beta\mathbf{m})))} \\ \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1}\mathbf{m} \, \mathrm{d}\alpha \, \mathrm{d}\beta \, \mathrm{d}S(\mathbf{m}) \quad (1.16)\end{aligned}$$

indexed by the dimensionless parameter $s \searrow 0_+$ which measures the non-locality.

Although the formulae for the tensors $\mathbf{P}$ and ν seem to be very different at first sight, the following theorem shows that their collapsed counterparts are surprisingly equal.

Theorem 1.3. *Let $\Omega \subset \mathbb{R}^3$ be bounded domain and $\overline{\Omega}$ denote its closure. Let moreover $\hat{\mathbf{f}} : \mathbb{R}^3 \times \mathbb{R}^3 \times \overline{\Omega} \to \mathbb{R}^3$ be continuous, $\mathbf{y} : \Omega \to \mathbf{y}(\Omega)$ and $\mathbf{y}^{-1} : \mathbf{y}(\Omega) \to \Omega$ continuously differentiable and $\det \nabla \mathbf{y} > 0$ in Ω. Then*

$$\mathbf{P}_0(\mathbf{x}) := \lim_{s \to 0_+} \mathbf{P}_s = \nu_0(\mathbf{x}).$$

Proof. It is easy to see that the integrand in (1.16) converges point-wisely to

$$\left(\frac{\alpha + \beta}{\det \nabla \mathbf{y}(\mathbf{x})} \right)^2 \hat{\mathbf{f}}((\alpha + \beta)\mathbf{m}, (\nabla \mathbf{y}(\mathbf{x}))^{-1}(\alpha + \beta)\mathbf{m}, \mathbf{x}) \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1}\mathbf{m}.$$

Thanks to our assumptions, we may use the Lebesgue dominated convergence theorem to interchange the order of limit and integration and hence

$$\mathbf{P}_0(\mathbf{x}) = \frac{1}{2 \det \nabla \mathbf{y}(\mathbf{x})} \int_{\mathbb{S}^2} \int_0^{+\infty} \int_0^{+\infty} (\alpha + \beta)^2 \hat{\mathbf{f}}((\alpha + \beta)\mathbf{m}, (\nabla \mathbf{y}(\mathbf{x}))^{-1}(\alpha + \beta)\mathbf{m}, \mathbf{x}) \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1}\mathbf{m} \, \mathrm{d}\alpha \, \mathrm{d}\beta \, \mathrm{d}S(\mathbf{m}).$$

Similarly as in Silling and Lehoucq [2008], we perform the substitution

$$\alpha = p - \beta, \quad \mathrm{d}\alpha = \mathrm{d}p, \quad p \in (\beta, +\infty)$$

leading to

$$\mathbf{P}_0(\mathbf{x}) := \frac{1}{2 \det \nabla \mathbf{y}(\mathbf{x})} \int_{\mathbb{S}^2} \int_0^{+\infty} \int_\beta^{+\infty} p^2 \, \hat{\mathbf{f}}(p\mathbf{m}, (\nabla \mathbf{y}(\mathbf{x}))^{-1} p\mathbf{m}, \mathbf{x}) \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1}\mathbf{m} \, \mathrm{d}p \, \mathrm{d}\beta \, \mathrm{d}S(\mathbf{m}).$$

Using the Fubini theorem, we may interchange the order of integration with respect to p and β and then integrate β form 0 to p which yields an additional power of p. Hence

$$\mathbf{P}_0(\mathbf{x}) = \frac{1}{2 \det \nabla \mathbf{y}(\mathbf{x})} \int_{\mathbb{S}^2} \int_0^{+\infty} p^2 \, \hat{\mathbf{f}}(p\mathbf{m}, (\nabla \mathbf{y}(\mathbf{x}))^{-1} p\mathbf{m}, \mathbf{x}) \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1} p\mathbf{m} \, \mathrm{d}p \, \mathrm{d}S(\mathbf{m}),$$

which is nothing but the volume integral over $\mathbb{R}^3$ with respect to $\tilde{\mathbf{y}} := p\mathbf{m}$, i.e.

$$\mathbf{P}_0(\mathbf{x}) = \frac{1}{2 \det \nabla \mathbf{y}(\mathbf{x})} \int_{\mathbb{R}^3} \hat{\mathbf{f}}(\tilde{\mathbf{y}}, (\nabla \mathbf{y}(\mathbf{x}))^{-1} \tilde{\mathbf{y}}, \mathbf{x}) \otimes (\nabla \mathbf{y}(\mathbf{x}))^{-1} \tilde{\mathbf{y}} \, \mathrm{d}\tilde{\mathbf{y}}.$$

Finally using a substitution

$$\tilde{\mathbf{y}} = \nabla \mathbf{y}(\mathbf{x}) \, \tilde{\mathbf{x}}, \quad \tilde{\mathbf{x}} \in \mathbb{R}^3$$

we see that

$$\mathbf{P}_0(\mathbf{x}) = \frac{1}{2} \int_{\mathbb{R}^3} \hat{\mathbf{f}}(\nabla \mathbf{y}(\mathbf{x})\tilde{\mathbf{x}}, \tilde{\mathbf{x}}, \mathbf{x}) \otimes \tilde{\mathbf{x}} \, \mathrm{d}\tilde{\mathbf{x}}$$

which is exactly $\nu_0(\mathbf{x})$ for bond-based peridynamics (see [Silling and Lehoucq, 2008, eq. (50)]). □

This result seems to be of a particular interest. It shows that the geometric inconsistency contained in the peridynamic tensor ν vanishes in the limit of small horizon. Moreover it implies that identifying of the 1st Piola-Kirchhoff stress tensor with the collapsed tensor ν_0 is now equivalent to identifying it with the collapsed tensor $\mathbf{P}_0$. In the next section we shall argue that such an identification is possible.

1.3 Correspondence Between Cauchy Stress Tensor and Peridynamic Stress Tensor $\mathbf{P}^{\mathbf{y}}$

A very natural question is whether the peridynamic tensor $\mathbf{P}^{\mathbf{y}}$ is indeed the Cauchy stress tensor $\mathbf{T}^{\mathbf{y}}$. We shall prove that it is *not* the case. We begin with a generalization of the procedure used in the Section 1.1 for determining the form of the peridynamic tensor $\mathbf{P}^{\mathbf{y}}$. This will lead us to a general expression for force flux between two sufficiently regular regions. Based on its knowledge we shall conclude what the relation between these tensors is.

The necessary connection between the local and non-local interaction is provided by the formulae (1.1), (1.6), and (1.2). For a given material and its deformation we need to find a vector field $\mathbf{t}^{\mathbf{y}} : \mathbf{y}(\Omega) \times \mathbb{S}^2 \to \mathbb{R}^3$ s.t. for any two adjacent spatial regions $A^{\mathbf{y}}, B^{\mathbf{y}} \subset \mathbf{y}(\Omega)$ the mutual force interaction can be expressed as the surface integral of $\mathbf{t}^{\mathbf{y}}$, i.e.

$$\int_{B^{\mathbf{y}}} \int_{A^{\mathbf{y}}} \mathbf{f}^{\mathbf{y}}(\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}) \, \mathrm{d}\mathbf{x}'^{\mathbf{y}} \mathrm{d}\mathbf{x}^{\mathbf{y}} = \int_{\partial A^{\mathbf{y}} \cap \partial B^{\mathbf{y}}} \mathbf{t}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}, \mathbf{n}^{\mathbf{y}}) \, \mathrm{d}S(\mathbf{s}^{\mathbf{y}}). \tag{1.17}$$

Moreover, in simple materials the vector $\mathbf{t}^{\mathbf{y}}$ can depend on the surface $\partial A^{\mathbf{y}} \cap \partial B^{\mathbf{y}}$ only through its normal vector $\mathbf{n}^{\mathbf{y}}$ at point $\mathbf{s}^{\mathbf{y}}$.

The problem is that the substitution (1.10), though it seems to be very natural, cannot be applied in general. For example there may be several intersections of the line segment $[\mathbf{x}'^{\mathbf{y}}, \mathbf{x}^{\mathbf{y}}]$ and $\partial A^{\mathbf{y}} \cap \partial B^{\mathbf{y}}$ or there may be even no intersection at all (see Fig. 1.3). Nevertheless, in the case there is exactly one intersection for every interacting pair (which holds for example for a convex set and its complement), we may proceed further. The difference is that now $\mathbf{s}^{\mathbf{y}}$ is a map which locally describes the boundary and the range of the lengths α and β may depend on the direction $\mathbf{m}$ (see Fig. 1.3 for illustration). Otherwise the calculations are performed in a similar way yielding the following form of the mutual force

$$\begin{aligned} &F(A^{\mathbf{y}}, B^{\mathbf{y}}) \\ &= \int_{\mathcal{S}} \int_{\mathbb{S}^2_+(\mathbf{s}^{\mathbf{y}})} \int_0^{\tilde{\beta}} \int_0^{\tilde{\alpha}} (\alpha + \beta)^2 \, \mathbf{f}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}} + \alpha\mathbf{m}, \mathbf{s}^{\mathbf{y}} - \beta\mathbf{m})(\mathbf{m} \cdot \mathbf{n}^{\mathbf{y}}) \, \mathrm{d}\alpha \, \mathrm{d}\beta \, \mathrm{d}S(\mathbf{m}) \, \mathrm{d}S(\mathbf{s}^{\mathbf{y}}), \end{aligned}$$

where

$$\mathcal{S} = \partial A^{\mathbf{y}} \cap \partial B^{\mathbf{y}}, \quad \mathbb{S}^2_+(\mathbf{s}^{\mathbf{y}}) = \{\mathbf{m} \in \mathbb{S}^2 : \mathbf{m} \cdot \mathbf{n}^{\mathbf{y}}(\mathbf{s}^{\mathbf{y}}) > 0\}$$

and $\tilde{\alpha}$ and $\tilde{\beta}$ are functions

$$\tilde{\alpha} = \tilde{\alpha}(A^{\mathbf{y}}, \mathbf{s}^{\mathbf{y}}, \mathbf{m}), \quad \tilde{\beta} = \tilde{\alpha}(B^{\mathbf{y}}, \mathbf{s}^{\mathbf{y}}, \mathbf{m})$$

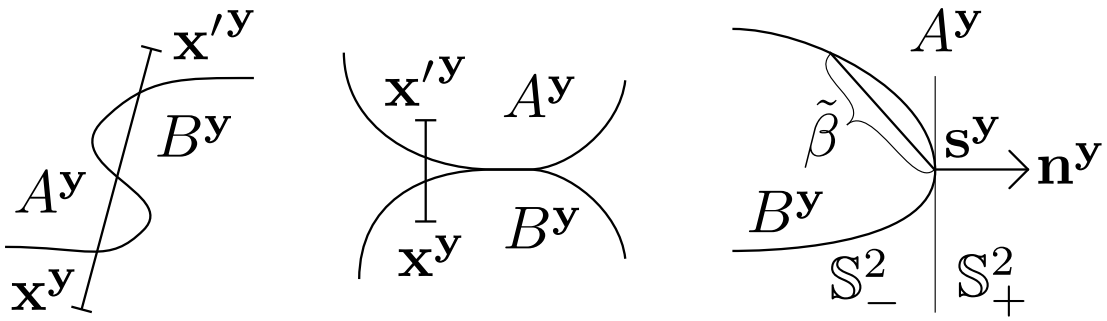

Figure 1.3: Issues arising from non-locality

such that

$$\forall \mathbf{s}^\mathbf{y} \in \mathcal{S}\, \forall \mathbf{m} \in \mathbb{S}^2_+(\mathbf{s}^\mathbf{y}): \quad \mathbf{s}^\mathbf{y} + \alpha\mathbf{m} \in A^\mathbf{y} \Leftrightarrow \alpha \in (0, \tilde{\alpha}) \text{ and } \mathbf{s}^\mathbf{y} - \beta\mathbf{m} \in B^\mathbf{y} \Leftrightarrow \beta \in (0, \tilde{\beta}).$$

Hence the force flux

$$\mathbf{t}^\mathbf{y}(\mathbf{s}^\mathbf{y}) = \int\limits_{\mathbb{S}^2_+(\mathbf{x}^\mathbf{y})} \int\limits_0^{\tilde{\beta}} \int\limits_0^{\tilde{\alpha}} (\alpha+\beta)^2\, \mathbf{f}^\mathbf{y}(\mathbf{s}^\mathbf{y} + \alpha\mathbf{m}, \mathbf{s}^\mathbf{y} - \beta\mathbf{m})(\mathbf{m}\cdot\mathbf{n}^\mathbf{y})\, \mathrm{d}\alpha\, \mathrm{d}\beta\, \mathrm{d}S(\mathbf{m}) \quad (1.18)$$

from $A^\mathbf{y}$ to $B^\mathbf{y}$ is strictly non-local since it depends on the contact surface $\partial A^\mathbf{y} \cap \partial B^\mathbf{y}$ not only through the normal vector $\mathbf{n}^\mathbf{y}$ at a point, but it involves its nontrivial part close to the point $\mathbf{s}^\mathbf{y}$. To see this, let us consider a ball $C^\mathbf{y} \subset \mathbf{y}(\Omega)$ and its tangent plane $\mathcal{P}^\mathbf{y}$. Let their intersection be denoted as $\mathbf{s}^\mathbf{y}$. Moreover let $A^\mathbf{y}$ be the half-space containing the ball $C^\mathbf{y}$ and $B^\mathbf{y}$ denote the other one (see Fig. 1.4). Although the normal vector $\mathbf{n}^\mathbf{y}$ at the point $\mathbf{s}^\mathbf{y}$ is the same for both surfaces, the fluxes from $A^\mathbf{y}$ to $B^\mathbf{y}$ and from $C^\mathbf{y}$ to its complement differ at this point. This fact actually shows that the peridynamic non-local force interaction cannot be described by a tensor in the sense of (1.2) and (1.3), which is, however, a fundamental assumption in the classical theory of simple materials.

This resembles to the situation in so-called non-simple materials (which can be, according to Bažant and Jirásek [2002], understood in some sense as non-local) where the Cauchy stress vector may depend, besides the surface normal vector $\mathbf{n}^\mathbf{y}$, also on the surface curvature (c.f. Toupin [1962], Toupin [1964] or Fried and E. [2006]). It should be also noted that the possible asymmetry in the integration bounds of α and β makes the step from (1.11) to (1.12) impossible in general. It is therefore very surprising that the tensor $\mathbf{P}^\mathbf{y}$ provides, by its divergence, the correct total force flux from $A^\mathbf{y}$ to $B^\mathbf{y}$ despite the fact that the two fluxes (1.12) and (1.18) differ at each point where the boundary is curved.

Yet we anticipate that in the limit of vanishing non-locality the situation changes and that the collapsed peridynamic tensor $\mathbf{P}^\mathbf{y}_0$ can be identified with the Cauchy stress tensor (and hence $\mathbf{P}_0$ with the 1st Piola-Kirchhoff tensor). The idea is as follows. Let two adjacent regions $\mathbf{A}^\mathbf{y}$, $\mathbf{B}^\mathbf{y} \subset \mathbf{y}(\Omega)$ be such that the interacting pairs ($\mathbf{x'^y}$, $\mathbf{x}^\mathbf{y}$) for which the substitution (1.10) cannot be used vanish in the limit. If moreover the common boundary at some point $\mathbf{s}^\mathbf{y} \in \partial A^\mathbf{y} \cap \partial B^\mathbf{y}$ can be approximated by its tangent plane, then the force flux (1.18) through the boundary at the point $\mathbf{s}^\mathbf{y}$ is likely to converge to the force flux (1.12)

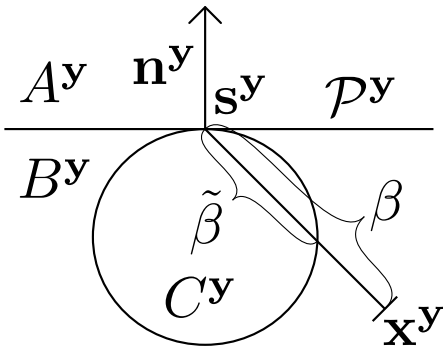

Figure 1.4: Different fluxes for the same unit normal vector.

through its tangent plane. Hence it seems that in the limit the equation (1.17) may hold for broader class of adjacent regions than just two parts of the deformed body divided by a plane.

2. Gradient Polyconvexity in Evolutionary Models of Shape Memory Alloys

The idea of non-simple materials can be traced back to 1901 when Korteweg considered a gradient of the density in his model of fluid capillarity. Considering more than only the first deformation gradient in the description of elastic behavior of solids goes back to the 1960's and appeared in the work of Toupin Toupin [1962, 1964], and Green and Rivlin Green and Rivlin [1964]. Such materials are usually called N-grade materials, where N refers to the highest deformation gradient appearing in the model. This approach has brought questions on thermodynamical consistency of such models, treated in Dunn and Serrin [1985], Capris [1985], for instance. From then on, it has been used in many works; see, e.g., Ball et al. [1981], Dell'Isola et al. [2009], Forest [2009], Kouranbaeva and Shkoller [2000], Mariano [2007], Segev [2017], Šilhavý [1985]. Mathematically, the presence of higher order gradients in the model brings additional compactness properties for the set of admissible functions and ensures the existence of minimizers. We refer to recent related results on the mathematical treatment of shape memory materials: Ball and Crooks [2011], Ball and Mora-Corral [2009]. We also refer to B. Benešová, and S. Krömer and M. Kružík [2015] for an overview.

The aim of this contribution is to apply a new class of non-simple material models introduced in Benešová et al. [2018] (called *gradient polyconvex materials*) to evolutionary problems of shape memory alloys. The novelty consists in considering only gradients of nonlinear minors in the stored energy density of the material. It is shown there, and also in Example 2.2 below, that corresponding deformations do not necessarily have integrable second weak derivatives. Nevertheless, it is possible to prove the existence of an energetic solution. The plan of the chapter is as follows. We first introduce necessary notation and tools in Section 2.1. The notion of gradient polyconvexity is thoroughly discussed in Section 2.2 and the quasistatic evolution in Section 2.3. Finally, we close our exposition with a short conclusion.

2.1 Preliminaries

Hyperelasticity is a special area of Cauchy elasticity, where one assumes that the first Piola-Kirchhoff stress tensor S possesses a potential (called stored energy density) $W : \mathbb{R}^{3\times 3} \to [-w, \infty]$, for some $w \geq 0$. In other words,

$$S := \frac{\partial W(F)}{\partial F} \tag{2.1}$$

on its domain, where $F \in \mathbb{R}^{3\times 3}$ is such that $\det F > 0$. This concept emphasizes that all work done by external loads on the specimen is stored in it. The principle of frame-indifference requires that W satisfies, for all $F \in \mathbb{R}^{3\times 3}$ and all proper rotations $R \in \mathrm{SO}(3)$,

$$W(F) = W(RF) = \tilde{W}(F^\top F) = \tilde{W}(C),$$

where $C := F^\top F$ is the right Cauchy-Green strain tensor and $\tilde{W} : \mathbb{R}^{3\times 3} \to [-w, \infty]$.

Additionally, every elastic material is assumed to resist extreme compression, which is modeled by assuming

$$W(F) \to +\infty, \text{ if } \det F \searrow 0. \tag{2.2}$$

Let the reference configuration be a bounded Lipshitz domain $\Omega \subset \mathbb{R}^3$. Deformation $y : \bar{\Omega} \to \mathbb{R}^3$ maps the points in the closure of the reference configuration $\bar{\Omega}$ to their positions in the deformation configuration. Solutions to the corresponding elasticity equations can then be formally found by minimizing the energy functional

$$I(y) := \int_\Omega W(\nabla y(x))\,\mathrm{d}x - \ell(y) \tag{2.3}$$

over the class of admissible deformations. Here, ℓ is a functional on the set of deformations, expressing (in a simplified way) the work of external loads on the specimen, and ∇y is the deformation gradient, which quantifies the strain. We only allow for deformations, which are orientation-preserving, i.e., if $a, b, c \in \mathbb{R}^3$ satisfy $(a \times b) \cdot c > 0$, then $(Fa \times Fb) \cdot Fc > 0$ for every $F := \nabla y(x)$ and $x \in \Omega$, which means that $\det F > 0$. This condition can be expressed by extending W by infinity on matrices with non-positive determinants, i.e.,

$$W(F) := +\infty, \text{ if } \det F \leq 0. \tag{2.4}$$

In view of (2.1), (2.2), and (2.4), we see that $W : \mathbb{R}^{3\times 3} \to [-w, +\infty]$, is continuous in the sense that if $F_k \to F$ in $\mathbb{R}^{3\times 3}$ for $k \to +\infty$, then $\lim_{k\to+\infty} W(F_k) = W(F)$. Furthermore, W is differentiable on the set of matrices with positive determinants.

A key question immediately appears: Under which conditions does the functional I in (2.3) possess minimizers? Relying on the direct method of the calculus of variations, the usual approach to address this question is to study (weak) lower semicontinuity of the functional I on appropriate Banach spaces containing the admissible deformations. For definiteness, we assume that $y \mapsto -\ell(y)$ is weakly sequentially lower semicontinuous. Thus, the question reduces to a discussion of the assumptions on W. It is well known that (2.2) prevents us from assuming convexity of W. See, e.g., Dacorogna [2008] or the recent review for a detailed exposition of weak lower semicontinuity. Following earlier work by C.B. Morrey, Jr., Morrey [1952], J.M. Ball Ball [1977] defined a polyconvex stored energy density W by assuming that there is a convex and lower semicontinuous function $\overline{W} : \mathbb{R}^{19} \to [-w, +\infty]$ such that

$$W(F) := \overline{W}(F, \operatorname{Cof} F, \det F) \quad \forall F \in \mathbb{R}^{3\times 3}.$$

Here, $\operatorname{Cof} F$ denotes the cofactor matrix of F, which, for F being invertible, satisfies Cramer's rule:

$$\operatorname{Cof} F = (\det F)(F^{-1})^\top.$$

It is well-known that polyconvexity is satisfied for a large class of constitutive functions and allows for the existence of minimizers of I under (2.2) and (2.4). On

the other hand, there are still situations where polyconvexity cannot be adopted. A prominent example are shape-memory alloys, where W has the so-called multi-well structure; see, e.g., Ball and James [1987], Bhattacharya [2003], Müller [1999]. Namely, there is a high-temperature phase, called austenite, which is usually of cubic symmetry, and a low-temperature phase, called martensite, which is less symmetric and exists in more variants, e.g., in three for the tetragonal structure (NiMnGa) or in twelve for the monoclinic one (NiTi). We can assume that

$$W(F) := \min_{0\le i\le M} W_i(F), \tag{2.5}$$

where $W_i : \mathbb{R}^{3\times 3} \to [-w_i, +\infty]$, $w_i \ge 0$, is the stored energy density of the i-th variant of martensite if $i > 0$, and W_0 is the stored energy density of the austenite. For every admissible i, we have $W_i(F) = -w_i$ if and only if $F = RF_i$ for a given matrix $F_i \in \mathbb{R}^{3\times 3}$ and an arbitrary proper rotation $R \in \mathrm{SO}(3)$. This means that each variant of the martensite and the austenite is modeled as a hyperelastic material with its own stored energy density W_i. We also assume that each W_i is differentiable on the set of matrices with positive determinants. Thus the variants can be described independently, e.g., the elastic constants can be chosen differently. The drawback is obviously the non-smoothness of W, however, physically realistic elastic strain values do not occur in the set where W is not differentiable.

To construct such energy densities explicitly, we can now proceed as follows. Assume that $V : \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{+\infty\}$ is minimized on $\mathrm{SO}(3)$ and that $V(F) = \varphi(F^\top F) = \varphi(C)$ for some function $\varphi : \mathbb{R}^{3\times 3}_{sym} \to \mathbb{R} \cup \{+\infty\}$ and the right-Cauchy-Green tensor $C = F^\top F$. It is easy to see that φ attains its minimum at the identity matrix $\mathbb{I}$. Considering the polar decomposition of $F_i \in \mathbb{R}^{3\times 3}$ with $\det F_i > 0$, we can write $F_i = R_i U_i$, where R_i is a rotation and U_i is symmetric and positive definite matrix. Note that $C_i := F_i^\top F_i = U_i^2$. Bearing this in mind, we define the energy of the i-th variant via a shift

$$W_i(F) := V(FU_i^{-1}) = \varphi(U_i^{-1} C U_i^{-1}),$$

which is clearly minimized on $\mathrm{SO}(3)F_i$. Notice also that if V is polyconvex, so is W_i.

Given a deformation gradient F, we need to decide if the corresponding deformation is in the well of the austenite, or in a martensitic variant. In order to do so, we define a volume fraction $\lambda(F)$ as follows: Let $\lambda : \mathbb{R}^{3\times 3} \to \mathbb{R}^{M+1}$. Set

$$\lambda^j(F) := \frac{1}{M}\left(1 - \frac{\operatorname{dist}(C, \mathcal{N}(C_j))}{\sum_{i=0}^{M} \operatorname{dist}(C, \mathcal{N}(C_i))}\right) \quad \forall\, C = F^T F \in \mathbb{R}^{3\times 3}, \quad j = 0, \dots, M, \tag{2.6}$$

where $\mathcal{N}(C_i)$ are pairwise disjoint neighborhoods of the strain tensors $C_i = F_i^\top F_i$, for $i \in \{0, \dots, M\}$. Notice that $\sum_{i=0}^{M} \lambda^j(F) = 1$ for every F, which, together with $\lambda^j > 0$, allows us to interpret λ as a volume fraction. Moreover, note that λ is continuous and frame-indifferent in the sense that $\lambda(F) = \lambda(RF)$ for every proper rotation R. Volume fractions will play an important role in the definition of our evolutionary model in Section 2.3. We refer, e.g. to Mielke and Roubíček [2015] for other models of the stored energy density of shape memory alloys.

Remark 2.1. *Note that this particular choice of λ allows for some elastic behavior close to the wells $\mathrm{SO}(3)F_i$, $i = 0, \dots, M$, since the volume fraction remains constant on the neighbourhoods $\mathcal{N}(C_i)$, $i = 0, \dots, M$.*

Let us emphasize that (2.5) ruins even generalized notions of convexity as, e.g., rank-one convexity. (We recall that rank-one convex functions are convex on line segments with endpoints differing by a rank-one matrix and that rank-one convexity is a necessary condition for polyconvexity; cf. Dacorogna [2008], for instance.) Namely, it is observed (see, e.g., Ball and James [1987], Bhattacharya [2003]) that $w_i = w_j$, whenever $i, j \neq 0$, and that there is a proper rotation R_{ij} such that $\operatorname{rank}(R_{ij}F_i - F_j) = 1$. Hence, generically, $W(R_{ij}F_i) = W(F_j) = -w_i$, but $W(F) > -w_i$ if F is on the line segment between $R_{ij}F_i$ and F_j. Nevertheless, not having a convexity property at hand that implied existence of minimizers is in accordance with experimental observations for these alloys.

Indeed, nonexistence of a minimizer corresponds to the formation of microstructure of strain-states. This is mathematically manifested via a faster and faster oscillation of deformation gradients in minimizing sequences, driving the functional I to its infimum. One can then formulate a minimization problem for a lower semicontinuous envelope of I, the so-called relaxation, see, e.g., Dacorogna [2008]. Such a relaxation yields information of the effective behaviour of the material and on the set of possible microstructures. Thus relaxation is not only an important tool for mathematical analysis, but also for applications. For numerical considerations it is a challenging problem, because the relaxation formula is generically not obtained in a closed form. Further difficulties come from the fact that a sound mathematical relaxation theory is developed only if W has p-growth; that is, for some $c > 1$, $p \in]1, +\infty[$ and all $F \in \mathbb{R}^{3\times 3}$, the inequality

$$\frac{1}{c}(|F|^p - 1) \leq W(F) \leq c(1 + |F|^p)$$

is satisfied. This in particular implies that $W < +\infty$. We refer, however, to Benešová and Kružík [2016], Conti and Dolzmann [2015], Koumatos et al. [2013] for results allowing for infinite energies. Nevertheless, these works include other assumptions that severely restrict their usage. Let us point out that the right Cauchy-Green strain tensor $F^\top F$ maps $\mathrm{SO}(3)F$ as well as $(\mathrm{O}(3)\backslash\mathrm{SO}(3))F$ to the same point. Here, $\mathrm{O}(3)$ are the orthogonal matrices with determinant ± 1. Thus, for example, $F \mapsto |F^\top F - \mathbb{I}|$ is minimized on two energy wells, on $\mathrm{SO}(3)$ and also on $\mathrm{O}(3)\backslash\mathrm{SO}(3)$. However, the latter set is not acceptable in elasticity, because the corresponding minimizing affine deformation is a mirror reflection. In order to distinguish between these two wells, it is necessary to incorporate $\det F$ in the model properly.

Besides relaxation, another approach guaranteeing existence of minimizers is to resort to non-simple materials, i.e., materials, whose stored energy density depends also on higher-order derivatives. Simple examples are functionals of the form

$$I(y) := \int_\Omega W(\nabla y(x)) + \varepsilon|\nabla^2 y(x)|^p \,\mathrm{d}x - \ell(y),$$

where $\varepsilon > 0$. Obviously, the second-gradient term brings additional compactness to the problem, which allows to require only strong lower semicontinuity of the

term

$$\nabla y \mapsto \int_\Omega W(\nabla y(x))\,\mathrm{d}x$$

for the existence of minimizers.

2.2 Gradient Polyconvexity

Here, we follow a different approach, recently suggested in Benešová et al. [2018], which is a natural extension of polyconvexity exploiting weak continuity of minors in Sobolev spaces. Instead of the full second gradient, it is assumed that the stored energy density of the material depends on the deformation gradient ∇y and on gradients of nonlinear minors of ∇y, i.e., on $\nabla[\operatorname{Cof}\nabla y]$ and on $\nabla[\det\nabla y]$. The corresponding functionals are then called gradient polyconvex. While we assume convexity of the stored energy density in the two latter variables, this is not assumed in the ∇y variable. The advantage is that minimizers are elements of Sobolev spaces $W^{1,p}(\Omega,\mathbb{R}^3)$, and no higher regularity is required.

The following example is inspired from Benešová et al. [2018]. It shows that there are maps with smooth nonlinear minors whose deformation gradient is *not* a Sobolev map. Hence, gradient polyconvex energies are more general than second-gradient ones.

Example 2.2. *Let $\Omega =]0,1[^3$. For functions $f, g :]0,1[\to]0,+\infty[$ to be specified later, let us consider the deformation*

$$y(x_1,x_2,x_3) := (x_1, x_2 f(x_1), x_3 g(x_1))\,.$$

Then,

$$\nabla y(x_1,x_2,x_3) = \begin{pmatrix} 1 & 0 & 0 \\ x_2 f'(x_1) & f(x_1) & 0 \\ x_3 g'(x_1) & 0 & g(x_1) \end{pmatrix},$$

$$\operatorname{Cof}\nabla y(x_1,x_2,x_3) = \begin{pmatrix} f(x_1)g(x_1) & -x_2 f'(x_1)g(x_1) & -x_3 f(x_1)g'(x_1) \\ 0 & g(x_1) & 0 \\ 0 & 0 & f(x_1) \end{pmatrix}$$

and

$$\det\nabla y(x_1,x_2,x_3) = f(x_1)g(x_1) > 0\ .$$

Finally, the non-zero entries of $\nabla^2 y(x_1,x_2,x_3)$ are

$$x_2 f''(x_1), \quad f'(x_1), \quad x_3 g''(x_1), \quad g'(x_1). \tag{2.7}$$

Note that we have in particular

$$|\nabla^2 y(x_1,x_2,x_3)| \geq |x_2||f''(x_1)|.$$

Any functions f, g such that $y \in W^{1,p}(\Omega;\mathbb{R}^3)$, $\operatorname{Cof}\nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3})$, $0 < \det\nabla y \in W^{1,r}(\Omega)$, $(\det\nabla y)^{-s} \in L^1(\Omega)$ for some $p,q,r \geq 1$ and $s > 0$, but such

that one of the quantities in (2.7) *is not a function in* $L^p(\Omega)$ *yield a useful example since then* $y \notin W^{2,p}(\Omega;\mathbb{R}^3)$. *To be specific, we choose, for* $1 > \varepsilon > 0$,

$$f(x_1) = x_1^{1-\varepsilon} \quad \textit{and} \quad g(x_1) = x_1^{1+\varepsilon}.$$

Hence

$$\begin{aligned} f'(x_1) &= (1-\varepsilon)x_1^{-\varepsilon}, & g'(x_1) &= (1+\varepsilon)x_1^{\varepsilon}, \\ f''(x_1) &= -\varepsilon(1-\varepsilon)x_1^{-1-\varepsilon}, & g''(x_1) &= \varepsilon(1+\varepsilon)x_1^{-1+\varepsilon}. \end{aligned}$$

Since $x_2 f''(x_1)$ *is not integrable, we have* $\nabla^2 y \notin L^1(\Omega;\mathbb{R}^{3\times 3\times 3})$ *and thus* $y \notin W^{2,1}(\Omega;\mathbb{R}^3)$. *We have only* $y \in W^{1,p}(\Omega;\mathbb{R}^3) \cap L^\infty(\Omega;\mathbb{R}^3)$ *for every* $1 \le p < 1/\varepsilon$. *Moreover, direct computation shows that both* $\operatorname{Cof}\nabla y$ *and* $\det\nabla y$ *lie in* $W^{1,\infty}$. *Finally,* $\det\nabla y = x_1^2 > 0$ *and* $(\det\nabla y)^{-s} \in L^1(\Omega)$ *for all* $0 < s < 1/2$.

Therefore, for any $r, q \ge 1$, $s > 0$, *requiring a deformation* $y : \Omega \to \mathbb{R}^3$ *to satisfy* $\det\nabla y \in W^{1,r}(\Omega)$, $(\det\nabla y)^{-s} \in L^1(\Omega)$ *and* $\operatorname{Cof}\nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3})$ *is a weaker assumption than* $y \in W^{2,1}(\Omega;\mathbb{R}^3)$.

Let us now state the definition of gradient polyconvex functionals.

Definition 2.3 (See Benešová et al. [2018])**.** *Let* $\hat{W} : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3} \times \mathbb{R}^3 \to \mathbb{R}\cup\{+\infty\}$ *be a lower semicontinuous function, and let* $\Omega \subset \mathbb{R}^3$ *be a bounded open domain. The functional*

$$J(y) = \int_\Omega \hat{W}(\nabla y(x), \nabla[\operatorname{Cof}\nabla y(x)], \nabla[\det\nabla y(x)])\mathrm{d}x, \tag{2.8}$$

defined for any measurable function $y : \Omega \to \mathbb{R}^3$ *for which the weak derivatives* ∇y, $\nabla[\operatorname{Cof}\nabla y]$, $\nabla[\det\nabla y]$ *exist and which are integrable, is called* gradient polyconvex *if the function* $\hat{W}(F,\cdot,\cdot)$ *is convex for every* $F \in \mathbb{R}^{3\times 3}$.

With J defined as in (2.8) and a functional $y \mapsto -\ell(y)$ expressing the work of external loads, we set

$$I(y) := J(y) - \ell(y). \tag{2.9}$$

Besides convexity properties, the results of weak lower semicontinuity of I on $W^{1,p}(\Omega;\mathbb{R}^3)$, in the case $1 \le p < +\infty$, rely on suitable coercivity properties. Here we assume that there are numbers $q, r > 1$ and $c, s > 0$ such that for every $F \in \mathbb{R}^{3\times 3}$, $\Delta_1 \in \mathbb{R}^{3\times 3\times 3}$, and every $\Delta_2 \in \mathbb{R}^3$

$$\hat{W}(F,\Delta_1,\Delta_2) \ge \begin{cases} c\Big(|F|^p + |\operatorname{Cof}F|^q + (\det F)^r + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r\Big), \\ \qquad\qquad \text{if } \det F > 0, \\ +\infty, \quad \text{otherwise.} \end{cases} \tag{2.10}$$

The following existence result is taken from Benešová et al. [2018]. For the reader's convenience, we provide a proof below.

Proposition 2.4. *Let* $\Omega \subset \mathbb{R}^3$ *be a bounded Lipschitz domain, and let* $\Gamma = \Gamma_0 \cup \Gamma_1$ *be an* $\mathcal{H}^2$*-measurable partition of* $\Gamma = \partial\Omega$ *with the area of* $\Gamma_0 > 0$. *Let further*

$-\ell : W^{1,p}(\Omega;\mathbb{R}^3) \to \mathbb{R}$ *be a weakly lower semicontinuous functional satisfying, for some* $\tilde{C} > 0$ *and* $1 \le \bar{p} < p$,

$$\ell(y) \le \tilde{C}\|y\|^{\bar{p}}_{W^{1,p}(\Omega;\mathbb{R}^3)}, \qquad \text{for all } y \in W^{1,p}(\Omega;\mathbb{R}^3). \tag{2.11}$$

Further, let J, *as in* (2.8), *be gradient polyconvex on* Ω *and such that there is a* $\hat{W}$ *as in Definition 2.3 which in addition satisfies* (2.10) *for* $p > 2$, $q \ge \frac{p}{p-1}$, $r > 1$, $s > 0$. *Moreover, assume that, for some given measurable function* $y_0 : \Gamma_0 \to \mathbb{R}^3$, *the following set*

$$\begin{aligned}\mathcal{A} := \Big\{ y \in W^{1,p}(\Omega;\mathbb{R}^3) :\ & \operatorname{Cof}\nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3}),\ \det\nabla y \in W^{1,r}(\Omega),\\ & (\det\nabla y)^{-s} \in L^1(\Omega),\ \det\nabla y > 0 \text{ a.e. in } \Omega,\ y = y_0 \text{ on } \Gamma_0 \Big\}\end{aligned}$$

is nonempty. If $\inf_{\mathcal{A}} I < \infty$ *for* I *from* (2.9), *then the functional* I *has a minimizer on* $\mathcal{A}$.

Proof. Our proof closely follows the approach in Benešová et al. [2018]. Let $\{y_k\} \subset \mathcal{A}$ be a minimizing sequence of I. Due to coercivity assumption (2.10), the bound on the loading (2.11), the Poincaré inequality, and the Dirichlet boundary conditions on Γ_0, we obtain that

$$\begin{aligned}\sup_{k\in\mathbb{N}} \Big(&\|y_k\|_{W^{1,p}(\Omega;\mathbb{R}^3)} + \|\operatorname{Cof}\nabla y_k\|_{W^{1,q}(\Omega;\mathbb{R}^{3\times 3})}\\ &+\|\det\nabla y_k\|_{W^{1,r}(\Omega)} + \|(\det\nabla y_k)^{-s}\|_{L^1(\Omega)}\Big) < \infty. \end{aligned}\tag{2.12}$$

Hence, by standard results on weak convergence of minors, see, e.g., [Ciarlet, 1988, Thm. 7.6-1], there are (not explicitly labeled) subsequences such that

$$\begin{aligned} y_k &\rightharpoonup y && \text{in } W^{1,p}(\Omega;\mathbb{R}^3),\\ \operatorname{Cof}\nabla y_k &\rightharpoonup \operatorname{Cof}\nabla y && \text{in } L^q(\Omega;\mathbb{R}^{3\times 3}),\\ \det\nabla y_k &\rightharpoonup \det\nabla y && \text{in } L^r(\Omega), \end{aligned}$$

for $k \to \infty$. Moreover, since bounded sets in uniformly convex Sobolev spaces are weakly sequentially compact,

$$\operatorname{Cof}\nabla y_k \rightharpoonup H \text{ in } W^{1,q}(\Omega;\mathbb{R}^{3\times 3}), \quad \det\nabla y_k \rightharpoonup D \text{ in } W^{1,r}(\Omega) \tag{2.13}$$

for some $H \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3})$ and $D \in W^{1,r}(\Omega)$. Since the weak limit is unique, we have $H = \operatorname{Cof}\nabla y$ and $D = \det\nabla y$. By compact embedding, also $\operatorname{Cof}\nabla y_k \to H$ in $L^q(\Omega;\mathbb{R}^{3\times 3})$ and hence we obtain a (not explicitly labeled) subsequence such that, for $k \to \infty$,

$$\operatorname{Cof}\nabla y_k \to \operatorname{Cof}\nabla y \quad \text{a.e. in } \Omega. \tag{2.14}$$

Since, by Cramer's formula, $\det(\operatorname{Cof}\nabla y) = (\det\nabla y)^2$, we have, for $k \to \infty$, that

$$\det\nabla y_k \to \det\nabla y \quad \text{a.e. in } \Omega. \tag{2.15}$$

Next we show that y belongs to the set of admissible functions $\mathcal{A}$. Notice that $\det\nabla y \ge 0$ since $\det\nabla y_k > 0$ for any $k \in \mathbb{N}$. Further, the conditions (2.10), (2.11), (2.12), and the Fatou lemma imply that

$$+\infty > \liminf_{k\to\infty} I(y_k) + \ell(y_k) \ge \liminf_{k\to\infty} \int_\Omega \frac{1}{(\det\nabla y_k(x))^s}\,\mathrm{d}x \ge \int_\Omega \frac{1}{(\det\nabla y(x))^s}\,\mathrm{d}x.$$

Hence, inevitably, $\det \nabla y > 0$ almost everywhere in Ω and $(\det \nabla y)^{-s} \in L^1(\Omega)$. Since the trace operator is continuous, we obtain that $y \in \mathcal{A}$.

By Cramer's rule, the inverse of the deformation gradient satisfies, for almost all $x \in \Omega$ and $k \to \infty$, that

$$(\nabla y_k(x))^{-1} = \frac{(\operatorname{Cof} \nabla y_k(x))^\top}{\det \nabla y_k(x)} \longrightarrow \frac{(\operatorname{Cof} \nabla y(x))^\top}{\det \nabla y(x)} = (\nabla y(x))^{-1}. \tag{2.16}$$

Notice that, for almost all $x \in \Omega$,

$$\begin{aligned}\sup_{k\in\mathbb{N}} |\nabla y_k(x)| &= \sup_{k\in\mathbb{N}} \det \nabla y_k(x)\ |((\operatorname{Cof}(\nabla y_k(x)))^{-1}))^\top| \\ &\le \sup_{k\in\mathbb{N}} \frac{3}{2} \det \nabla y_k(x)\ |(\nabla y_k(x))^{-1}|^2 < \infty\end{aligned}$$

because of the pointwise convergence of $\{\det \nabla y_k\}$ and (2.16).

Due to (2.16), we have, for almost all $x \in \Omega$ and $k \to \infty$, that

$$\begin{aligned}\nabla y_k(x) = ((\operatorname{Cof}(\nabla y_k(x))^{-1})^\top \det \nabla y_k(x) \longrightarrow \\ \longrightarrow ((\operatorname{Cof}(\nabla y(x))^{-1})^\top \det \nabla y(x) = \nabla y(x),\end{aligned}$$

where we have used that the cofactor of some matrix is invertible whenever the matrix itself is invertible too. As the Lebesgue measure on Ω is finite, we get by the Egoroff theorem, c.f. [Fonseca and Leoni, 2007, Thm. 2.22],

$$\nabla y_k \to \nabla y \ \text{ in measure.} \tag{2.17}$$

Since $\hat{W}$ is non-negative and continuous and $\hat{W}(F, \cdot, \cdot)$ is convex, we may use [Fonseca and Leoni, 2007, Cor. 7.9] to conclude, from (2.17) and (2.13), that

$$\begin{aligned}&\int_\Omega \hat{W}(\nabla y(x), \nabla \operatorname{Cof} \nabla y(x), \nabla \det \nabla y(x))\, \mathrm{d}x \\ &\le \liminf_{k\to\infty} \int_\Omega \hat{W}(\nabla y_k(x), \nabla \operatorname{Cof} \nabla y_k(x), \nabla \det \nabla y_k(x))\, \mathrm{d}x\ .\end{aligned}$$

To pass to the limit in the functional $-\ell$, we exploit its weak lower semicontinuity. Therefore, the whole functional I is weakly lower semicontinuous along $\{y_k\} \subset \mathcal{A}$ and hence $y \in \mathcal{A}$ is a minimizer of I. □

Remark 2.5. *Note that the pointwise convergence* (2.15) *of the determinant, necessary for obtaining the crucial convergence in* (2.17)*, was not achieved by compact embedding, as it was done for* $\operatorname{Cof} \nabla y$ *in* (2.14)*. Hence, the coercivity in* $\nabla[\det \nabla y]$ *is of minor importance and can be relaxed, provided the function* $\hat{W}$ *from* (2.8) *does not depend on its last argument, c.f. [Benešová et al., 2018, Prop. 5.1]. On the other hand, although only* $\nabla[\operatorname{Cof} \nabla y]$ *is necessary for regularizing the whole problem, making the functional in* (2.8) *dependent also on* $\nabla[\det \nabla y]$ *may be interesting from the applications point of view.*

Let $\mathcal{L}^3$ denote the Lebesgue measure in $\mathbb{R}^3$. If $p > 3$ and $y \in W^{1,p}(\Omega; \mathbb{R}^3)$ is such that $\det \nabla y > 0$ almost everywhere in Ω, then the so-called Ciarlet-Nečas condition

$$\int_\Omega \det \nabla y(x)\, \mathrm{d}x \le \mathcal{L}^3(y(\Omega)), \tag{2.18}$$

derived in Ciarlet and Nečas [1987], ensures almost-everywhere injectivity of deformations. We also refer to [Giaquinta et al., 1989, Sec. 6, Thm.2] and to Ball [1981] for other conditions ensuring injectivity of deformations, requiring, however, a prescribed Dirichlet boundary datum on the whole $\partial\Omega$, which is difficult to ensure in a physical lab. If

$$\frac{|\nabla y|^3}{\det \nabla y} \in L^\delta(\Omega) \tag{2.19}$$

for some $\delta > 2$ and (2.18) holds, then we even get invertibility everywhere in Ω due to [Hencl and Koskela, 2014, Theorem 3.4]. Namely, this then implies that y is an open map. Hence, we get the following corollary of Proposition 2.4.

Corollary. *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma = \Gamma_0 \cup \Gamma_1$ be an $\mathcal{H}^2$-measurable partition of $\Gamma = \partial\Omega$ with the area of $\Gamma_0 > 0$. Let further $\ell : W^{1,p}(\Omega;\mathbb{R}^3) \to \mathbb{R}$ be a weakly upper semicontinuous functional and J as in* (2.8) *be gradient polyconvex on Ω such that $\hat{W}$ satisfies* (2.10)*. Finally, let $p > 6$, $q \geq \frac{p}{p-1}$, $r > 1$, $s > 2p/(p-6)$, and assume that, for some given measurable function $y_0 : \Gamma_0 \to \mathbb{R}^3$, the following set*

$$\begin{aligned}\mathcal{A} := \{y \in W^{1,p}(\Omega;\mathbb{R}^3) :\ & \operatorname{Cof}\nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3}),\ \det\nabla y \in W^{1,r}(\Omega),\\ & (\det\nabla y)^{-s} \in L^1(\Omega),\ \det\nabla y > 0 \text{ a.e. in } \Omega,\ y = y_0 \text{ on } \Gamma_0,\ (2.18) \text{ holds}\}\end{aligned}$$

is nonempty. If $\inf_{\mathcal{A}} I < \infty$ for I from (2.9)*, then the functional I has a minimizer on $\mathcal{A}$ which is injective everywhere in Ω.*

A simple example of an energy density which satisfies the assumptions of Proposition 2.2 and Corollary 2.2 is

$$\hat{W}(F,\Delta_1,\Delta_2) = \begin{cases} W(F) + \epsilon\Big(|F|^p + |\operatorname{Cof} F|^q + (\det F)^r + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r\Big), \\ \qquad\qquad \text{if } \det F > 0, \\ +\infty, \qquad \text{otherwise,} \end{cases}$$

where $\epsilon > 0$ is a small number and W is defined in (2.5).

Remark 2.6 (Gradient polyconvex materials and smoothness of stress)**.** *Gradient polyconvex materials enable us to control regularity of the first Piola-Kirchhoff stress tensor by means of smoothness of the Cauchy stress. Assume that the Cauchy stress tensor $T^y : y(\Omega) \to \mathbb{R}^{3\times 3}$ is Lipschitz continuous, for instance. If $\operatorname{Cof}\nabla y : \Omega \to \mathbb{R}^{3\times 3}$ is Lipschitz continuous too, then the first Piola-Kirchhoff stress tensor S inherits the Lipschitz continuity from T^y because*

$$S(x) := T^y(x^y)\operatorname{Cof}\nabla y(x),$$

where $x^y := y(x)$. In a similar fashion, one can transfer Hölder continuity of T^y to S via Hölder continuity of $x \mapsto \operatorname{Cof}\nabla y$.

2.3 Evolution

If the loading changes in time or if the boundary condition becomes time-dependent, then the specimen evolves as well. We consider here the case, in which

evolution is connected with energy dissipation. Experimental evidence shows that considering a rate-independent dissipation mechanism is a reasonable approximation in a wide range of rates of external loads. We hence need to define a suitable dissipation function. Since we consider solely rate-independent processes, this dissipation will be positively one-homogeneous. We associate the dissipation with the magnitude of the time derivative of the dissipative variable $z \in \mathbb{R}^{M+1}$, where $M \in \mathbb{N}$, i.e., with $|\dot{z}|_{M+1}$, where $|\cdot|_{M+1}$ denotes a norm on $\mathbb{R}^{M+1}$ (in our setting, the internal variable z can be seen as a vector of volume fractions of austenite and M variants of martensite). Therefore, the specific dissipated energy associated with a change from state z^1 to z^2 is postulated as

$$D(z^1, z^2) := |z^1 - z^2|_{M+1}.$$

Hence, for $z^i : \Omega \to \mathbb{R}^{M+1}$, $i = 1, 2$, the total dissipation reads

$$\mathcal{D}(z^1, z^2) := \int_\Omega D(z^1(x), z^2(x))\, dx,$$

and the total $\mathcal{D}$-dissipation of a time dependent curve $z : t \in [0, T] \mapsto z(t)$, where $z(t) : \Omega \to \mathbb{R}^{M+1}$ is defined as

$$\mathrm{Diss}_{\mathcal{D}}(z, [s, t]) := \sup\Big\{ \sum_{j=1}^{N} \mathcal{D}(z(t_{i-1}), z(t_i)) : N \in \mathbb{N}, s = t_0 \le \ldots \le t_N = t \Big\}.$$

Let $\mathcal{Z}$ denote the set of all admissible states of internal variables $z : \Omega \to \mathbb{R}^{M+1}$ and $\mathcal{A}$ be the set of admissible deformations as before. For a given triple $(t, y, z) \in [0, T] \times \mathcal{A} \times \mathcal{Z}$, we define the total energy of the system by

$$\mathcal{E}(t, y, z) = \begin{cases} J(y) - L(t, y), & \text{if } z = \lambda(\nabla y) \text{ a.e. in } \Omega, \\ +\infty, & \text{otherwise,} \end{cases}$$

where $L(t, \cdot)$ is a functional on deformations expressing time-dependent loading of the specimen, and λ is defined in (2.6).

Energetic Solution

Suppose, that we look for the time evolution of $t \mapsto y(t) \in \mathcal{A}$ and $t \mapsto z(t) \in \mathcal{Z} := L^\infty(\Omega, \mathbb{R}^{M+1})$ during a process on a time interval $[0, T]$, where $T > 0$ is the time horizon. We use the following notion of solution from Francfort and Mielke [2006], see also Mielke and Theil [2004], Mielke et al. [2002].

Definition 2.7 (Energetic solution)**.** *Let an energy $\mathcal{E} : [0, T] \times \mathcal{A} \times \mathcal{Z} \to \mathbb{R} \cup \{+\infty\}$ and a dissipation distance $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R} \cup \{+\infty\}$ be given. The set of admissible configurations is defined as*

$$\mathcal{Q} := \{(y, z) \in \mathcal{A} \times \mathcal{Z} : \lambda(\nabla y) = z \text{ a.e. in } \Omega\}.$$

We say that $(y, z) : [0, T] \to \mathcal{Q}$ is an energetic solution to $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, if the mapping $t \mapsto \partial_t \mathcal{E}(y(t), z(t))$ is in $L^1(0, T)$ and if, for all $t \in [0, T]$, the stability condition

$$\mathcal{E}(t, y(t), z(t)) \le \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \qquad \forall (\tilde{y}, \tilde{z}) \in \mathcal{Q}. \tag{2.20}$$

and the energy balance

$$\mathcal{E}(t, y(t), z(t)) + \mathrm{Diss}_{\mathcal{D}}(z; [s,t]) = \mathcal{E}(s, y(s), z(s)) + \int_s^t \partial_t \mathcal{E}(\vartheta, y(\vartheta), z(\vartheta))\, \mathrm{d}\vartheta \tag{2.21}$$

are satisfied for any $0 \le s < t \le T$.

An important role is played by the set of so-called stable states, defined for each $t \in [0,T]$ as

$$\begin{aligned}\mathcal{S}(t) := \{(y,z) \in \mathcal{Q} : \mathcal{E}(t,y,z) < +\infty \quad &\text{and} \\ \mathcal{E}(t,y,z) \le \mathcal{E}(t,\tilde{y},\tilde{z}) + \mathcal{D}(z,\tilde{z}) \;\; &\forall (\tilde{y},\tilde{z}) \in \mathcal{Q}\}.\end{aligned}$$

Existence of an Energetic Solution

A standard way how to prove the existence of an energetic solution is to construct time-discrete minimization problems and then to pass to the limit. Before we give the existence proof we need some auxiliary results. For given $N \in \mathbb{N}$ and for $0 \le k \le N$, we define the time increments $t_k := kT/N$. Furthermore, we use the abbreviation $q := (y,z) \in \mathcal{Q}$. We assume that there exists an admissible deformation y^0 being compatible with the initial volume fraction z^0, i.e., $q^0 := (y^0, z^0) \in \mathcal{S}(0)$. For $k = 1, \dots, N$, we define a sequence of minimization problems

$$\text{minimize } \mathcal{I}_k(y,z) := \mathcal{E}(t_k, y, z) + \mathcal{D}(z, z^{k-1}), \quad (y,z) \in \mathcal{Q}. \tag{2.22}$$

We denote a minimizer of (2.22), for a given k, as $q_k^N := (y^k, z^k) \in \mathcal{Q}$ for $1 \le k \le N$. The following lemma shows that a minimizer always exists if the elastic energy is not identically infinite on $\mathcal{Q}$:

Lemma 2.8. *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma = \Gamma_0 \cup \Gamma_1$ be an $\mathcal{H}^2$-measurable partition of $\Gamma = \partial\Omega$ with the area of $\Gamma_0 > 0$. Let J, of the from (2.8), be gradient polyconvex on Ω and such that the stored energy density $\hat{W}$ satisfies (2.10). Moreover, let $L \in C^1([0,T]; W^{1,p}(\Omega;\mathbb{R}^3))$ be such that, for some $C > 0$ and $1 \le \alpha < p$,*

$$L(t,y) \le C\|y\|^{\alpha}_{W^{1,p}}, \quad \textit{for all } t \in [0,T]$$

and $y \mapsto -L(t,y)$ is weakly lower semicontinuous on $W^{1,p}(\Omega;\mathbb{R}^3)$ for all $t \in [0,T]$. Finally, let $p > 6$, $q \ge \frac{p}{p-1}$, $r > 1$, $s > 2p/(p-6)$.

If there is $(y,z) \in \mathcal{Q}$ such that $\mathcal{I}_k(y,z) < \infty$ for $\mathcal{I}_k$ from (2.22), then the functional $\mathcal{I}_k$ has a minimizer $q_k^N = (y^k, z^k) \in \mathcal{Q}$ such that y_k is injective everywhere in Ω. Moreover, $q_k^N \in \mathcal{S}(t_k)$ for all $1 \le k \le N$.

Proof. Since the discretized problem (2.22) has a purely static character, we can follow the proof of Proposition 2.4. Let $\{(y_j^k, z_j^k)\}_{j\in\mathbb{N}} \subset \mathcal{Q}$ be a minimizing sequence. As

$$\nabla y_j^k \longrightarrow \nabla y^k \quad \text{ strongly in } L^{\tilde{p}}(\Omega, \mathbb{R}^{3\times 3}) \text{ as } j \to \infty$$

for every $1 \le \tilde{p} < p$ and $\lambda \in C(\mathbb{R}^{3\times 3}, \mathbb{R}^{M+1})$ is bounded, we obtain that

$$z_j^k = \lambda(\nabla y_j^k) \longrightarrow \lambda(\nabla y^k) \quad \text{ strongly in } L^{\tilde{p}}(\Omega, \mathbb{R}^{M+1}) \text{ as } j \to \infty.$$

Since $\|z_j^k\|_{L^1(\Omega,\mathbb{R}^{M+1})}$ is uniformly bounded in j, there is a subsequence (not explicitly relabeled) such that $z_j^k \overset{*}{\rightharpoonup} \mu^k$ in Radon measures on Ω. This shows that $z^k := \mu^k = \lambda(\nabla y^k)$ and hence $q_k^N = (y^k, z^k) \in \mathcal{Q}$. Since $\mathcal{D}(\cdot, z^{k-1})$ is convex, we obtain that q_k^N is indeed a minimizer of $\mathcal{I}_k$. Moreover, y_k is injective everywhere by the reasoning used for proving Corollary 2.2. The stability $q_k^N \in \mathcal{S}(t_k)$ follows by standard arguments; see, e.g., Francfort and Mielke [2006]. □

Denoting by $B([0,T];\mathcal{A})$ the set of bounded maps $t \in [0,T] \mapsto y(t) \in \mathcal{A}$, we have the following result showing the existence of an energetic solution to the problem $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$:

Theorem 2.9. *Let $T > 0$ and let the assumptions in Lemma 2.8 be satisfied. Moreover, let the initial condition be stable, i.e., $q^0 := (y^0, z^0) \in \mathcal{S}(0)$. Then there is an energetic solution to $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ satisfying $q(0) = q^0$ and such that $y \in B([0,T];\mathcal{A})$, $z \in \mathrm{BV}\left([0,T]; L^1(\Omega;\mathbb{R}^{M+1})\right) \cap L^\infty(0,T;\mathcal{Z})$, and such that for all $t \in [0,T]$ the identity $\lambda(\nabla y(t,\cdot)) = z(t,\cdot)$ holds a.e. in Ω. Moreover, for all $t \in [0,T]$, the deformation $y(t)$ is injective everywhere in Ω.*

Proof. Let $q_k^N := (y^k, z^k)$ be the solution of (2.22), which exists by Lemma 2.8, and let $q^N : [0,T] \to \mathcal{Q}$ be given by

$$q^N(t) := \begin{cases} q_k^N, & \text{if } t \in [t_k, t_{k+1}[\text{ if } k = 0, \dots, N-1, \\ q_N^N, & \text{if } t = T. \end{cases}$$

Following Francfort and Mielke [2006], we get, for some $C > 0$ and for all $N \in \mathbb{N}$, the estimates

$$\|z^N\|_{BV(0,T;L^1(\Omega;\mathbb{R}^{M+1}))} \le C, \qquad \|z^N\|_{L^\infty(0,T;BV(\Omega;\mathbb{R}^{M+1}))} \le C, \tag{2.23a}$$

$$\|y^N\|_{L^\infty(0,T;W^{1,p}(\Omega;\mathbb{R}^3))} \le C, \tag{2.23b}$$

as well as the following two-sided energy inequality

$$\begin{aligned} \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q_k^N)\,\mathrm{d}\theta &\le \mathcal{E}(t_k, q_k^N) + \mathcal{D}(z^k, z^{k-1}) - \mathcal{E}(t_{k-1}, q_{k-1}^N) \\ &\le \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q_{k-1}^N)\,\mathrm{d}\theta. \end{aligned} \tag{2.24}$$

The second inequality in (2.24) follows since q_k^N is a minimizer of (2.22) and by comparison of its energy with $q := q_{k-1}^N$. The lower estimate is implied by the stability of $q_{k-1}^N \in \mathcal{S}(t_{k-1})$, see Lemma 2.8, when compared with $\tilde{q} := q_k^N$. By this inequality, the a-priori estimates and a generalized Helly's selection principle [Mielke et al., 2002, Cor. 2.8], we get that there is indeed an energetic solution obtained as a limit for $N \to \infty$.

Let us comment more on the two main properties of the minimizer, namely, that it is orientation preserving and injective everywhere in Ω. The condition $\det \nabla y > 0$ a.e. in Ω follows from the fact that if $t_j \to t$, $(y_{(j)}, z_{(j)}) \in \mathcal{S}(t_j)$ and $(y_{(j)}, z_{(j)}) \rightharpoonup (y, z)$ in $W^{1,p}(\Omega;\mathbb{R}^3) \times BV(\Omega;\mathbb{R}^{M+1})$, then $(y, z) \in \mathcal{S}(t)$. Indeed, we have $z_{(j)} \to z$ in $L^1(\Omega;\mathbb{R}^{M+1})$ in our setting and hence for all $(\tilde{y}, \tilde{z}) \in \mathcal{Q}$, we get

$$\begin{aligned} \mathcal{E}(t, y, z) &\le \liminf_{j\to\infty} \mathcal{E}(t_j, y_{(j)}, z_{(j)}) \le \liminf_{j\to\infty} (\mathcal{E}(t_j, \tilde{y}, \tilde{z}) + \mathcal{D}(z_{(j)}, \tilde{z})) \\ &= \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z, \tilde{z}). \end{aligned}$$

In particular, as $\mathcal{E}(t_j, \tilde{y}, \tilde{z})$ is finite for some $(\tilde{y}, \tilde{z}) \in \mathcal{Q}$, we get $\mathcal{E}(t, y, z) < +\infty$ and thus $\det \nabla y > 0$ a.e. in Ω in view of (2.10).

To prove injectivity, we profit again from the fact that quasistatic evolution of energetic solutions is very close to a purely static problem. In view of (2.23b), we obtain, for each $t \in [0, T]$, all necessary convergences that were used in the proof of Corollary 2.2 to pass to the limit in the conditions (2.18) and (2.19). $\square$

3. Separately Global Solutions to Rate-Independent Processes in Large-Strain Inelasticity

Rate independent systems (RIS) are characterized by their lack of any internal time length scale; rescaling of the input of the system in time leads to the very same rescaling of its solution. In continuum mechanics, rate-independent models represent a suitable approximation when the external conditions change slowly enough so that the system can always reach its equilibrium. This applies if inertial, viscous, and thermal effects are neglected. Rate independent systems have proven to be useful in modeling of hysteresis, phase transitions in solids, elastoplasticity, damage, or fracture in small and large strain regimes. We refer to Mielke and Roubíček [2015] for a thorough overview of various results and applications.

In the context of continuum mechanics, the approximation of the original system has the form a so called generalized gradient system, shortly denoted by $(\mathcal{Q}, \mathcal{E}, \mathcal{R})$, defined by the state space $\mathcal{Q}$, the energy functional $\mathcal{E} : [0,T] \times \mathcal{Q} \to (-\infty, +\infty]$ and a dissipation potential $\mathcal{R} : T\mathcal{Q} \to [0, +\infty]$, where $[0,T]$ is the time interval and $T\mathcal{Q}$ denotes the tangent bundle of $\mathcal{Q}$. Solutions to generalized gradient systems satisfy the so-called Biot's inclusion

$$0 \in \partial_{\dot{q}} \mathcal{R}(q(t), \dot{q}(t)) + \partial_q \mathcal{E}(t, q(t)), \quad t \in [0,T], \tag{3.1}$$

where ∂ denotes a (generalized) subdifferential; see Section 3.2 for a specific choice of $(\mathcal{Q}, \mathcal{E}, \mathcal{R})$. The dissipation potential $\mathcal{R}$ is usually non-negative, convex in its second argument, and satisfies $\mathcal{R}(q, 0) = 0$ for all $q \in \mathcal{Q}$. Equation (3.1) represents a force balance where the elastic forces $\partial_q \mathcal{E}$ are in equilibrium with static friction forces $\partial_{\dot{q}} \mathcal{R}$, and where both of them are in general multi-valued. The formulation fully relies on the theory of generalized standard materials; see Halphen and Nguyen [1975], Frémond [2002]. The rate-independence is expressed by the positive one-homogeneity of $\mathcal{R}(q, \cdot)$, leading to a zero homogeneity of the subdifferential $\partial_{\dot{q}} \mathcal{R}$, which makes the system clearly time-scale invariant.

On the other hand, this invariance property of the dissipation potential makes the system somewhat degenerate and determines the non-smooth nature of rate-independent processes (RIP). In particular, when the energy $\mathcal{E}$ is not convex, solutions may develop jumps, making the strong derivative $\dot{q}$ ill-defined; a reformulation of the equation (3.1) is therefore necessary. To this point, we utilise a characterisation of the positive 1-homogeneity stating

$$\mathcal{R}(q, \dot{q}) = \langle \eta, \dot{q} \rangle \quad \text{whenever} \quad \eta \in \partial_{\dot{q}} \mathcal{R}(q, \dot{q}), \tag{3.2}$$

with $\langle \cdot, \cdot \rangle$ denoting the duality pairing between $T\mathcal{Q}$ and $T\mathcal{Q}^*$. Using the definition of the subdifferential and the characterisation (3.2), we see that the Biot's equation (3.1) is equivalent to the following two conditions

$$\text{local stability:} \quad 0 \in \partial_{\dot{q}} \mathcal{R}(q(t), 0) + \partial_q \mathcal{E}(t, q(t)), \tag{3.3a}$$

$$\text{power balance:} \quad 0 = \langle \partial_q \mathcal{E}(t, q(t)), \dot{q}(t) \rangle + \mathcal{R}(q(t), \dot{q}(t)), \tag{3.3b}$$

we refer to Mielke and Roubíček [2015] for the detailed derivation. Note that the local stability is a purely static condition, saying that the static friction forces have to be strong enough to balance the elastic forces. The second, scalar equation relates the power of the change of state with the dissipation rate $\mathcal{R}(q, \dot{q})$. It is a remarkable feature of RIS that one purely static condition together with a single scalar equation is enough to characterize their evolution. Integration of the power balance over $[0, T]$ then yields the energy equality

$$\mathcal{E}(T, q(T)) + \int_0^T \mathcal{R}(q(t), \dot{q}(t)) \, \mathrm{d}t = \mathcal{E}(0, q(0)) + \int_0^T \partial_t \mathcal{E}(t, q(t)) \, \mathrm{d}t, \tag{3.4}$$

where the total $\mathcal{R}$-variation $\int_0^T \mathcal{R}(q(t), \dot{q}(t)) \, \mathrm{d}t$ expresses the total amount of dissipated energy, and $\int_0^T \partial_t \mathcal{E}(t, q(t)) \, \mathrm{d}t$ the reduced work of the loading; note that here ∂_t stands for the *partial* derivative of $\mathcal{E}$ with respect to its first argument. The sought weaker reformulation, completely free of any time derivatives, is then finally obtained by substituting the total $\mathcal{R}$-variation by an equivalent formula

$$\mathrm{Diss}_{\mathcal{R}}(q; [0, T]) := \sup \left\{ \sum_{j=1}^{N} \mathcal{R}(q(t_i) - q(t_{i-1})); N \in \mathbb{N}, 0 \leq t_0 \leq \ldots \leq t_N \leq T \right\}, \tag{3.5}$$

which is valid when $\mathcal{Q}$ is a vector space, the tangent bundle simplifies to $T\mathcal{Q} = \mathcal{Q} \times \mathcal{Q}$, and also only for dissipation potentials $\mathcal{R}(q, \dot{q})$ not depending on the state q.

Apart from the non-existence of the strong derivative, the aforementioned non-smoothness has yet another, peculiar side effect, that is the existence of a variety of different notions of solutions to RIS which differ significantly in the occurrence of jumps. As mentioned already in Roubíček [2015], the proper definition of the solution to the problem is here a vital part of the modelling.

The most general notion, encompassing all others, is that of *local solution*, first introduced by R. Toader and C. Zanini in Toader and Zanini [2009]. It is defined by the local stability (3.3a) and an *upper energy inequality*, i.e. "=" in (3.4) is replaced by "$\leq$", stating that the energy in the system cannot increase. It is exactly the energy inequality which makes the existence of local solutions easier to prove, however, at the same time, it represents its main drawback. Since the equality in (3.4) is lost, the energetics of the system are not fully under control. In other words, the dissipative mechanisms, and hence the underlying physics of the system, are not specified entirely. From the mathematical point of view the indefiniteness of the dissipative mechanisms leads to a selectivity gap for this concepts as there may exist even an uncountable family of local solutions to a given problem; see e.g. Roubíček [2015]. Also from the computational point of view the mere inequality is disadvantageous since when the solution is approximated numerically, it is not known whether the energy decreases due to unspecified physical dissipation or rather to rounding errors.

A generally stronger concept of *energetic solutions* was first introduced by Mielke and Theil Mielke and Theil [2004] and then advocated by many authors (see Mielke and Roubíček [2015] and the references therein). The local stability (3.3a) is replaced by the *global stability* condition

$$\forall \tilde{q} \in \mathcal{Q}: \quad \mathcal{E}(q(t)) \leq \mathcal{E}(\tilde{q}) + \mathcal{D}(q(t), \tilde{q}), \tag{3.6}$$

where $\mathcal{D}(q_1, q_2)$ is the so-called dissipation distance, expressing the amount of dissipated energy when the state changes from q_1 to q_2. In the case in which $\mathcal{Q}$ is a vector space coinciding with its tangent space, the dissipation distance is related to the dissipation potential by $\mathcal{D}(q_1, q_2) = \mathcal{R}(q_2 - q_1)$, provided that $\mathcal{R}(q, \dot{q})$ is again state independent; we refer to [Mielke and Roubíček, 2015, Subsec.3.2.2] for a thorough discussion about the relation between the dissipation potential $\mathcal{R}$ and the dissipation distance $\mathcal{D}$. Energetic solutions are very flexible and applicable to convex as well as nonconvex problems. In nonconvex problems, however, they do not necessarily provide us with proper predictions as the jump of the solution in time appears "too early" when compared to physical experiments in several applications, for example in models predicting damage and fracture. In fact, they jump immediately when there is enough energy available, as can be seen directly from (3.6), representing hence, in a sense, the worst case scenario. For this reason, the global stability condition is sometimes called in literature the *energetic criterion*, in contrast to the Biot's equation (3.1) representing a *stress criterion*. In other applications, e.g. for shape memory alloys, the energetic criterion may provide a reasonable simplification of the problem that makes its modelling feasible. The global stability condition also implies the lower energy inequality (i.e. the opposite to the one in the definition of the local solution) holds. Energetic solutions therefore satisfy even energy *equality* (3.4), so that the only dissipation is due to $\int_0^T \mathcal{R}(q, \dot{q}) \, \mathrm{d}t$; in particular, there is no extra energy dissipated on jumps. We again refer to Mielke and Roubíček [2015] for further properties of energetic solutions and their applications to materials science.

Completely on the other side of the spectrum than energetic solutions lie the so-called *BV solutions*, introduced by A. Mielke, R. Rossi and G. Savaré in Mielke et al. [2009], which 'jump as late as possible'. BV solutions also satisfy the energy equality, but with an extra dissipation counting for time discontinuities, which is given by a detailed resolution of the jump during which the viscous dissipative mechanism, not present in the rate-independent limit, is again activated. This notion of solution stems from models considering also viscous dissipation as a limit for vanishing viscosity. However, as opposed to the vanishing viscosity solutions, BV solutions are not defined as a pointwise limit of solutions to a viscous perturbation of the original RIS. Unlike for energetic solutions, however, the so far developed existence theory for BV solutions requires very strong assumptions on the data that can be barely expected to hold in the engineering practice. Apart from the analytical point of view, also the numerical approximation of BV solutions represents a fairly challenging task.

The list of possible notions of solutions presented here is by no means exhaustive and the reader is encouraged to consult for example Mielke [2011], Mielke and Roubíček [2015], Rindler et al. [2017, 2019] for a more detailed survey of both the mentioned and unmentioned solution strategies for RIS and for recent developments.

Given the overview above, we regard the concept of local solutions as a certain compromise between physical requirements and mathematical restrictions, taking into account the state of art of contemporary mathematical and numerical analysis. As they are the most general concept, local solutions do not exclude solutions jumping 'late enough' and represent a well defined object towards which

the numerical solutions may converge, the numerics for local solutions being also more understood today than for BV solutions; see Knees and Negri [2017]. A use of local solutions in continuum mechanics, was presented in Roubíček [2015] with a special regard to damage and delamination. In this setting, the state space is linear and poses a product structure $Q = U \times Z$, where U denoted the vector space of displacements u, also called elastic variables, and Z is the vector space of general internal variables z, describing, e.g. the damage field. In Roubíček [2015], the author proves the existence of local solutions to a rich class of problems in which the energy functional $\mathcal{E}(t, \cdot, \cdot)$ is not convex, but at least is separately convex in the last two variables, i.e.

$$\mathcal{E}(t, \cdot, z) : U \to (-\infty, +\infty] \quad \text{is convex and} \tag{3.7}$$
$$\mathcal{E}(t, u, \cdot) : Z \to (-\infty, +\infty] \quad \text{is convex} \tag{3.8}$$

and the Biot's equation (3.1) is replaced by the system

$$0 \in \partial_u \mathcal{E}(t, u(t), z(t)),$$
$$0 \in \partial_{\dot{z}} \mathcal{R}(\dot{z}(t)) + \partial_z \mathcal{E}(t, u(t), z(t)).$$

Note that the dissipation potential is assumed to be state independent. The reason for calling u the elastic variable is that the dissipation potential does not depend on its rate, i.e. its change never dissipates energy. The three convexities of $\mathcal{R}(\cdot)$, $\mathcal{E}(t, \cdot, z)$, and $\mathcal{E}(t, u, \cdot)$ make the strong formulation (3.7) equivalent to global stability in u and the so-called semi-stability in z

$$\forall \tilde{u} \in U : \quad \mathcal{E}(t, u(t), z(t)) \leq \mathcal{E}(t, \tilde{u}, z(t)), \tag{3.9}$$
$$\forall \tilde{z} \in Z : \quad \mathcal{E}(t, u(t), z(t)) \leq \mathcal{E}(t, u(t), \tilde{z}) + \mathcal{R}(\tilde{z} - z(t)). \tag{3.10}$$

The convexity in u is also important for controlling the jump-behavior in u, which is not directly encoded by the dissipation as is instead the case for the internal variable z. The two separately global conditions in (3.9) are then supplemented with an energy inequality where the total dissipation is given by (3.5). It should be noted that the paper Roubíček [2015] also deals with one of the main drawbacks of local solutions, i.e their weak selectivity behavior, and suggests to impose an additional criterion the solutions have to satisfy, giving rise to so called maximally dissipative local solutions; however, proving existence in this narrower class of solutions is still an open problem.

The main goal of this chapter is to generalize the concept of local solutions also to energies that are not necessarily convex in the elastic variable and hence extending significantly its applicability by including inelastic processes at large strain. As already mentioned, the advantage over energetic solutions is that 'too early' jumps can be avoided. The novelty of our analysis is that the physical requirements typical for large strain mechanics, in particular the local and global invertibility of the deformations, are met within our setting. We also stress that our analysis encompasses energies depending on Eulerian gradients of the Eulerian fields, which after rewriting into Lagrangian coordinates introduce a nonlinear coupling between the deformation and the Lagrangian field of the internal variable; we refer to Section 3.6 for a specific example.

The chapter is organized as follows: in Section 3.1 we describe our notion of separately global solutions, in Section 3.2 we present our concrete case study, in Section 3.3 we exhibit a simplified statement of our main result, discuss its implication, and present the proof strategy. Its precise statement is postponed to Theorem 3.21 in Section 3.6. In Section 3.4 we describe the precise mathematical setting. Section 3.5 is devoted to the proof of Theorem 3.21.

3.1 Separately Global Solutions

As in Roubíček [2015], dealing with local solutions with separately convex energies, we will suppose the state space poses a product structure $\mathcal{Q} = \mathcal{Y} \times Z$, where $\mathcal{Y}$ is the space of elastic variables, here a deformations y, and Z is a vector space of internal variables z. For a time interval $[0, T]$ we consider the energy functional $\mathcal{E} : [0, T] \times \mathcal{Y} \times Z \to (-\infty, +\infty]$ and the dissipation functional $\mathcal{R} : X \to [0, +\infty]$, which is for simplicity not state dependent. For analytical reasons we suppose $X \supset Z$, i.e. the tangent space is larger than the state space of internal variables.

Since we plan to work within the large deformations framework, we do not impose any convexity assumption on the functional

$$\mathcal{E}(t, \cdot, z) : \mathcal{Y} \to (-\infty, +\infty]; \tag{3.11}$$

nevertheless, we will require convexity of the energy in the second gradient of deformation, which is here the highest order term. Regarding the internal parameter instead we work under the assumption that

$$\mathcal{E}(t, y, \cdot) : Z \to (-\infty, +\infty] \quad \textit{is} \text{ convex.} \tag{3.12}$$

Concerning the dissipation potential, we assume that $\mathcal{R}$ is a so-called gauge, i.e.

$$\mathcal{R} : X \to [0, +\infty] \text{ is convex}, \quad \forall a \geq 0, \forall z \in \operatorname{Dom} \mathcal{R} : \mathcal{R}(az) = a\mathcal{R}(z), \tag{3.13}$$

where $\operatorname{Dom} \mathcal{R} := \{z \in Z : \mathcal{R}(z) < +\infty\}$. The positive degree-1 homogeneity of $\mathcal{R}$ also implies $\mathcal{R}(0) = 0$ and, together with convexity, it guarantees the dissipation potential satisfies the triangle inequality $\mathcal{R}(a + b) \leq \mathcal{R}(a) + \mathcal{R}(b))$ for every $a, b \in X$. We point out that still a broad class of problems (such as delamination and bulk damage) can be formulated within this framework of (3.11), (3.12), and (3.13).

In the strong formulation of the problem we seek a solution $(y, z) : [0, T] \to \mathcal{Y} \times Z$ satisfying

$$z(0) = z_0, \tag{3.14a}$$

$$y(t) \in \operatorname*{ArgLocMin}_{y \in \mathcal{Y}} \mathcal{E}(t, y, z(t)), \tag{3.14b}$$

$$0 \in \partial \mathcal{R}(\dot{z}(t)) + \partial_z \mathcal{E}(t, y(t), z(t)), \tag{3.14c}$$

where z_0 is a given initial condition, ∂ and ∂_z denote the (partial) sub-differentials, and ArgLocMin is the set of local minimizers since in the quasi-static evolution we seek exclusively for stable deformations. The weak formulation relies on the convexity of the dissipation potential and of the energy in the internal variable. Following Roubíček [2015], we rewrite (3.14c) using the concept of *semi-stability*

for the internal parameter z. The condition of local minimum for the elastic variable is replaced by a global one, both because of its stability and mathematical benefits; in proving the existence we rely on global minimization in several aspects. Denoting $\mathrm{B}([0,T];U)$ the collection of functions defined everywhere in $[0,T]$ and bounded in a space U and by

$$\mathrm{Diss}_{\mathcal{R}}(z;[r,s]) := \sup\left\{\sum_{j=1}^{N}\mathcal{R}(z(t_{i-1}),z(t_i)); N\in\mathbb{N}, r\le t_0\le\ldots\le t_N\le s\right\}$$

the total dissipation on the interval $[r,s]\subset[0,T]$, our notion of solution to the system (3.14) reads as follows.

Definition 3.1 (a.e.-Separately Global Solution)**.** *The mapping $(y,z) : t \mapsto (y(t),z(t)) \in \mathcal{Q}$ with $y\in \mathrm{B}(I;\mathcal{Y})$ and $z\in \mathrm{B}(I;Z)\cap\mathrm{BV}(I;X)$ is called an a.e.-separately global solution if $t\mapsto\partial_t\mathcal{E}(t,y(t),z(t))$ is integrable, and the following conditions are satisfied:*

$$\begin{aligned}
&& z(0) &= z_0,\\
\forall_{a.e.} t\in I,\ \forall\tilde{y}\in\mathcal{Y}: && \mathcal{E}(t,y(t),z(t)) &\le \mathcal{E}(t,\tilde{y},z(t)),\\
\forall_{a.e.} t\in I,\ \forall\tilde{z}\in Z: && \mathcal{E}(t,y(t),z(t)) &\le \mathcal{E}(t,y(t),\tilde{z})+\mathcal{R}(\tilde{z}-z(t)),\\
\forall_{a.e.} t_1,t_2\in I,\ t_1<t_2: && \mathcal{E}(t_2,y(t_2),z(t_2))&+\mathrm{Diss}_{\mathcal{R}}(z;[t_1,t_2])\\
&&&\le \mathcal{E}(t_1,y(t_1),z(t_1))+\int_{t_1}^{t_2}\partial_t\mathcal{E}(t,y(t),z(t))\,\mathrm{d}t.
\end{aligned}$$

We point out that this concept of solutions does not require any time-differentiability of the internal variable z. As in Roubíček [2015], though, no measurability in time of the deformation and no absolute-continuity in time of the internal variable are a-priori guaranteed.

Separate global energy minimization is beneficial from the mathematical point of view and unlike a mere first optimality condition it guaranties the necessary stability of the solution, which is required by the underlying physics. On the other hand, in some situations it inevitably leads to a completely flawed predictions; especially when time dependent dead surface load is considered. In order to avoid the most pathological situations we hence consider only time dependent Dirichlet boundary conditions (sometimes referred to as 'hard device'), or at least their relaxation via a penalty method, sometimes also called 'soft-device'.

3.2 Specific Example of Rate-Independent System

Before proceeding further, let us visualize the abstract framework of RIS on a concrete example from continuum mechanics, postponing the full mathematical details to Section 3.4; see also Mielke and Roubíček [2015] for a rich list of applications to continuum mechanics. In the problem of bulk gradient damage the state space $\mathcal{Q}=\mathcal{Y}\times Z$ consists of deformations $y:\Omega\to\mathbb{R}^3$, $\Omega\subset\mathbb{R}^3$ denoting the body in the reference configuration, and of damage field $z:\Omega\to[0,1]$, where $z(x)=1$ means the material at the point $x\in\Omega$ is flawless, while $z(x)=0$

corresponds to fully damaged material, completely unable to sustain any stress (perhaps with the exception of a pure compression).

The energy functional then may take the form

$$\mathcal{E}(t,y,z)=\int_\Omega V(z,\nabla y,\nabla^2 y)+\phi\left((\nabla y)^{-\top}\nabla z\right)\,\mathrm{d}x-\ell(t,y,z),\tag{3.15}$$

where $V:\mathbb{R}\times\mathbb{R}^{3\times3}\times\mathbb{R}^{3\times3\times3}\to[0,+\infty)$ is the stored energy density, $\phi:\mathbb{R}^3\to\mathbb{R}$ prevents formation of a microstructure by penalizing the 'crack length' (in gradient damage relaxed by a smooth interface), and $\ell(t,y,z):[0,T]\times\mathcal{Y}\times Z\to\mathbb{R}$ denotes the time dependent loading. All the functions can be in principle x-dependent, including also materials not homogeneous in the reference configuration.

For bulk damage, the stored energy density has usually the form

$$V(\nabla y,\nabla^2 y,z)=\gamma(z)W(\nabla y,\nabla^2 y),$$

where $W:\mathbb{R}^{3\times3}\times\mathbb{R}^{3\times3}\to[0,+\infty)$ is the stored energy density of undamaged material, and the function $\gamma:\mathbb{R}\to(0,+\infty)$ models incomplete bulk damage, meaning its values are bounded from zero by some small positive constant and hence preserving the coercivity of the stored energy density; we refer to Bouchitté et al. [2009], Mielke et al. [2010] for modeling of complete damage. A particular choice of W may be

$$\begin{aligned}W(\nabla y,\nabla^2 y)&=\psi(\nabla y)+\Phi(\nabla^2 y)\\&=a|\nabla y|^p+b|\operatorname{Cof}\nabla y|^q+c(\det\nabla y)^r-d\ln(\det\nabla y)^2+\frac{\epsilon}{p}|\nabla^2 y|^p.\end{aligned}$$

The positive coefficients a,b,c,d may yield arbitrary Lamé constants; see Ciarlet [1988] for $p=2$ and a general function of $(\det\nabla y)^{-1}$. The last term serves as a mathematical regularisation, the coefficient $\epsilon>0$ being small enough not to influence the material response considerably. Thanks to the regularisation by $\Psi(\nabla^2 y)$ the $\psi(\nabla y)$ term can be in principle non-convex, including for example the St. Venant–Kirchhoff material

$$\psi(\nabla y)=\frac{1}{8}\mathcal{C}\left((\nabla y)^\top\nabla y-\mathbb{I}\right):\left((\nabla y)^\top\nabla y-\mathbb{I}\right),$$

where $\mathcal{C}$ is a fourth order tensor of elastic constants, which is easy to use in an engineering practise thanks to its direct connection to the small strain mechanics. A very common choice of γ is

$$\gamma(z)=\begin{cases}z^2+\epsilon, & \text{for } z\geq0,\\ \epsilon, & \text{for } z<0.\end{cases}$$

The function ϕ depends on the Eulerian gradient of the Eulerian field $\zeta(y(x))=z(x),x\in\Omega$, denoted $\nabla^y\zeta$, and it may be of the form

$$\int_\Omega\phi\left((\nabla y)^{-\top}\nabla z\right)\,\mathrm{d}x=\int_\Omega\frac{\rho_0}{\alpha}\left|(\nabla y)^{-\top}\nabla z\right|^\alpha\,\mathrm{d}x=\int_{\Omega^y}\frac{\rho}{\alpha}\,|\nabla^y\zeta|^\alpha\,\mathrm{d}y,$$

where $\alpha>0$ and $\rho_0(x)=\rho(y(x))\det\nabla y(x)$ is the relation between the Lagrangian and Eulerian field of density with respect to the volume in the reference and

deformed configuration, respectively. This choice favors the onset of damage at points where the density ρ is smaller. A similar behaviour would be achieved by replacing $\phi\left((\nabla y)^{-\top}\nabla z\right)$ with $\phi_d(\mathrm{Cof}\,\nabla y\nabla z)$ and considering

$$\int_\Omega \phi_d(\mathrm{Cof}\,\nabla y\nabla z)\,\mathrm{d}x = \int_\Omega |\mathrm{Cof}\,\nabla y\nabla z|\,\mathrm{d}x = \int_{\Omega^y} |\nabla^y\zeta|\,\mathrm{d}y. \tag{3.16}$$

This example corresponds to a relaxed penalization of perimeter of the set of undamaged material, i.e. a criterion based only on the geometry of the deformed body and not taking its density into account.

A typical example of the loading functional ℓ, in large deformations typically non-linear, would be

$$\ell(t,y,z) = \int_\Omega B(t)\cdot y\,\mathrm{d}x + \int_{\Gamma_N} S(t)\cdot y\,\mathrm{d}\mathcal{H}^2(x) \tag{3.17}$$

$$-\frac{1}{2\varepsilon}\int_{\Gamma_\mathrm{d}} |y-y_D(t)|^2\,\mathrm{d}\mathcal{H}^2 - \int_\Omega \pi(t,y)\det\nabla y\,\mathrm{d}x, \tag{3.18}$$

where B and S stand for bulk and surface dead-loads, respectively, the third term penalizes for $\varepsilon\to 0$ the mismatch between the deformation value and the prescribed Dirichlet boundary condition y_D, and the last term is a potential for a surface pressure load, π being the pressure field in the deformed configuration.

Remark 3.2 (Hyper-loading)**.** *The second grade materials, whose stored energy density depends also on $\nabla^2 y$, may model various physical phenomena, for example flow of Korteweg fluids (depending on the Eulerian gradient of the Eulerian density field) or deformation of woven fabrics; see Korteweg [1901], dell'Isola and Steigmann [2014] for the example mentioned and Toupin [1962, 1964], Green and Rivlin [1964], Ball et al. [1981], Šilhavý [1985], Pideri and Seppecher [1997], Kouranbaeva and Shkoller [2000], Mariano [2007], Dell'Isola et al. [2009], Forest [2009], Ball and Mora-Corral [2009], Ball and Crooks [2011], Seppecher et al. [2011], Segev [2017] for further works on the so-called non-simple continua, the list definitely not being exhaustive. However, here they rather arise from the mathematical need for compactness. It is therefore not necessary to incorporate the hyper-loading, an additional terms representing conservative forces, typically in a form of an edge traction or the so-called couple-stress or double force acting on the boundary; see Podio-Guidugli and Caffarelli [1990], Mindlin [1964]. No such physical phenomena is expected in our intended applications. Nevertheless, such terms might be useful for another mathematical or numerical regularization, e.g. preventing the mesh to degenerate near the boundary.*

Apart energy, the second constitutive quantity in the gradient system is the dissipation potential, for applications to the unidirectional bulk damage being

$$\mathcal{R}(\dot z) = \begin{cases} \displaystyle\int_\Omega G\rho_0|\dot z(x)|\,\mathrm{d}x = \int_{\Omega^y} G\rho(x)|\dot\zeta(y)|\,\mathrm{d}y, & \text{for } \dot z\le 0 \text{ a.e. in } \Omega,\\ +\infty, & \text{otherwise,}\end{cases} \tag{3.19}$$

where G is the so-called fracture toughness and $z(x)=\zeta(y(x)), x\in\Omega$ are respectively the Lagrangian and Eulerian damage field. In this model the material cannot heal as $\dot z>0$ is prohibited. The unidirectionality can be relaxed by allowing small healing, which may be useful from the analytical point of view; see Roubíček [2015].

Remark (Delamination)**.** *A particular example of the loading functional $\ell(t, y, z)$ depending also on the internal variable z could be provided by delamination, where the 'elastic constants' in the boundary term in* (3.17) *may depend on z, simulating then a damageable adhesive. The dissipation potential in* (3.19) *would include then the corresponding surface term; see Roubíček [2015] for a specific example in small strain regime.*

3.3 Main Result

Leaving the precise assumptions and formulations to Sections 3.4 and 3.6, we state roughly the main result, explain the crucial steps, and highlight the novelties.

Theorem 3.3. *Under suitable assumptions on the system $(\mathcal{Q}, \mathcal{E}, \mathcal{R})$, the problem* (3.14) *admits a separately global solution in the sense of Definition 3.1.*

The proof strategy relies on a classical procedure: after performing Rothe-type time discretization, we establish uniform estimates for the piecewise constant interpolants and select suitable convergent subsequences. Using the convexity of the energy in the highest order terms we improve their convergence, which is in turn instrumental for showing the limiting stability, semi-stability, and energy inequality.

The most important novelty of our contribution consists in extending the notion of local solutions to the large-strain setting for RIS, as well as to energies $\mathcal{E}$ which are not convex in the deformation, and which include energies depending on the Eulerian gradient of the internal variable, which rewritten to the Lagrangian coordinates equals $\nabla y^{-\top} \nabla z$.

One difficulty caused by the term $\nabla y^{-\top} \nabla z$ lies in uniform estimates and the related integrability of the fields, because only the coupled term is under control. This in turn leads to worse integrability of ∇z and hence weaker compactness properties of the sequence of interpolants. The latter is crucial since due to the coupling the term $\phi(\nabla y^{-\top} \nabla z)$ does not cancel in the discrete (semi-)stability, as it would happen if it depended solely on the Lagrangian gradient ∇z, and is therefore present on the right hand side, as opposed to Roubíček [2015]. When passing to the limit the strong convergence is therefore used for proving upper semi-continuity of this term.

We overcome this difficulty by having both ∇y and $\nabla y^{-\top}$ in $L^\infty(\Omega)$, because then the integrability and compactness of the Eulerian and Lagrangian gradient is not affected. While the desired integrability of ∇y is obtained by regularizing the energy with the second gradient $\nabla^2 y$, the latter is not trivial. We achieve it by using the Healey-Krömer Lemma 3.4, see Healey and Krömer [2009], which assures that $\det \nabla y$ is bounded from zero uniformly for the approximating sequence. The integrability and compactness of $\nabla y^{-\top}$ then follows by the Cramer's rule

$$(\nabla y)^{-\top} = \frac{\operatorname{Cof} \nabla y}{\det \nabla y}.$$

This regularization is necessary for passing from time-discrete to time-continuous solutions. However, in proving the existence of the discrete solutions it can be

avoided, and the first gradient with polyconvex energies is sufficient. This simplification is possible thanks to the alternating minimization scheme which decouples the discrete problem effectively.

Although the decoupling of the discrete system is advantageous in this sense, it leads to additional complications on the continuous level. While in the discrete stability condition the *right*-continuous interpolant (3.51) of the internal variable appears, in the discrete semi-stability the *left*-continuous interpolant (3.52) is present. In turn, only for the *left*-continuous interpolant the convergence is improved. The problem is that the standard estimates for the error between the two interpolants are not sufficient for proving strong convergence of the highest order terms of the other interpolant. We hence have to proceed in Lemma 3.13 differently, proving, however, strong convergence of the right-continuous interpolant only for almost every time.

The strong convergence of the right-continuous interpolant of the internal variable can be used in the stability condition for improving the convergence of the elastic variable, as far as convergence for almost every time is not enough. In order to achieve strong convergence of the elastic variable for *all* times we regularize the energy on the discrete level by an additional term (3.28), which improves the integrability of the internal variable, but disappears for the discretization parameter tending to zero. Due to the regularization we cannot use elements of Z as competitors in the semi-stability and hence we use their Lipschitz truncation instead; for the same reason also the initial condition z_0 has to be truncated. The reason for using the Lipschitz truncation does not lie in the smallness of the set where the truncation differs, but only in quantification of the Lipschitz constant of the truncated function.

Apart from the problems arising from geometric nonlinearities due to large strains, we also have to face the non-uniqueness of solutions caused by the lack of convexity in the elastic variable. Hence the selection of the t-dependent of subsequences in Lemma 3.15 is more subtle, as it is for the energetic solutions in Francfort and Mielke [2006], and leads to solutions where the elastic variable is not measurable in time; nevertheless, the method from Mielke and Roubíček [2015] used for measurable selection of the energetic solution might be adopted. Unlike energetic solutions, however, local solutions are characterized by an energy inequality evaluated at *two time instants*, which makes the selection of t-dependent subsequences even more complicated; for solving this issue in Lemma 3.20 the global stability separately in the elastic variable is essential. While we keep the t-dependence of the subsequences explicit in statements, we skip it in the proofs for the ease of notation.

In addition, the energy inequality has on its right hand side an energy term evaluated at arbitrary times and hence continuity of the energy, implied by strong convergence of the sequences, is needed; as opposed to the left hand side where mere lower semi-continuity of the energy functional is enough. For improving the convergences in Lemmata 3.13 and 3.16 we use energies that are convex in the higher order terms. The strong convergence is also needed for identifying the reduced power in Lemma 3.19 since for non-linear loading a mere weak convergence is not enough.

Although the stored energy density is suited for bulk damage, a more general ansatz could be considered. The general proof strategy is based on splitting

the highest order terms of the elastic and internal variable. The loading, on the other hand, is kept fully general and we closely follow the procedure from Roubíček [2015]. Rather than to impose the (lower semi-)continuity assumptions on the loading $\ell(t, y, z)$ alone, we suppose that the differences

$$\ell(t, y, \tilde{z}) - \ell(t, y, z) \quad \text{or} \quad \ell(t, \tilde{y}, z) - \ell(t, y, z) \tag{3.20}$$

have suitable properties; the variables $\tilde{y}$ and $\tilde{z}$ are to be replaced by a recovery sequence. While for the elastic variable y a constant sequence is sufficient, for the inelastic variable z one has to handle the energy regularization on the discrete time level or eventually the constraint expressed by infinite values of the dissipation potential $\mathcal{R}$, e.g. the unidirectional damage. The reason for the formulation (3.20) is that it allows for a notable cancellation effect when the highest order terms are fully decoupled. Note that the coupling in the ϕ term is exactly the reason why the procedure from Roubíček [2015] cannot be directly applied here. Nevertheless, this formulation is still fruitful for improving the convergence in Lemmata 3.13 and 3.16, where only weak convergence is at disposal, but the sequences are such that the limits cancels; as opposed to proof of (semi-)stability where the limit is general, but the strong convergence holds.

3.4 Mathematical Setup

Now we introduce the precise setting of our work and present the key mathematical ingredients for our proof. In the whole chapter we suppose the body's reference configuration $\Omega \subset \mathbb{R}^3$ is a bounded Lipschitz domain.

State Space

The state space $\mathcal{Q}$ is assumed to pose the product structure

$$\mathcal{Q} := \mathcal{Y} \times Z, \tag{3.21}$$

consisting of admissible deformations and fields of internal variable, given by

$$\mathcal{Y} := \{y \in W^{2,p}(\Omega, \mathbb{R}^3) : (\det \nabla y)^{-1} \in L^s(\Omega), \tag{3.22}$$

$$\det \nabla y > 0 \text{ a.e. in } \Omega, (3.25) \text{ holds}\}, \tag{3.23}$$

where (3.25) is the Ciarlet–Nečas condition defined below, and

$$Z := \{z \in W^{1,\alpha}(\Omega) : 0 \leq z \leq 1 \text{ a.e. in } \Omega\}, \tag{3.24}$$

for some $p, q, r \geq 1$, $s \geq 0$, and $\alpha \geq 1$. Note that instead of time-dependent Dirichlet data, representing a load by a hard device, we consider their relaxation via a penalty method, in contrast to the former called soft-device. While the relaxation is still sufficient for Poincaré-type inequalities on $\mathcal{Y}$, it does not relies on extension theorems for locally invertible mappings, which are up to now not available.

Injectivity

As outlined in the introduction, the utmost physical requirement in large deformations is that the material does not interpenetrate. Our analysis relies on the classical Ciarlet–Nečas condition on the deformation

$$\int_\Omega \det \nabla y \, \mathrm{d}x \leq \mathcal{L}^3(y(\Omega)), \tag{3.25}$$

where $\mathcal{L}^3$ denote the Lebesgue measure in $\mathbb{R}^3$ [1]. The original statement from Ciarlet and Nečas [1987] states that whenever $p > 3$ and $y \in W^{1,p}(\Omega;\mathbb{R}^3)$ is such that $\det \nabla y > 0$ almost everywhere in Ω, then the deformation y is injective almost-everywhere in Ω. Apart the Ciarlet–Nečas condition we use also the result from [Hencl and Koskela, 2014, Theorem 3.4] by which the additional condition to (3.25)

$$\frac{|\nabla y|^3}{\det \nabla y} \in L^\delta(\Omega), \tag{3.26}$$

satisfied for some $\delta > 2$, implies invertibility *everywhere* in Ω. The crucial observation is that (3.26) then implies y is an open map. Although the Ciarlet–Nečas condition (3.25) is well suited for proving the existence of minimizer by the direct method, it is by no means trivial to incorporate the non-local constraint numerically. We refer e.g. to Krömer and Valdman [2019], Krömer [2019] for its relaxation, more feasible for numerical computations, and further generalizations.

Boundedness of $\det \nabla y$ from Zero

Another important ingredient for our proof, helping to overcome the difficulties arising from the Eulerian gradient of the damage field, is the following corollary of the result from Healey and Krömer [2009]. For convenience of the reader we provide an alternative proof in the Appendix A.1.

Corollary (Healey-Krömer)**.** *Let $p > 3$, $s \geq \frac{3p}{p-3}$, Then for every $y \in \mathcal{Y}$ there exists $\varepsilon_y > 0$ s.t.*

$$\det \nabla y \geq \varepsilon_y > 0 \quad \textit{in } \overline{\Omega}. \tag{3.27}$$

Moreover, if a sequence $\{y_\tau\} \subset \mathcal{Y}$ is uniformly bounded in $W^{2,p}(\Omega)$, and the sequence $\{(\det \nabla y_\tau)^{-1}\}$ is uniformly bounded in $L^s(\Omega)$, then the bound on the determinant in (3.27) *is uniform.*

The corollary implies that for the class Z of internal variables, the Lagrangian gradient with respect to the set $\mathcal{Y}$ of admissible deformations is integrable if and only if the Eulerian gradient has the same property. In other words, we have

$$\nabla^y z := (\nabla y)^{-\top} \nabla z = \frac{\operatorname{Cof} \nabla y^\top}{\det \nabla y} \nabla z \in L^1(\Omega) \quad \text{iff} \quad \nabla z \in L^1(\Omega).$$

[1] For other conditions ensuring injectivity we refer to [Giaquinta et al., 1989, Sec. 6, Thm.2] and to Ball [1981]; however, these require Dirichlet boundary datum to be prescribed on the whole $\partial\Omega$.

This observation is crucial for proving the stability condition for the deformation y.

Apart from the integrability of the Lagrangian gradient, the Healey-Krömer lemma also allows us to prove continuity of elastic energies that blow-up as the determinant of their argument converges to zero.

Corollary (Continuity of W on $\mathcal{Y}$)**.** *Let $\{y_\tau\} \subset \mathcal{Y}$ be such that $\{(\det \nabla y_\tau)^{-1}\}$ is uniformly bounded in $L^s(\Omega)$ and $y_\tau \to y$ in $W^{2,p}(\Omega)$, where $p > 3$ and $s \geq \frac{3p}{p-3}$. If the stored energy density $W : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3} \to [0, +\infty)$ is continuous and satisfies the growth condition*

$$|W(F, G)| \leq C(|F|^p + (\det F)^{-s} + |G|^p + 1),$$

then

$$W(\nabla y_\tau, \nabla^2 y_\tau) \to W(\nabla y, \nabla^2 y) \quad \text{in } L^1(\Omega).$$

Proof. Thanks to Corollary 3.4 the function W has p-growth on the sequence. The thesis follows then from the standard argument for the continuity of the Nemytskii operator. □

Strong Convergence Implied by Strict Convexity

The well-known result for uniformly convex Banach spaces, that weak convergence together with convergence of the norms implies strong convergence (see e.g. Fan and Glicksberg [1958]), has been generalised by Visintin [1984], where, roughly speaking, convergence of the norms is replaced by convergence of a strictly convex functional. Since the case of multiple variables is not treated there, we introduce here its slight generalisation for integrands which are strictly convex in the last variable. Reader interested in proof is referred to the Appendix A.1.

Lemma 3.4. *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Assume that $C, c > 0$ and $h : \Omega \times \mathbb{R} \times \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3} \to \mathbb{R}$ is a Carathéodory integrand such that for all $(x, z, F, G) \in \Omega \times \mathbb{R} \times \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3}$ and some $p, q \in (1, +\infty)$*

$$c(|z|^q + |F|^{p*} + |G|^p) - C \leq h(x, z, F, G) \leq C(1 + |z|^q + |F|^{p^*} + |G|^p) \ ,$$

where $h(x, z, F, \cdot)$ is strictly convex and

$$p^* := \begin{cases} pn/(n-p) & \text{if } 1 < p < n, \\ \text{any number in } [1, +\infty) & \text{otherwise.} \end{cases}$$

If $y_k \rightharpoonup y$ in $W^{2,p}(\Omega; \mathbb{R}^n)$, $z_k \to z$ in $L^q(\Omega)$, and

$$\int_\Omega h(x, z_k, \nabla y_k, \nabla^2 y_k)\, \mathrm{d}x \to \int_\Omega h(x, z, \nabla y, \nabla^2 y)\, \mathrm{d}x,$$

then $y_k \to y$ in $W^{2,p}(\Omega; \mathbb{R}^n)$.

Discrete Space Regularization

For improving the integrability of the discrete solution we introduce the following energy regularization on the time-discrete level

$$\mathcal{H}_\tau(z) := \tau^\kappa \int_\Omega |\nabla z|^\beta \,\mathrm{d}x, \tag{3.28}$$

where $\kappa > 0$ and $\beta > \alpha + \kappa$. The role of this additional regularization is to improve weak convergence of gradients for the time-interpolants associated to the damage field z. The semi-stability condition by itself, is enough to proof their strong convergence, i.e. exclude oscillations and concentrations, but only for almost every time. Our analysis relies on the observation that, in proving strong convergence of the elastic variable y, it is enough to handle just eventual concentrations of ∇z. These are localised by the decomposition lemma (see Lemma A.3) and suppressed by the space regularisation (3.28).

On the other hand, the space regularization prevents us from using $z \in Z$ as a competitor in the discrete semi-stability. We hence use its Lipschitz truncation instead; see Lemma A.4. In our application, we do not rely on the smallness of the set where the functions are truncated, but only on the quantification of the Lipschitz constant.

Free-Energy Assumptions

For simplicity we confine ourselves to slightly simplified ansatz of the energy functional $\mathcal{E} : [0,T] \times \mathcal{Y} \times Z \to \mathbb{R}$

$$\mathcal{E}(t,y,z) = \int_\Omega \gamma(z) W(\nabla y, \nabla^2 y) + \phi\left((\nabla y)^{-\top}\nabla z\right) \,\mathrm{d}x - \ell(t,y,z), \tag{3.29}$$

where $\kappa > 0$, and $\alpha + \kappa < \beta$; in general the proof's strategy would work for any energy that splits the highest order terms of y and z. We will assume that the functions γ, W, ϕ and the loading ℓ satisfy the following coercivity and growth conditions. The function $\gamma : \mathbb{R} \to (0, +\infty)$ satisfies

$$\gamma \in C^1(\mathbb{R}) \text{ is positive and convex, and it is constant on } (-\infty, 0]. \tag{3.30}$$

The function ϕ is required to be strictly convex and satisfy polynomial growth assumptions from above and below, whereas W is assumed to be convex in $\nabla^2 y$ and its growth conditions on are compatible with the modeling of impenetrability and blow-up of the elastic energy under strong compression. Namely

$$c|u|^\alpha - C \le \phi(u) \le C(|u|^\alpha + 1), \tag{3.31}$$

for every $u \in \mathbb{R}^3$, and

$$c(|F|^p + (\det F)^{-s} + |G|^p) \le W(F,G) \le C(|F|^p + (\det F)^{-s} + |G|^p + 1), \tag{3.32}$$

for every $F \in \mathbb{R}^{3\times 3}$ and $G \in \mathbb{R}^{3\times 3\times 3}$, for some $p > 1$ and $s \ge 0$. Finally, we assume the nonlinear loading to fulfill the following coercivity assumption:

$$\begin{aligned} &-\ell(t,y,z) \\ &\ge c\left(\left|\int_{\Gamma_D} y \,\mathrm{d}\mathcal{H}^2\right| - \|\nabla y\|_p^{\tilde{p}} - \|\nabla^2 y\|_p^{\tilde{p}} - \|(\det \nabla y)^{-1}\|_s^{\tilde{s}} - \|(\nabla y)^{-\top}\nabla z\|_\alpha^{\tilde{\alpha}}\right) - C, \end{aligned} \tag{3.33}$$

for every $(y,z) \in \mathcal{Q}$, for some $0 \le \tilde{p} < p$, $0 \le \tilde{s} < s$, and $0 \le \tilde{\alpha} < \alpha$.

In addition, for the loading ℓ we consider a slightly modified version of an assumption in Roubíček [2015]. We assume that the loading functional $\ell : \mathbb{R} \times \mathcal{Y} \times Z \to \mathbb{R}$ is such that either for each $\tilde{y} \in \mathcal{Y}$ the map

$$(t,y,z) \mapsto \ell(t,\tilde{y},z) - \ell(t,y,z) \tag{3.34}$$

or the map

$$(t,y,z,\tilde{z}) \mapsto \ell(t,y,\tilde{z}) - \ell(t,y,z) \tag{3.35}$$

pose suitable (lower semi-)continuity properties; see the hypothesis of Lemmata 3.13, 3.16, 3.17, and 3.18. For the proving the energy inequality we need continuity of the reduced power $-\partial_t \ell$; see Lemma 3.20. Finally, in order to obtain the standard uniform estimates for the solutions of the system discertized in time, we assume the loading enjoys the following structural properties

$$\operatorname{Dom} \ell = [0,T] \times \operatorname{Dom} \ell(0,\cdot,\cdot), \tag{3.36}$$

$$\forall (y,z) \in \mathcal{Q}: \quad \ell(\cdot,y,z) \in W^{1,1}(0,T), \tag{3.37}$$

$$\forall_{\text{a.e.}} t \in (0,T),\ \forall (y,z) \in \mathcal{Q}: \quad \partial_t \ell(\cdot,y,z) \text{ exists.} \tag{3.38}$$

While for most of the time we have to work with a more specific structure of the energy (because of the product structure of the state space and the separate global minimization), the time discretization is fully covered by the abstract approach from Mielke and Roubíček [2015]. Conditions (3.30) - (3.38) imply the energetic control of power, described by the equations below

$$\begin{aligned}
&\operatorname{Dom} \mathcal{E} = [0,T] \times \operatorname{Dom} \mathcal{E}(0,\cdot,\cdot),\\
&\forall (y,z) \in \mathcal{Q}: \quad \mathcal{E}(\cdot,y,z) \in W^{1,1}(0,T),\\
&\forall_{\text{a.e.}} t \in (0,T),\ \forall (y,z) \in \mathcal{Q}: \quad \partial_t \mathcal{E}(\cdot,y,z) \text{ exists},\\
&\exists C^0 \in \mathbb{R} \text{ and } \lambda \in L^1(0,T) \text{ such that } \forall_{\text{a.e.}} t \in (0,T) \text{ and } \forall (y,z) \in \mathcal{Q}:\\
&|\partial_t \mathcal{E}(t,y,z)| \le \lambda(t)(\mathcal{E}(t,y,z) + C^0).
\end{aligned} \tag{3.39}$$

The above properties, together with Gronwall's inequality, imply

$$\mathcal{E}(t,y,z) + C^0 \le (\mathcal{E}(s,y,z) + C^0)\mathrm{e}^{|\Lambda(t)-\Lambda(s)|}, \quad \text{where } \Lambda(t) := \int_0^t \lambda(r)\,\mathrm{d}r, \tag{3.40}$$

which finally yields, when combined again with (3.39),

$$|\partial_t \mathcal{E}(t,y,z)| \le \lambda(t)(\mathcal{E}(s,y,z) + C^0)\mathrm{e}^{|\Lambda(t)-\Lambda(s)|}, \tag{3.41}$$

for every $s,t \in [0,T]$. In particular, $t \mapsto \mathcal{E}(t,y,z)$ is absolutely continuous for every $(y,z) \in \mathcal{Q}$

Dissipation Potential Assumptions

Unlike the energy functional, the dissipation potential does not require any structural assumptions. For simplicity we consider $\mathcal{R} : L^1(\Omega) \to [0,+\infty)$ that is coercive in the sense

$$\inf_{v \neq 0} \frac{\mathcal{R}(v)}{\|v\|_1} > 0, \tag{3.42}$$

and enjoys suitable semi-continuity properties to be specified later. Note that the convexity and positively 1-homogeneity together with $\mathcal{R}(0) = 0$ implies

$$\forall z_1, z_2, z_3 \in Z: \quad \mathcal{R}(z_3 - z_1) \leq \mathcal{R}(z_3 - z_2) + \mathcal{R}(z_2 - z_1), \tag{3.43}$$

$$\forall v \in Z: \quad \mathcal{R}(v) = 0 \Longleftrightarrow v = 0, \tag{3.44}$$

i.e. $\mathcal{R}$ defines the so-called extended metric.

Remark. *Although we consider in general $\mathcal{R}$ which is finite everywhere, the unidirectional damage is also covered, but discussed separately; see Remark 3.14.*

3.5 Proof of the Existence Theorem

Having fixed all the details we are now ready to prove the existence of a separately global solution. As already mentioned, the proof follows the standard scheme, namely the Rothe time discretization, existence of discrete solutions, compactness, improving of convergence, passing to limit on (semi-)stability, and proving the energy inequality. Since we regularize the problem on the discrete level, we have to modify the initial condition and hence the last step consists of proving its convergence to the original value z_0.

3.5.1 Rothe Time Discretization

Let $z^0 \in Z$ be the initial condition and let $y^0 \in \mathcal{Y}$ be a minimizer of the function $y \mapsto \mathcal{E}(0, y, z^0)$. Due to the regularization of the discrete problem we need to construct our discrete solutions for a slightly modified initial condition. We replace it by its Lipschitz truncation $(z^0)_{\lambda(\tau)}$, where the truncation parameter $\lambda(\tau)$ depends on the time step τ in such a way that

$$\mathcal{H}_\tau((z^0)_{\lambda(\tau)}) = \tau^\kappa \int_\Omega |\nabla (z^0)_{\lambda(\tau)}|^\beta \,\mathrm{d}x \leq C(\alpha, \Omega)\mathcal{L}^3(\Omega)\tau^\kappa \lambda^\beta(\tau) \to 0, \tag{3.45}$$

where $C(\alpha, \Omega)$ is the constant from the bound on $\|(z^0)_{\lambda(\tau)}\|_{1,\infty}$. In other words, $\lambda(\tau)$ blows-up sufficiently slow. After performing a time discretization of $[0, T]$, where $k \in \{1, \dots, N\}$, $N \in \mathbb{N}$ and $\tau = T/N$, the regularised discrete problem reads as follows.

$$z_\tau^0 = (z^0)_{\lambda(\tau)}, \tag{3.46a}$$

$$y_\tau^0 \text{ minimizes } y \mapsto \mathcal{E}(0, y, z_\tau^0) + \mathcal{H}_\tau(z_\tau^0) \tag{3.46b}$$

$$y_\tau^k \text{ minimizes } y \mapsto \mathcal{E}(k\tau, y, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) \tag{3.46c}$$

$$z_\tau^k \text{ minimizes } z \mapsto \mathcal{E}(k\tau, y_\tau^k, z) + \mathcal{H}_\tau(z) + \mathcal{R}(z - z_\tau^{k-1}). \tag{3.46d}$$

We postpone the study of existence of solutions to (3.46) to the next subsection and proceed by showing the properties of discrete solutions. The next lemma show that, provided these solution exists, then they satisfy standard uniform energy estimates.

Lemma 3.5 (Discrete Solution)**.** *Let* $\operatorname{Dom}\mathcal{E} = [0,T]\times\mathcal{Y}\times Z$*,* (3.39) *hold, and* $z^0 \in Z$*. Then any solution of the problem* (3.46) *satisfies for all* $k \in \{1,\dots,N\}$ *the discrete (semi)-stability and energy inequality*

$$\forall\tilde{y}: \quad \mathcal{E}(k\tau, y_\tau^k, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) \le \mathcal{E}(k\tau, \tilde{y}, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}), \tag{3.47}$$

$$\forall\tilde{z}: \quad \mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) \le \mathcal{E}(k\tau, y_\tau^k, \tilde{z}) + \mathcal{H}_\tau(\tilde{z}) + \mathcal{R}(\tilde{z} - z_\tau^k), \tag{3.48}$$

$$\begin{aligned}&\mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1})\\ &\qquad \le \mathcal{E}((k-1)\tau, y_\tau^{k-1}, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) + \int_{(k-1)\tau}^{k\tau} \partial_t\mathcal{E}(t, y_\tau^{k-1}, z_\tau^{k-1})\,\mathrm{d}t.\end{aligned} \tag{3.49}$$

In addition, we have the uniform estimate

$$\begin{aligned}&\mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) + C^0 + \sum_{j=1}^{k} \mathcal{R}(z_\tau^j - z_\tau^{j-1})\\ &\qquad \le (\mathcal{E}(0, y_\tau^0, z_\tau^0) + \mathcal{H}_\tau(z_\tau^0) + C^0)\mathrm{e}^{\Lambda(k\tau)}.\end{aligned} \tag{3.50}$$

Proof. The discrete (semi)-stability is a direct consequence of (3.46c) and (3.46d), respectively. Further, testing (3.46d) by z_τ^{k-1}, then (3.46c) by y_τ^{k-1}, and finally integrating in time (thanks to the absolute continuity of $\mathcal{E}(\cdot, y, z)$ implied by (3.41)) yield

$$\begin{aligned}&\mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1})\\ &\quad \le \mathcal{E}(k\tau, y_\tau^k, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) \le \mathcal{E}(k\tau, y_\tau^{k-1}, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1})\\ &\quad = \mathcal{E}((k-1)\tau, y_\tau^{k-1}, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) + \int_{(k-1)\tau}^{k\tau} \partial_t\mathcal{E}(t, y_\tau^{k-1}, z_\tau^{k-1})\,\mathrm{d}t.\end{aligned}$$

Finally, the former estimate combined with (3.40) implies (note that $\mathcal{H}_\tau$ does not depend on t and hence we may apply the inequality also for $(\mathcal{E}+\mathcal{H}_\tau)$)

$$\begin{aligned}&\mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) + C^0 + \mathcal{R}(z_\tau^k - z_\tau^{k-1})\\ &\qquad \le \mathcal{E}(k\tau, y_\tau^k, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) + C^0\\ &\qquad \le (\mathcal{E}((k-1)\tau, y_\tau^{k-1}, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1}) + C^0)\mathrm{e}^{\Lambda(k\tau)-\Lambda((k-1)\tau)}.\end{aligned}$$

Since $\mathcal{R}(z_\tau^k - z_\tau^{k-1}) \ge 0$ and for $k \in \{0,\dots,N\}$ we have $\mathcal{E}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{H}_\tau(z_\tau^k) < +\infty$, the desired estimates follows by induction; see e.g. Francfort and Mielke [2006] or [Mielke and Roubíček, 2015, Thm 2.1.5] for details. □

The discrete stability for arbitrary time $t \in [0,T]$ will be proven in terms of piecewise constant in-time interpolants. We collect the main definitions below. For $(k-1)\tau \le t < k\tau$ we define the right-continuous piecewise constant interpolants

$$\underline{z}_\tau(t) := z_\tau^{k-1}, \qquad \underline{y}_\tau(t) := y_\tau^{k-1}, \tag{3.51}$$

while the left-continuous piecewise constant are defined for $(k-1)\tau < t \le k\tau$ as

$$\bar{z}_\tau(t) := z_\tau^k, \qquad \bar{y}_\tau(t) := y_\tau^k \qquad \bar{\mathcal{E}}_\tau(t,y,z) := \mathcal{E}(k\tau, y, z). \tag{3.52}$$

Note that the interpolants are related by

$$\underline{y}_\tau(t+\tau) = \bar{y}_\tau(t), \quad \text{for any } t \in I \text{ not belonging to the partition,} \tag{3.53}$$

but they coincide at the nodes, i.e.

$$\underline{y}_\tau(t) = \bar{y}_\tau(t) \quad \text{for any } t = k\tau \in I, k \in \mathbb{N},$$

where they differ only by their left/right continuity. The same holds for $\underline{z}_\tau$ and $\bar{z}_\tau$. For notational convenience, we introduce the quantity

$$\underline{\theta}_\tau(t) := \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t)),$$

which will arise in the energy inequality, and its analogue

$$\bar{\theta}_\tau(t) := \partial_t \mathcal{E}(t, \bar{y}_\tau(t), \bar{z}_\tau(t)),$$

depending on the left-continuous interpolants. Eventually, we define the pointwise limit

$$\bar{\theta}^{\sup}(t) := \limsup_{\tau \to 0} \bar{\theta}_\tau(t).$$

In the next lemma we show that these interpolants satisfy the standard discrete (semi)-stability, energy inequality and uniform estimates.

Lemma 3.6 (Interpolated Solution)**.** *Let the hypothesis of Lemma 3.5 and* (3.43) *hold. Then the interpolants satisfy for all $t \in [0,T]$ and all $0 \le t_1 < t_2 \le T$ of the form $t_1 = k_1\tau$ and $t_2 = k_2\tau$ with $k_1, k_2 \in \mathbb{N}$*

$$\bar{z}_\tau(0) = \underline{z}_\tau(0) = (z^0)_{\lambda(\tau)}, \tag{3.54}$$

$$\forall \tilde{y} \in \mathcal{Y}: \quad \bar{\mathcal{E}}_\tau(t, \bar{y}_\tau(t), \underline{z}_\tau(t)) \le \bar{\mathcal{E}}_\tau(t, \tilde{y}, \underline{z}_\tau(t)), \tag{3.55}$$

$$\forall \tilde{z} \in Z: \quad \bar{\mathcal{E}}_\tau(t, \bar{y}_\tau(t), \bar{z}_\tau(t)) + \mathcal{H}_\tau(\bar{z}_\tau(t)) \le \bar{\mathcal{E}}_\tau(t, \bar{y}_\tau(t), \tilde{z}) + \mathcal{H}_\tau(\tilde{z}) + \mathcal{R}(\tilde{z} - \bar{z}_\tau(t)), \tag{3.56}$$

$$\begin{aligned} &\bar{\mathcal{E}}_\tau(t_2, \bar{y}_\tau(t_2), \bar{z}_\tau(t_2)) + \mathcal{H}_\tau(\bar{z}_\tau(t_2)) + \mathrm{Diss}_{\mathcal{R}}(\bar{z}_\tau; [t_1, t_2]) \\ &\quad \le \bar{\mathcal{E}}_\tau(t_1, \bar{y}_\tau(t_1), \bar{z}_\tau(t_1)) + \mathcal{H}_\tau(\bar{z}_\tau(t_1)) + \int_{t_1}^{t_2} \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t)) \,\mathrm{d}t. \end{aligned} \tag{3.57}$$

Moreover, for every $t \in [0,T]$ either of the interpolants*, denoted here by $(\hat{y}_\tau, \hat{z}_\tau)$, satisfy the uniform estimates*

$$\begin{aligned} &\mathcal{E}(t, \hat{y}_\tau(t), \hat{z}_\tau(t)) + \mathcal{H}_\tau(\hat{z}_\tau(t)) + C^0 + \mathrm{Diss}_{\mathcal{R}}(\hat{z}_\tau; [0,t]) \\ &\quad \le \mathrm{e}^{\Lambda(t)}(\mathcal{E}(0, y_\tau^0, z_\tau^0) + \mathcal{H}_\tau(z_\tau^0) + C^0) \le \mathrm{e}^{\Lambda(t)}(\mathcal{E}(0, y^0, z_\tau^0) + \mathcal{H}_\tau(z_\tau^0) + C^0). \end{aligned}$$

Finally, if for every $y \in \mathcal{Y}$ the energy $\mathcal{E}(0, y, \cdot)$ is strongly continuous on Z

$$\mathrm{e}^{\Lambda(t)}(\mathcal{E}(0, y^0, z_\tau^0) + \mathcal{H}_\tau(z_\tau^0) + C^0) \to \mathrm{e}^{\Lambda(t)}(\mathcal{E}(0, y^0, z^0) + C^0) < +\infty \tag{3.58}$$

as $\tau \to 0$, for every $t \in [0,T]$.

Proof. The stability follows directly by Lemma 3.5 and the definition of the interpolants, the regularizing term $\mathcal{H}_\tau(\underline{z}_\tau(t))$ is finite and cancels. For the semi-stability we further use the triangular inequality for $\mathcal{R}$. Further, for the uniform estimate for arbitrary $t \in [0,T]$ we need to exploit (3.41) once more; see Francfort and Mielke [2006]. Finally, the convergence of the energy associated to the initial condition follows by the strong convergence of the truncated initial condition, with respect to which the energy is continuous, and by the choice of the truncation parameter (3.45). □

3.5.2 Existence of Discrete Solutions

Let us move to proving the existence of discrete solutions defined in Subsection 3.5.1. We first show that existence of solutions is guaranteed in the setting described in Subsection 3.4. Then we prove the existence of the discrete solution under relaxed assumptions that does not include coercivity in $\nabla^2 y$, which is necessary only for the limit passages.

Lemma 3.7 (Existence of Discrete Solutions - Second Gradient)**.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Assume that the damage function $\gamma : \mathbb{R} \to (0, +\infty)$ is continuous, and that the stored energy density $W : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3} \to [0, +\infty)$ is continuous in its first argument, is convex in its second argument, and satisfies the coercivity condition* (3.32)*, with $p > 3$. Assume also that $\phi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is convex, and that the dissipation potential $\mathcal{R} : L^1(\Omega) \to [0, +\infty]$ is lower semi-continuous with respect to the $L^1(\Omega)$ norm topology. Further, let $\partial\Omega = \Gamma_D \cup \Gamma_N$ be a measurable partition, with Γ_D having a positive two dimensional Hausdorff measure. Finally, let $k\tau \in [0, T]$, $y_\tau^k \in \mathcal{Y}$, and $z_\tau^{k-1} \in Z$, and assume that the coercivity condition* (3.33) *is satisfied. Under the further assumption that the functional $y \mapsto -\ell(k\tau, y, z_\tau^{k-1})$ is lower semi-continuous with respect to the weak topology on $W^{2,p}(\Omega)$, and that the functional $z \mapsto -\ell(k\tau, y_\tau^k, z)$ is lower semi-continuous with respect to the weak topology on $W^{1,\alpha}(\Omega)$, then, the functional*

$$\begin{aligned}\mathcal{G}(z) &:= \mathcal{E}(k\tau, y_\tau^k, z) + \mathcal{H}_\tau(z) + \mathcal{R}(z - z_\tau^{k-1})\\ &= \int_\Omega \left(\gamma(z) W(\nabla y_\tau^k, \nabla^2 y_\tau^k) + \phi\left((\nabla y_\tau^k)^{-\top} \nabla z\right) + \tau^\kappa |\nabla z|^\beta\right) \mathrm{d}x - \ell(k\tau, y_\tau^k, z)\\ &\quad + \mathcal{R}(z - z_\tau^{k-1})\end{aligned}$$

has a minimizer $z_\tau^k \in Z$, and the functional

$$\begin{aligned}&\mathcal{F}(y) := \mathcal{E}(k\tau, y, z_\tau^{k-1}) + \mathcal{H}_\tau(z_\tau^{k-1})\\ &= \int_\Omega \left(\gamma(z_\tau^{k-1}) W(\nabla y, \nabla^2 y) + \phi\left((\nabla y)^{-\top} \nabla z_\tau^{k-1}\right) + \tau^\kappa |\nabla z^{k-1}|^\beta\right) \mathrm{d}x - \ell(k\tau, y, z_\tau^{k-1})\end{aligned}$$

has a minimizer $y_\tau^k \in \mathcal{Y}$ which is injective almost everywhere in Ω. If moreover $p > 6$ and $s > 2p/(p-6)$, then the minimizer is injective everywhere *in Ω.*

Proof. The existence of a global minimizer follows by the direct method, while the injectivity is assured by (3.25) and (3.26). Note that for $p > 3$ we have $(\nabla y_\tau^k)^{-\top} \in L^\infty$ together with its pointwise convergence and hence Fatou's lemma yields the desired inequality. □

Now we proceed by proving existence of discrete solutions in the case when the elastic energy density satisfies weaker growth assumptions than in Lemma 3.7. Namely we suppose $W(\nabla y, \nabla^2 y) = W_{\mathrm{d}}(\nabla y)$, i.e. no coercivity in higher-order derivatives of the deformations is assumed. We hence switch to state space $\mathcal{Q}_{\mathrm{d}}$, defined as

$$\mathcal{Q}_{\mathrm{d}} := \{(y, z) \in \mathcal{Y}_{\mathrm{d}} \times Z_{\mathrm{d}} : \operatorname{Cof} \nabla y \nabla z \in L^\alpha(\Omega)\} \subset \mathcal{Y}_{\mathrm{d}} \times Z_{\mathrm{d}},$$

with

$$\begin{aligned}\mathcal{Y}_{\mathrm{d}} := \{&y \in W^{1,p}(\Omega, \mathbb{R}^3) : \operatorname{Cof} \nabla y \in L^q(\Omega), \det \nabla y \in L^r(\Omega),\\ &(\det \nabla y)^{-1} \in L^s(\Omega), \det \nabla y > 0 \text{ a.e. in } \Omega, (3.25) \text{ holds}\},\end{aligned}$$

and

$$Z_{\mathrm{d}} := \{z \in W^{1,1}(\Omega) : 0 \le z \le 1 \text{ a.e. in } \Omega\},$$

and replace the energy functional $\mathcal{E}$ by

$$\mathcal{E}_{\mathrm{d}}(t, y, z) := \int_\Omega \left(\gamma_{\mathrm{d}}(z) W_{\mathrm{d}}(\nabla y) + \phi_{\mathrm{d}}\left(\operatorname{Cof} \nabla y \nabla z\right)\right) \mathrm{d}x - \ell_{\mathrm{d}}(t, y, z). \tag{3.59}$$

In the definition in (3.59) we suppose that

$$\gamma_{\mathrm{d}} \in C(\mathbb{R}) \text{ and positive}, \tag{3.60}$$

and that the energy density $W_{\mathrm{d}} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is polyconvex and satisfies the following coercivity assumptions

$$W_{\mathrm{d}}(F) \ge c(|F|^p + |\operatorname{Cof} F|^q + (\det F)^r + (\det F)^{-s} - 1), \tag{3.61}$$

for every $F \in \mathbb{R}^{3\times 3}$, for $p, q, r > 1$ and $s \ge 0$. Further, we assume that

$$\phi_{\mathrm{d}}(u) \ge c(|u|^\alpha - 1), \tag{3.62}$$

for every $u \in \mathbb{R}^3$, and that the nonlinear loading satisfies

$$\begin{aligned} -\ell_{\mathrm{d}}(t, y, z) \ge c \Big(\Big| \int_{\Gamma_D} y \, \mathrm{d}\mathcal{H}^2 \Big| - \|\nabla y\|_p^{\tilde p} - \|\operatorname{Cof} \nabla y\|_q^{\tilde q} - \|\det \nabla y\|_r^{\tilde r} \\ - \|(\det \nabla y)^{-1}\|_s^{\tilde s} - \|\operatorname{Cof} \nabla y \nabla z\|_\alpha^{\tilde\alpha} - 1 \Big), \end{aligned} \tag{3.63}$$

for every $(y, z) \in \mathcal{Q}_{\mathrm{d}}$, for $0 \le \tilde p < p$, $0 \le \tilde q < q$, $0 \le \tilde r < r$, $0 \le \tilde s < s$, and $0 \le \tilde\alpha < \alpha$.

Having defined the system $(\mathcal{Q}_{\mathrm{d}}, \mathcal{E}_{\mathrm{d}}, \mathcal{R})$ we are now ready to state the two existence result to the discrete problem (3.46c) and (3.46d).

Lemma 3.8 (Existence of Discrete Solutions - Deformation)**.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, let $\gamma_{\mathrm{d}} : \mathbb{R} \to (0, +\infty)$ specify the incomplete damage, and let the stored energy density $W_{\mathrm{d}} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be polyconvex and satisfy the coercivity assumption* (3.61) *with $p \ge 2$, $q > p/(p-1)$, $r > 1$, $s \ge 1$. Let also $\phi_{\mathrm{d}} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be convex, and satisfy the coercivity condition* (3.62)*, where α is such that $1/p + 1/s + 1/\alpha \le (q-1)/q$. Let $\partial\Omega = \Gamma_D \cup \Gamma_N$ be a measurable partition, with Γ_D having a positive two dimensional Hausdorff measure. Finally, let $k\tau \in [0, T]$ and $z_\tau^{k-1} \in Z_{\mathrm{d}}$ be such that there exists $\tilde y \in \mathcal{Y}_{\mathrm{d}}$ satisfying*

$$(\tilde y, z_\tau^{k-1}) \in \mathcal{Q}_{\mathrm{d}}, \qquad \mathcal{E}_d(k\tau, \tilde y, z_\tau^{k-1}) < +\infty, \tag{3.64}$$

and let the loading $y \mapsto -\ell_{\mathrm{d}}(k\tau, y, z_\tau^{k-1})$ be lower semi-continuous with respect to the weak product topology on $W^{1,p}(\Omega) \times L^q(\Omega) \times L^r(\Omega) \ni (y, \operatorname{Cof} \nabla y, \det \nabla y)$, and satisfy the coercivity condition (3.63)*.*

Then, the functional

$$\begin{aligned} \mathcal{F}_{\mathrm{d}}(y) := \mathcal{E}_d(k\tau, y, z_\tau^{k-1}) = \int_\Omega \left(\gamma_{\mathrm{d}}(z_\tau^{k-1}) W_{\mathrm{d}}(\nabla y) + \phi_{\mathrm{d}}(\operatorname{Cof} \nabla y \nabla z_\tau^{k-1})\right) \mathrm{d}x \\ - \ell_{\mathrm{d}}(k\tau, y, z_\tau^{k-1}) \end{aligned}$$

has a minimizer $y_\tau^k \in \mathcal{Y}_{\mathrm{d}}$ such that

$$(y_\tau^k, z_\tau^{k-1}) \in \mathcal{Q}_{\mathrm{d}}, \qquad \mathcal{E}_d(k\tau, y_\tau^k, z_\tau^{k-1}) < +\infty.$$

If $p > 3$, then the minimizer is injective almost everywhere in Ω. If $p > 6$ and $s > 2p/(p-6)$, then the minimizer is injective everywhere *in Ω.*

Proof. Since $\gamma_{\rm d}(z_\tau^{k-1}) > 0$, by the growth assumptions in (3.63), we need to address only the coercivity and lower-semicontinuity of the $\phi_{\rm d}$ term. The remaining part of the proof would then follow from standard results on polyconvex energies; see e.g. Ciarlet [1988]. Let $y_n \rightharpoonup y_\tau^k$ be a minimizing sequence for $\mathcal{F}_{\rm d}$ which thanks to (3.64) has finite energy. By the coercivity of $\phi_{\rm d}$ we may further suppose that there exists $f \in L^\alpha(\Omega)$ such that, up to extracting not relabelled subsequences,

$$\operatorname{Cof} \nabla y_n \nabla z_\tau^{k-1} \rightharpoonup f \quad \text{in } L^\alpha(\Omega).$$

Since $\phi_{\rm d}$ is convex and finite, the corresponding part of $\mathcal{E}$ is weakly lower semicontinuous with respect to the weak convergenc in L^α, and hence it remains to identify the limit $f \in L^\alpha(\Omega)$. Thanks to the estimate

$$|\nabla z_\tau^{k-1}| \le C \left| \frac{\nabla y_n^\top}{\det \nabla y_n} \right| |\operatorname{Cof} \nabla y_n \nabla z_\tau^{k-1}| \le \frac{C}{\det \nabla y_n} |\nabla y_n| |\operatorname{Cof} \nabla y_n \nabla z_\tau^{k-1}|, \tag{3.65}$$

and the choice of p, s, and α we have $\nabla z_\tau^{k-1} \in L^{q'}(\Omega)$, since the right-hand side is bounded by the coercivity of $W_{\rm d}$ and $\phi_{\rm d}$. Therefore, for every $\psi \in L^\infty(\Omega)$ we may choose $\varphi := \psi \otimes \nabla z_\tau^{k-1}$ as a test function for the weak convergence $\operatorname{Cof} \nabla y_n \rightharpoonup \operatorname{Cof} \nabla y_\tau^k$ in $L^q(\Omega)$, which yields

$$f = \operatorname{Cof} \nabla y_\tau^k \nabla z_\tau^{k-1} \in L^\alpha(\Omega).$$

This completes the proof of the lemma. □

Remark 3.9. *Let us explain how the assumptions on the exponents p, q, s, and α interact. Normally the existence of minimizers for polyconvex energies is known even for $q \ge p/(p-1)$, i.e. $(q-1)/q \ge 1/p$. However, due to the requirements on α, we have $1/p < 1/p + 1/s + 1/\alpha \le (q-1)/q$. Therefore, for smaller values of s or α, larger values of q are needed.*

Lemma 3.10 (Existence of Discrete Solutions - Damage)**.** *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Assume that the damage function $\gamma_{\rm d} : \mathbb{R} \to (0, +\infty)$ is continuous, and let the stored energy density $W_{\rm d} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be bounded from below. Let $\phi_{\rm d} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ be convex, and satisfy the coercivity condition* (3.62)*, with α such that $1/p + 1/s \le (\alpha - 1)/\alpha$. Eventually, let the dissipation potential $\mathcal{R} : L^1(\Omega) \to [0, +\infty]$ be lower semi-continuous with respect to the strong L^1-topology. Let $k\tau \in [0, T]$, $y_\tau^k \in \mathcal{Y}_{\rm d}$, and $z_\tau^{k-1} \in Z_{\rm d}$ be such that there exists $\tilde z \in Z_{\rm d}$ satisfying*

$$(y_\tau^k, \tilde z) \in \mathcal{Q}_{\rm d}, \qquad \mathcal{E}_{\rm d}(k\tau, y_\tau^k, \tilde z) + \mathcal{R}(\tilde z - z_\tau^{k-1}) < +\infty. \tag{3.66}$$

Let the loading $z \mapsto -\ell(k\tau, y_\tau^k, z)$: be lower semi-continuous with respect to the weak $W^{1,1}$-topology, and satisfy the coercivity condition (3.63)*. Then, the functional*

$$\begin{aligned} \mathcal{G}_{\rm d}(z) &:= \mathcal{E}_{\rm d}(k\tau, y_\tau^k, z) + \mathcal{R}(z - z_\tau^{k-1}) \\ &= \int_\Omega \left(\gamma_{\rm d}(z) W_{\rm d}(\nabla y_\tau^k) + \phi_{\rm d}(\operatorname{Cof} \nabla y_\tau^k \nabla z) \right) \mathrm{d}x - \ell_{\rm d}(k\tau, y_\tau^k, z) + \mathcal{R}(z - z_\tau^{k-1}) \end{aligned}$$

has a minimizer $z_\tau^k \in Z_{\rm d}$ such that

$$(y_\tau^k, z_\tau^k) \in \mathcal{Q}_{\rm d}, \qquad \mathcal{E}_{\rm d}(k\tau, y_\tau^k, z_\tau^k) + \mathcal{R}(z_\tau^k - z_\tau^{k-1}) < +\infty.$$

Proof. Let $\{z_n\}$ be a minimizing sequence for $\mathcal{G}$. We first observe that, thanks to (3.66), $\{z_n\}$ has finite energy. By the continuity of $\gamma_{\rm d}$ and by the boundedness of $W_{\rm d}$ from below we have

$$\int_\Omega \gamma_{\rm d}(z_n) W_{\rm d}(\nabla y_\tau^k)\,{\rm d}x \geq -c\mathcal{L}(\Omega) \max_{z\in[0,1]} \gamma_{\rm d}(z) > -\infty.$$

Since $\mathcal{R} \geq 0$, we infer from the coercivity assumptions on $\phi_{\rm d}$ and $\ell_{\rm d}$ that $\operatorname{Cof} \nabla y_\tau^k \nabla z_n$ is bounded in $L^\alpha(\Omega)$. Since $\{z_n\}$ is bounded in $L^\infty(\Omega)$ by the definition of $Z_{\rm d}$, up to subsequences we deduce

$$\begin{aligned} \operatorname{Cof} \nabla y_\tau^k \nabla z_n &\rightharpoonup f \quad \text{in } L^\alpha(\Omega), \\ z_n &\rightharpoonup^* z_\tau^k \quad \text{in } L^\infty(\Omega), \end{aligned}$$

for some $f \in L^\alpha(\Omega)$ and $z_\tau^k \in L^\infty(\Omega)$.

To conclude, we need to characterize the limit f, and to show that ∇z_τ^k is $L^1(\Omega)$. Thanks to the choice of p, s, and α, the bound

$$|(\operatorname{Cof} \nabla y_\tau^k)^{-T}| \leq \frac{|\nabla y_\tau^k|}{\det \nabla y_\tau^k}$$

guarantees that for an arbitrary $\psi \in L^\infty(\Omega)$ we have $\varphi := (\operatorname{Cof} \nabla y_\tau^k)^{-\top} \psi \in L^{\alpha'}(\Omega)$. Hence, we obtain

$$\nabla z_n \rightharpoonup (\operatorname{Cof} \nabla y_\tau^k)^{-1} f \quad \text{in } L^1(\Omega).$$

Since also $z_n \rightharpoonup z_\tau^k$ in $L^1(\Omega)$, we have by the definition of the distributional gradient

$$\nabla z_\tau^k = (\operatorname{Cof} \nabla y_\tau^k)^{-1} f \in L^1(\Omega),$$

which in turn provides an identification of f. As a by product we have also obtained, for a suitable (not relabeled) subsequence, that the following convergences hold true

$$z_n \rightharpoonup z_\tau^k \quad \text{in } W^{1,1}(\Omega), \qquad z_n \to z_\tau^k \quad \text{in } L^{\hat\alpha}(\Omega), \qquad z_n \to z_\tau^k \quad \text{a.e. in } \Omega,$$

for every $1 \leq \hat\alpha < 3/2$, which follows by the compact embedding $W^{1,1}(\Omega) \Subset L^{\hat\alpha}(\Omega)$.

To conclude the proof it remains to show the lower semi-continuity of the functional $\mathcal{G}_{\rm d}(z)$ with respect to these convergences. The lower semicontinuity of the first term is ensured by the continuity of $\gamma_{\rm d}$ and by Fatou's lemma. For the second term, we deduce it arguing as in Lemma 3.8. Finally, the loading ℓ and the dissipation potential $\mathcal{R}$ are lower semi continuous with respect to the given convergences by assumption. □

Remark 3.11. *Note that here small values of p or s imply large values of α, and hence in turn, recalling Remark 3.9, of q.*

We close this subsection by observing that the assumptions of these lemmata are fulfilled for the problem (3.46), provided the initial condition is energetically stable. For $k = 1$, in fact, we can choose $\tilde y := y^0$ and $\tilde z := (z_0)_{\lambda(\tau)}$ because the domain of $\mathcal{E}$ is independent of time and $\mathcal{R}(0) = 0$. The same conclusion holds for every larger k arguing by induction.

3.5.3 Selection of Subsequences

Having proven the existence of time discrete solution we may proceed with analyzing the compactness properties of the sequences of the time-interpolants (3.51) and (3.52) as the time-step τ converges to zero. First, from the uniform estimate (3.58) and the coercivity of $\mathcal{E}$ and $\mathcal{R}$ we deduce the following convergence result for the piecewise constant interpolants. Let us recall that although the weak* limits of the left- and right-continuous interpolants coincide in the appropriate Bochner product space (see [Roubíček, 2013, proof of Thm. 8.9] which works also for piece-wise constant interpolants), the pointwise-in-time limits $\underline{y}(t)$ and $\bar{y}(t)$ of the t-dependent subsequences may differ in general.

Lemma 3.12 (Compactness I)**.** *Let the hypothesis of Lemma 3.5, 3.6, and 3.7 be satisfied. Further, let $\phi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ satisfy the coercivity and growth condition* (3.31) *with $\alpha > 1$. Let $\partial\Omega = \Gamma_D \cup \Gamma_N$ be a measurable partition, with Γ_D having a positive two dimensional Hausdorff measure and let the loading $(t, y, z) \mapsto -\ell(t, y, z)$: satisfy the coercivity condition* (3.33)*. Finally, let the dissipation potential $\mathcal{R} : L^1(\Omega) \to [0, +\infty]$ define an extended quasi-metric, i.e. assume that* (3.43) *and* (3.44) *hold. Then, we have the following uniform bounds*

$$\begin{aligned}
\|\bar{y}_\tau\|_{L^\infty((0,T),W^{2,p}(\Omega))} &\le C, & \|(\det \nabla \bar{y}_\tau)^{-1}\|_{L^\infty((0,T),L^s(\Omega)))} &\le C,\\
\|\bar{z}_\tau\|_{L^\infty((0,T),L^\infty(\Omega))} &\le C, & \|(\nabla \bar{y}_\tau)^{-\top}\nabla \bar{z}_\tau\|_{L^\infty((0,T),L^\alpha(\Omega))} &\le C,\\
\mathrm{Var}_{L^1}(\bar{z}_\tau; [0,T]) &\le C & \|\nabla \bar{z}_\tau\|_{L^\infty((0,T),L^\alpha(\Omega))} &\le C,\\
\|\bar{\theta}_\tau\|_{L^1(0,T)} &\le C, & \|\underline{\theta}_\tau\|_{L^1(0,T)} &\le C,
\end{aligned}$$

where $\{|\bar{\theta}_\tau|\}$ and $\{|\underline{\theta}_\tau|\}$ are equiintegrable. Up to a (not relabeled) subsequence, the following convergences of the piecewise interpolants associated to the internal variable hold true

$$\forall t \in [0,T]: \quad \bar{z}_\tau(t) \rightharpoonup^* z(t) \quad \text{and} \quad \underline{z}_\tau(t) \rightharpoonup^* \underline{z}(t) \quad \text{in } L^\infty(\Omega), \tag{3.67}$$

$$\nabla \bar{z}_\tau(t) \rightharpoonup \nabla z(t) \quad \text{and} \quad \nabla \underline{z}_\tau(t) \rightharpoonup \nabla \underline{z}(t) \quad \text{in } L^\alpha(\Omega). \tag{3.68}$$

The limiting map z satisfies $z, \underline{z} \in \mathrm{BV}([0,T]; L^1(\Omega)) \cap \mathrm{B}([0,T]; Z)$, and there exists an at most countable set $J \subset [0,T]$ such that

$$\forall t \in [0,T] \setminus J: \quad z(t) = \underline{z}(t). \tag{3.69}$$

The dissipations associated to the right-continuous piecewise constant interpolants of the internal variable fulfill

$$\forall t \in [0,T]: \quad \mathrm{Diss}_{\mathcal{R}}(\bar{z}_\tau, [0,t]) \to \delta(t). \tag{3.70}$$

The limiting map δ is such that $\delta \in \mathrm{BV}[0,T]$, and

$$\forall 0 \le t_1 < t_2 \le T: \quad \mathrm{Diss}_{\mathcal{R}}(z, [t_1, t_2]) \le \delta(t_2) - \delta(t_1). \tag{3.71}$$

The norms of the gradients of the interpolants of the internal variable satisfy

$$\|\nabla \bar{z}_\tau\|_{L^\alpha(\Omega;\mathbb{R}^{3\times 3})} \rightharpoonup^* \bar{f} \quad \text{and} \quad \|\nabla \underline{z}_\tau\|_{L^\alpha(\Omega;\mathbb{R}^{3\times 3})} \rightharpoonup^* \underline{f} \qquad \text{in } L^\infty(0,T), \tag{3.72}$$

for some $\bar{f}, \underline{f} \in L^\infty(0,T)$ *such that for almost every* $t \in (0,T)$

$$\underline{f} \geq \underline{f}^{inf}(t) := \liminf_{\tau \to 0} \|\nabla \underline{z}_\tau(t)\|_\alpha. \tag{3.73}$$

There exist $\bar{\theta}, \underline{\theta} \in L^1(0,T)$ *such that, up to a (not relabeled) subsequence,*

$$\underline{\theta}_\tau \rightharpoonup \underline{\theta} \quad \textit{and} \quad \bar{\theta}_\tau \rightharpoonup \bar{\theta} \qquad \textit{in } L^1(0,T). \tag{3.74}$$

Eventually, for the regularizing term we have the uniform bounds

$$\mathcal{H}_\tau(\bar{z}_\tau(t)) \leq C, \quad \textit{i.e.} \quad \int_\Omega |\nabla \underline{z}_\tau(t,x)|^\beta \,\mathrm{d}x \leq \frac{C}{\tau^\kappa} \tag{3.75}$$

for almost every $t \in (0,T)$.

Proof. For convenience of the reader, we subdivide the proof into three steps.

Step I: Uniform estimates. Since γ is positive and continuous, the uniform estimates on $\bar{y}_\tau$ and $\bar{z}_\tau$ are direct consequences of (3.58), the coercivity of ϕ (3.31), W (3.32), ℓ (3.33), and $\mathcal{R}$, and the definition of the space Z; see (3.24). Note that

$$|\nabla \bar{z}_\tau| \leq C|\nabla \bar{y}_\tau^\top||(\nabla \bar{y}_\tau)^{-\top} \nabla \bar{z}_\tau|,$$

and that thanks to the embedding of $W^{2,p}(\Omega)$ into $C(\bar{\Omega})$ for $p > 3$, we have that $\{\nabla \bar{y}_\tau^\top\}$ is uniformly bounded in $L^\infty((0,T), L^\infty(\Omega))$. Using again the coercivity of ϕ (3.31), we thus obtain the boundedness of $\{\nabla \bar{z}_\tau\}$ in $L^\infty((0,T), L^\alpha(\Omega))$.
Finally, the equi-integrability of $\bar{\theta}_\tau$ and $\underline{\theta}_\tau$, as well as the corresponding uniform bounds, follow by (3.39), (3.41) and (3.58). Indeed, for either of the interpolants, denoted $\hat{\theta}$, we have

$$\begin{aligned} |\hat{\theta}_\tau(t)| &= |\partial_t \mathcal{E}(t, \hat{y}_\tau(t), \hat{z}_\tau(t))| \leq \lambda(t)(\mathcal{E}(t, \hat{y}_\tau(t), \hat{z}_\tau(t)) + C^0) \\ &\leq \lambda(t) \mathrm{e}^{\Lambda(t)} (\mathcal{E}(0, y^0, z^0) + C^0 + 1), \end{aligned}$$

provided $\tau > 0$ is sufficiently small.

Step II: Selection of sub-sequences. By the convexity and positive 1-homogeneity of $\mathcal{R}$ we know it satisfies the triangle inequality, and since it is also non-negative, zero at the origin and coercive in the $L^1(\Omega)$ norm, it defines an extended quasi-distance. In view of its lower semi-continuity with respect to the strong $L^1(\Omega)$ convergence, we deduce that $\mathcal{R}$ is weakly lower semi-continuous in the $L^1(\Omega)$ topology. Finally, functions $z : \Omega \to [0,1]$ form a compact subset of $L^\infty(\Omega)$ in the weak* topology and thanks to the uniform bounds proven in Step I, the sequence $\{\bar{z}_\tau\}$ is also weakly compact in $W^{1,\alpha}$ for almost every t. We hence may apply the generalized Helly's selection principle from Mielke and Roubíček [2015] to obtain a subsequence $\{\bar{z}_\tau\}$, not relabeled, satisfying (3.67) - (3.71).
Further, the convergence properties of $\{\underline{z}_\tau\}$, as well as the equality of z and $\underline{z}$ almost everywhere in $[0,T]$ follow from the fact that $\bar{z}_\tau - \underline{z}_\tau \to 0$ in $L^1((0,T), L^1(\Omega))$; see Roubíček [2015]. As both z and $\underline{z}$ are in $\mathrm{BV}([0,T]; L^1(\Omega))$ they may differ only at discontinuity points which form an at most countable subset of $[0,T]$.
Finally, the compactness for $\|\bar{z}_\tau(t)\|_\alpha$, $\|\bar{z}_\tau(t)\|_\alpha$, $\bar{\theta}_\tau$, and $\underline{\theta}_\tau$ is straightforward from the estimates in Step I, while the inequality (3.73) follows by Fatou's lemma; for

a fixed test function on one side the weak convergence is used, while on the other the lower-semicontinuity of the integral, localizing the test functions around a given point yields the result.

Step III: Boundedness of the regularizing term. The bounds (3.75) follows directly from (3.28) and the uniform estimate (3.58). □

3.5.4 Improving Convergence of Internal Variable

Before selecting a t-dependent subsequence of $\{\bar{y}_\tau(t)\}$ we improve the convergence (3.68) first. The strong convergence for (almost) every $t \in [0,T]$ is needed for passing to the limit in the right-hand side of the energy inequality, and also for identifying the reduced power. Finally, we suppose for simplicity that the dissipation potential is finite, while possible generalizations are discussed afterwards.

Lemma 3.13 (Improved Convergence in z)**.** *Let the hypothesis of Lemma 3.12 hold. Further, let $W : \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3\times3} \to [0,+\infty)$ satisfy the coercivity condition (3.32), with $s \geq \frac{3p}{p-3}$. Let $\phi : \mathbb{R}^{3\times3} \to \mathbb{R}$ be strictly convex and satisfy the coercivity and growth condition (3.31), with $\alpha > 3$. Moreover, let the dissipation potential $\mathcal{R} : L^1(\Omega) \to [0,+\infty]$ be finite on $L^1(\Omega)$, i.e. $\operatorname{Dom}\mathcal{R} = L^1(\Omega)$, and be continuous with respect to the $L^1(\Omega)$ norm topology. Finally, let the loading functional $\ell : \mathbb{R} \times \mathcal{Y} \times Z \to \mathbb{R}$ be such that*

$$\forall \tilde{z}_\tau \to z(t) \text{ in } W^{1,\alpha}(\Omega): \quad \liminf_{\tau\to0} \left(\ell(k\tau, \bar{y}_\tau(t), \tilde{z}_\tau) - \ell(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t))\right) \geq 0.$$

Then,

$$\forall t \in [0,T]: \quad \bar{z}_\tau(t) \to z(t) \quad \text{in } W^{1,\alpha}(\Omega), \tag{3.76}$$

and there exists a (not relabeled) subsequence such that

$$\forall_{a.e.} t \in (0,T): \quad \underline{z}_\tau(t) \to z(t) \quad \text{in } W^{1,\alpha}(\Omega). \tag{3.77}$$

Moreover, for the regularizing term we have

$$\forall t \in [0,T]: \quad \mathcal{H}_\tau(\bar{z}_\tau(t)) \to 0. \tag{3.78}$$

Proof. We first prove the strong convergence (3.76). Let $t \in [0,T]$ be given. Since we cannot use the limit $z(t) \in Z$ as a competitor in the discrete semi-stability (3.56), because it may not lie in $W^{1,\beta}(\Omega)$, we use its Lipschitz truncation $\tilde{z}_\tau := (z(t))_{\lambda(\tau)}$ instead. The dependence of the truncation parameter λ on the time step τ is chosen to blow up sufficiently slow, i.e.

$$\lim_{\tau\to0} \tau^\kappa \lambda^\beta(\tau) = 0. \tag{3.79}$$

This gives

$$\bar{\mathcal{E}}_\tau(t, \bar{y}_\tau(t), \bar{z}_\tau(t)) + \mathcal{H}_\tau(\bar{z}_\tau(t)) \leq \bar{\mathcal{E}}_\tau(t, \bar{y}_\tau(t), \tilde{z}_\tau(t)) + \mathcal{H}_\tau(\tilde{z}_\tau(t)) + \mathcal{R}(\tilde{z}_\tau(t) - \bar{z}_\tau(t)). \tag{3.80}$$

Thanks to this uniform bound, and to the coercivity assumptions in the statement of the lemma, we extract a t-dependent subsequence $\tau'(t) \to 0$ (*for ease of notation henceforth* **denoted by $\boldsymbol{\tau'}$**) for which

$$\bar{y}_{\tau'}(t) \rightharpoonup \xi(t) \qquad \text{in } W^{2,p}(\Omega), \tag{3.81}$$

$$(\nabla \bar{y}_{\tau'})^{-\top}(t)\nabla \bar{z}_{\tau'}(t) \rightharpoonup (\nabla \xi)^{-\top}(t)\nabla z(t) \qquad \text{in } L^{\alpha}(\Omega), \tag{3.82}$$

$$\mathcal{H}_{\tau'}(\bar{z}_{\tau'}(t)) \to E(t) \geq 0, \tag{3.83}$$

for some $\xi(t) \in \mathcal{Y}$. Subtracting from both sides of (3.80) the term $\int_\Omega \phi((\nabla\xi)^{-\top}(t)\nabla\tilde{z}_{\tau'})\,\mathrm{d}x$, which is finite thanks to the growth conditions, we obtain after a rearrangement

$$\begin{aligned}
&\int_\Omega \phi\left((\nabla \bar{y}_{\tau'}(t))^{-\top}\nabla\bar{z}_{\tau'}(t)\right) - \phi\left((\nabla\xi(t)^{-\top}\nabla\tilde{z}_{\tau'}\right)\mathrm{d}x + \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(t)) \qquad (3.84)\\
&\quad\leq \int_\Omega (\gamma(\tilde{z}_{\tau'}) - \gamma(\bar{z}_{\tau'}(t)))W(\nabla\bar{y}_{\tau'}(t), \nabla^2\bar{y}_{\tau'}(t))\,\mathrm{d}x\\
&\qquad + \mathcal{R}(\tilde{z}_{\tau'} - \bar{z}_{\tau'}(t))\\
&\qquad + \int_\Omega \phi\left((\nabla\bar{y}_{\tau'}(t))^{-\top}\nabla\tilde{z}_{\tau'}\right) - \phi\left((\nabla\xi(t))^{-\top}\nabla\tilde{z}_{\tau'}\right)\mathrm{d}x\\
&\qquad - \ell(k\tau', \bar{y}_{\tau'}(t), \tilde{z}_{\tau'}) + \ell(k\tau', \bar{y}_{\tau'}(t), \bar{z}_{\tau'}(t)) + \mathcal{H}_{\tau'}(\tilde{z}_{\tau'}),
\end{aligned}$$

where $k\tau' \searrow t$ as $\tau' \to 0$.

Since ϕ is convex and finite, we have that the first term on the left-hand side of (3.84) is lower semi-continuous with respect to the convergence (3.82) and hence together with the convergence of $\mathcal{H}_{\tau'}(\bar{z}_{\tau'}(t))$ in (3.83) we have

$$\begin{aligned}
&0 \leq E(t)\\
&\quad\leq \liminf_{\tau'\to 0} \int_\Omega \phi\left((\nabla\bar{y}_{\tau'})^{-\top}(t)\nabla\bar{z}_{\tau'}(t)\right) - \phi\left((\nabla\xi)^{-\top}(t)\nabla\tilde{z}_{\tau'}\right)\mathrm{d}x + \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(t)).
\end{aligned}$$

Concerning the right-hand side of (3.84), for the elastic energy from (3.81) and the growth assumptions on W (see (3.32)), we deduce

$$\begin{aligned}
&\int_\Omega (\gamma(\tilde{z}_{\tau'}) - \gamma(\bar{z}_{\tau'}(t)))W(\nabla\bar{y}_{\tau'}(t), \nabla^2\bar{y}_{\tau'}(t))\,\mathrm{d}x\\
&\quad\leq \|\gamma(\tilde{z}_{\tau'}) - \gamma(\bar{z}_{\tau'}(t))\|_\infty \int_\Omega W(\nabla\bar{y}_{\tau'}(t), \nabla^2\bar{y}_{\tau'}(t))\,\mathrm{d}x\\
&\quad\leq C\|\gamma(\tilde{z}_{\tau'}) - \gamma(\bar{z}_{\tau'}(t))\|_\infty \to 0.
\end{aligned}$$

The latter convergence follows from the uniform continuity of γ on the compact interval $[0,1]$ and the uniform convergence of $\tilde{z}_{\tau'} - \bar{z}_{\tau'}(t)$ to zero. This, in turn, is achieved by the strong convergence of the Lipschitz truncation and the weak convergence (3.68) of $\bar{z}_{\tau'}(t)$ in $W^{1,\alpha}(\Omega)$, both combined with the (compact) Sobolev embedding of $W^{1,\alpha}(\Omega)$ into $C(\bar{\Omega})$ for $\alpha > 3$.

Concerning the third term on the right-hand side of (3.84), the growth condition (3.31) for ϕ implies continuity with respect to the following convergences

$$\begin{aligned}
(\nabla\bar{y}_{\tau'})^{-\top}(t)\nabla\tilde{z}_{\tau'} &\to (\nabla\xi)^{-\top}(t)\nabla z(t) \quad \text{in } L^\alpha(\Omega),\\
(\nabla\xi)^{-\top}(t)\nabla\tilde{z}_{\tau'} &\to (\nabla\xi)^{-\top}(t)\nabla z(t) \quad \text{in } L^\alpha(\Omega),
\end{aligned}$$

which in turn hold thanks to the strong convergence of the Lipschitz truncation $\tilde{z}_{\tau'}$ and the weak convergence of $\bar{y}_{\tau'}$ (3.81). By the Cramer's rule,

$$(\nabla \bar{y}_{\tau'})^{-\top} = \frac{\operatorname{Cof} \nabla \bar{y}_{\tau'}}{\det \nabla \bar{y}_{\tau'}},$$

the compact embedding of $W^{2,p}(\Omega)$ into $C(\bar{\Omega})$ for $p > 3$, and Corollary (3.4), which for our uniform bounds on $\bar{y}(t)$ in $W^{2,p}(\Omega)$ and $(\det \nabla \bar{y}_{\tau'}(t))^{-1}$ in $L^s(\Omega)$ implies

$$\left\| \frac{1}{\det \nabla \bar{y}_{\tau'}} \right\|_{\infty} \leq C,$$

also uniformly with respect to τ, we obtain

$$(\nabla \bar{y}_{\tau'})^{-\top}(t) \to (\nabla \xi)^{-\top}(t) \quad \text{in } L^{\infty}(\Omega). \tag{3.85}$$

Since $\tilde{z}_{\tau'} \to z(t)$ strongly in $W^{1,\alpha}(\Omega)$ we have for the loading directly by the assumptions (originally formulated for $\liminf_{\tau' \to 0}$)

$$\limsup_{\tau' \to 0} \left(-\ell(k\tau', \bar{y}_{\tau'}(t), \tilde{z}_{\tau'}) + \ell(k\tau', \bar{y}_{\tau'}(t), \bar{z}_{\tau'}(t)) \right) \leq 0.$$

Finally, the regularization term on the right-hand side satisfies

$$\mathcal{H}_{\tau'}(\tilde{z}_{\tau'}) = (\tau')^{\kappa} \int_{\Omega} |\nabla \tilde{z}_{\tau'}|^{\beta} \, \mathrm{d}x \leq C\mathcal{L}^3(\Omega)(\tau')^{\kappa} \|\tilde{z}_{\tau'}\|_{1,\infty}^{\beta} \leq C\mathcal{L}^3(\Omega)(\tau')^{\kappa}\lambda^{\beta}(\tau') \to 0, \tag{3.86}$$

owing to (3.79).

Altogether we have

$$\limsup_{\tau' \to 0} \int_{\Omega} \phi\left((\nabla \bar{y}_{\tau'})^{-\top}(t) \nabla \bar{z}_{\tau'}(t) \right) - \phi\left((\nabla \xi)^{-\top}(t) \nabla z(t) \right) \mathrm{d}x \leq 0,$$

as well as $E(t) = 0$. Consequently we have the convergence

$$\int_{\Omega} \phi\left((\nabla \bar{y}_{\tau'})^{-\top}(t) \nabla \bar{z}_{\tau'}(t) \right) \mathrm{d}x \to \int_{\Omega} \phi\left((\nabla \xi)^{-\top}(t) \nabla z(t) \right) \mathrm{d}x.$$

By the strict convexity of ϕ it even holds (cf. Visintin [1984])

$$(\nabla \bar{y}_{\tau'})^{-\top}(t) \nabla \bar{z}_{\tau'}(t) \to (\nabla \xi)^{-\top}(t) \nabla z(t) \quad \text{in } L^{\alpha}(\Omega),$$

and since we also have $(\nabla \bar{y}_{\tau'})^{\top}(t) \to (\nabla \xi)^{\top}(t)$ in $L^{\infty}(\Omega)$ by (3.81), and by the compact embedding of $W^{2,p}(\Omega)$ into $C(\bar{\Omega})$ for $p > 3$, it also holds

$$\nabla \bar{z}_{\tau'}(t) \to \nabla z(t) \quad \text{in } L^{\alpha}(\Omega). \tag{3.87}$$

Since the same procedure applies to any subsequence $\tau' \to 0$, we deduce that the convergence holds for the full sequence $\{\bar{z}_{\tau}\}$.

To finish the proof, we need to show the strong convergence of $\{\underline{z}_{\tau}(t)\}$ in $W^{1,\alpha}(\Omega)$. Since for $1 < \alpha < +\infty$ the space $L^{\alpha}(\Omega)$ is uniformly elliptic, it suffices

to show the convergence of the norms of the gradients. Using the already proven strong convergence (3.76) and Lebesgue theorem we infer

$$\forall_{\text{a.e.}} t \in [0,T]: \quad \bar{f}(t) = \|\nabla z(t)\|_\alpha,$$

where $\bar{f}$ is the map introduced in (3.72). The weak convergence (3.68) implies

$$\forall t \in [0,T] \setminus J: \quad \|\nabla z(t)\|_\alpha \le \liminf_{\tau\to 0} \|\nabla \underline{z}_\tau(t)\|_\alpha = \underline{f}^{\inf}(t),$$

where we used the equality of the limits (3.69). Recalling (3.73) we have for almost every $t \in (0,T)$

$$\bar{f}(t) = \|\nabla z(t)\|_\alpha \le \underline{f}^{\inf}(t) \le \underline{f}(t). \tag{3.88}$$

The last step is to show the equality of $\bar{f}$ and $\underline{f}$ in $L^\infty(0,T)$. This is based on the relation (3.53) between the left- and right-continuous interpolants, holding almost everywhere in $(0,T)$. For any $\varphi \in L^1(0,T)$ we use the substitution $t = s+\tau$ and obtain

$$\begin{aligned}\int_0^T \|\nabla \underline{z}_\tau(t)\|_\alpha \varphi(t)\,\mathrm{d}t &\\ = \int_0^\tau \|\nabla \underline{z}_\tau(t)\|_\alpha \varphi(t)\,\mathrm{d}t + \int_0^T \|\nabla \bar{z}_\tau(s)\|_\alpha \chi_{(0,T-\tau)}(s)\varphi(s+\tau)\,\mathrm{d}s &\\ \to \int_0^T \bar{f}\varphi(s)\,\mathrm{d}s,&\end{aligned}$$

where the convergence follows by the absolute continuity of the Lebesgue integral and the strong continuity of translations in $L^1(0,T)$. Hence the inequalities in (3.88) are in fact equalities and we may apply [Francfort and Mielke, 2006, Lemma 3.5] to conclude that

$$\|\nabla \underline{z}_\tau\|_\alpha \to \|\nabla z\|_\alpha \quad \text{in } L^1(0,T).$$

In particular, there is a subsequence such that for almost every $t \in (0,T)$ we have $\|\nabla \underline{z}_\tau(t)\|_\alpha \to \|\nabla z(t)\|_\alpha$. □

Remark 3.14 (Unidirectional Damage)**.** *In the setting of unidirectional damage, for which* $\operatorname{Dom}\mathcal{R} = \{v \in L^1(\Omega) : v \le 0 \text{ a.e. in } \Omega\}$ *we can use a slight modification of the recovery sequence from Mielke and Roubíček [2006]*

$$\tilde{z}_\tau := \Big(z(t))_{\lambda(\tau)} - \|\underline{z}_\tau(t) - (z(t))_{\lambda(\tau)}\|_\infty\Big)^+ \to z(t) \quad \textit{in } W^{1,\alpha}(\Omega).$$

Since we need to have α strictly greater than dimension anyway, we unfortunately cannot profit from the recovery sequence from Thomas and Mielke [2010], which works for energetic solution even for any $\alpha > 1$.

3.5.5 Selection of t-Dependent Subsequences

Considering the subsequence $\tau \to 0$ identified in Lemma 3.13, and for which particularly (3.77) holds, we now select further t-dependent subsequences whose limits will define the solution $y(t) \in \mathrm{B}([0,T];\mathcal{Y})$. As in Francfort and Mielke [2006], only those subsequences which 'maximize in the limit' the reduced power $\bar{\theta}_\tau(t)$ are considered in this definition.

Lemma 3.15 (Compactness II - t-Dependent)**.** *Let the hypothesis of Lemma 3.13 be satisfied. Then for almost every $t \in (0,T)$*

$$\bar{\theta}(t) \le \bar{\theta}^{sup}(t) := \limsup_{\tau\to 0} \bar{\theta}_\tau(t), \tag{3.89}$$

and for all $t \in [0,T]$ there exists a t-dependent subsequence $\{\tau(t)\}$ such that

$$\bar{\theta}_{\tau(t)}(t) \to \bar{\theta}^{sup}(t), \tag{3.90}$$
$$\bar{y}_{\tau(t)}(t) \rightharpoonup y(t) \qquad \text{in } W^{2,p}(\Omega), \tag{3.91}$$

where $y \in \mathrm{B}([0,T];\mathcal{Y})$, and consequently

$$(\nabla \bar{y}_{\tau(t)})^{-\top}(t) \to (\nabla y)^{-\top}(t) \qquad \text{in } L^\infty(\Omega), \tag{3.92}$$
$$(\nabla \bar{y}_{\tau(t)})^{-\top}(t)\nabla \bar{z}_{\tau(t)}(t) \to (\nabla y)^{-\top}(t)\nabla z(t) \qquad \text{in } L^\alpha(\Omega). \tag{3.93}$$

Moreover, there exists a sequence $\{v_{\tau(t)}(t)\} \subset W^{1,\alpha}(\Omega)$ such that

$$\|v_{\tau(t)}(t)\|_{1,\infty} \le \frac{C(\alpha,\Omega,t)}{\tau(t)}, \tag{3.94}$$
$$\mathcal{L}^3(M_{\tau(t)}(t)) \le C(t)(\tau(t))^\alpha, \tag{3.95}$$
$$\{|\nabla v_{\tau(t)}(t)|^\alpha\} \text{ is equiintegrable}, \tag{3.96}$$

where $M_{\tau(t)}(t) := \{x \in \Omega : \underline{z}_{\tau(t)}(t) \neq v_{\tau(t)}(t) \text{ or } \nabla \underline{z}_{\tau(t)}(t) \neq \nabla v_{\tau(t)}(t)\}$.

Proof. The convergence (3.90) can be achieved by a proper choice of the subsequence. Thanks to the uniform estimates proven in Lemma 3.12, a further selection yields (3.91). To prove that $y(t) \in \mathcal{Y}$ we first observe that the weak convergence in $W^{2,p}(\Omega)$ in (3.91) yields pointwise convergence of $\det \nabla \bar{y}_{\tau(t)}(t)$. Hence the uniform energy bounds in Lemma 3.6, together with Fatou's lemma, imply

$$+\infty > \int_\Omega \frac{\mathrm{d}x}{(\det \nabla \bar{y}_{\tau(t)}(t))^s} \ge \int_\Omega \frac{\mathrm{d}x}{(\det \nabla y(t))^s},$$

i.e. $(\det \nabla y(t))^{-1} \in L^s(\Omega)$ and consequently $\det \nabla y(t) > 0$ a.e. in Ω. Second, we recall that the Ciarlet-Nečas condition is stable even under weak $W^{1,p}$ convergence; c.f. Ciarlet and Nečas [1987].

The strong convergence of $(\nabla \bar{y}_{\tau(t)})^{-\top}(t)$ in $L^\infty(\Omega)$ follows by the very same argument as in the proof of Lemma 3.13. The last convergence then follows easily from (3.76). The existence of the sequence $\{v_{\tau(t)}(t)\}$ is a consequence of Lemma A.3.

□

3.5.6 Improving Convergence of Elastic Variable

Now, in a similar manner as in Lemma 3.13, we improve the convergence of the elastic variable. Since it is not necessary to modify the competitor $\tilde{y} \in \mathcal{Y}$, the assumptions are slightly weaker. On the other hand, since we want the result to hold for all $t \in [0,T]$, we cannot rely on the strong convergence of $\underline{z}_\tau(t)$.

Lemma 3.16 (Convergence of the Elastic Energy)**.** *Let the hypothesis of Lemma 3.15 hold and for every $t \in [0,T]$ let $\{\tau(t)\}$ be the subsequence identified in Lemma 3.15. Further, let $W : \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3\times 3} \to [0,+\infty)$ satisfy the growth condition* (3.32)*. Let the loading functional $\ell : \mathbb{R} \times \mathcal{Y} \times Z \to \mathbb{R}$ be such that* $\liminf_{\tau\to 0} \left(\ell(k\tau, y(t), \underline{z}_\tau(t)) - \ell(k\tau, \bar{y}_\tau(t), \underline{z}_\tau(t))\right) \geq 0$.

Then, for all $t \in [0,T]$ we have

$$\int_\Omega \gamma(\underline{z}_{\tau(t)}(t)) W(\nabla \bar{y}_{\tau(t)}(t), \nabla^2 \bar{y}_{\tau(t)}(t))\,\mathrm{d}x \to \int_\Omega \gamma(\underline{z}(t)) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x, \tag{3.97}$$

and

$$\bar{y}_{\tau(t)}(t) \to y(t) \quad \text{in } W^{2,p}(\Omega). \tag{3.98}$$

In particular, for every $t \in [0,T]$

$$\int_\Omega \gamma(\bar{z}_{\tau(t)}(t)) W(\nabla \bar{y}_{\tau(t)}(t), \nabla^2 \bar{y}_{\tau(t)}(t))\,\mathrm{d}x \to \int_\Omega \gamma(z(t)) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x. \tag{3.99}$$

Proof. Let $t \in [0,T]$. *For ease of notation throughout this proof we will simply write* $\boldsymbol{\tau}$ **instead of** $\boldsymbol{\tau}(\mathbf{t})$. *We point out, nevertheless, that all sequences will be t-dependent.* By using the limit $y(t) \in \mathcal{Y}$ as a competitor in the discrete stability (3.55) and subtracting from both sides the term $\int_\Omega \gamma(\underline{z}(t)) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x$, which is bounded from below thanks to its lower semi-continuity, we obtain after rearranging some terms (also finite since the minimizer $\bar{y}\tau(t)$ has finite energy)

$$\begin{aligned}
&\int_\Omega \Big(\gamma(\underline{z}_\tau(t)) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) - \gamma(\underline{z}(t)) W(\nabla y(t), \nabla^2 y(t))\Big)\,\mathrm{d}x \qquad (3.100)\\
&\quad \leq \int_\Omega (\gamma(\underline{z}_\tau(t)) - \gamma(\underline{z}(t))) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x\\
&\qquad + \int_\Omega \phi\left((\nabla y)^{-\top}(t) \nabla \underline{z}_\tau(t)\right) - \phi\left((\nabla \bar{y}_\tau)^{-\top}(t) \nabla \underline{z}_\tau(t)\right)\,\mathrm{d}x\\
&\qquad - \ell(k\tau, y(t), \underline{z}_\tau(t)) + \ell(k\tau, \bar{y}_\tau(t), \underline{z}_\tau(t)),
\end{aligned}$$

where $k\tau \searrow t$ as $\tau \to 0$. Note that the regularizing terms $\mathcal{H}_\tau(\underline{z}_\tau(t))$ are finite thanks to the uniform estimate (3.58), and hence have canceled each other. Since γ and W are lower semi-continuous, by the convexity of W in its last argument and by classical Sobolev embeddings, we have lower semi-continuity of the left-hand side of (3.100) with respect to the convergences (3.91) and (3.68). Namely,

$$0 \leq \liminf_{\tau\to 0} \int_\Omega \Big(\gamma(\underline{z}_\tau(t)) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) - \gamma(\underline{z}(t)) W(\nabla y(t), \nabla^2 y(t))\Big)\,\mathrm{d}x; \tag{3.101}$$

see e.g. Eisen [1979] or [Fonseca and Leoni, 2007, Cor. 7.9].

Concerning the right-hand side of (3.100), for the elastic energy for every $t \in [0,T]$ we have

$$\begin{aligned}
&\int_\Omega (\gamma(\underline{z}_\tau(t)) - \gamma(\underline{z}(t))) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x\\
&\quad \leq \|\gamma(\underline{z}_\tau(t)) - \gamma(\underline{z}(t))\|_\infty \int_\Omega W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x\\
&\quad \leq C \|\gamma(\underline{z}_\tau(t)) - \gamma(\underline{z}(t))\|_\infty \to 0,
\end{aligned}$$

since γ is continuous and hence uniformly continuous on $[0,1]$. The second inequality is a consequence of the fact that $y(t) \in \mathcal{Y}$ for almost every $t \in [0,T]$, and of the growth condition (3.32). The uniform convergence $\|\underline{z}_\tau(t) - \underline{z}(t)\|_\infty \to 0$ follows by (3.77), and by the compact Sobolev embedding of $W^{1,\alpha}(\Omega)$ into $C(\bar{\Omega})$ for $\alpha > 3$.

For the second term on the right-hand side of (3.100), we need to exclude concentrations of $\{\nabla \underline{z}_\tau(t)\}$; let us recall that the improved convergence of $\nabla \underline{z}_\tau(t)$ in (3.77) holds only almost everywhere in $(0,T)$, while we aim to prove (3.99) for all times. Although $\{\nabla \bar{y}_\tau(t)\}$ converges uniformly, a blow up of $\{\nabla \underline{z}_\tau(t)\}$ may still keep the difference bounded away from zero. We hence split this term using the equiintegrable sequence $\{\nabla v_\tau(t)\}$ provided by Lemma 3.15, and satisfying (3.94)–(3.96). On the bad set $M_\tau(t)$ we use the growth and coercivity condition (3.31), as well as the bound (3.75) in $L^\beta(\Omega)$ and the convergence in (3.92), which by (3.95) yield

$$\begin{aligned}
&\limsup_{\tau\to 0} \int_{M_\tau(t)} \left|\phi\left((\nabla y)^{-\top}(t)\nabla \underline{z}_\tau(t)\right) - \phi\left((\nabla \bar{y}_\tau)^{-\top}(t)\nabla \underline{z}_\tau(t)\right)\right| \,\mathrm{d}x \\
&\quad \le C \limsup_{\tau\to 0} \int_{M_\tau(t)} |\nabla \underline{z}_\tau(t)|^\alpha \,\mathrm{d}x \le C \limsup_{\tau\to 0} \mathcal{L}^3(M_\tau(t))^{1-\frac{\alpha}{\beta}} \left(\int_\Omega |\nabla \underline{z}_\tau(t)|^\beta\right)^{\frac{\alpha}{\beta}} \\
&\quad \le C \limsup_{\tau\to 0} |\tau^\alpha|^{1-\frac{\alpha}{\beta}} \left(\tau^{-\kappa}\right)^{\frac{\alpha}{\beta}} \le C \limsup_{\tau\to 0} \tau^{\alpha(1-(\alpha+\kappa)/\beta)} = 0,
\end{aligned}$$

for $\alpha + \kappa < \beta$. On the good set $\Omega \setminus M_\tau(t)$, in view of (3.31), (3.92), and (3.96), the sequence $\{\phi\left((\nabla y)^{-\top}(t)\nabla \underline{z}_\tau(t)\right) - \phi\left((\nabla \bar{y}_\tau)^{-\top}(t)\nabla \underline{z}_\tau(t)\right)\}$ is equi-integrable. Therefore, since $\mathcal{L}^3(\Omega) < +\infty$ it suffices to show that

$$\left|\phi\left((\nabla y)^{-\top}(t)\nabla \underline{z}_\tau(t)\right) - \phi\left((\nabla \bar{y}_\tau)^{-\top}(t)\nabla \underline{z}_\tau(t)\right)\right| \to 0 \quad \text{in measure.} \tag{3.102}$$

Equivalently, we need to show that for every $\varepsilon > 0$ and $n \in \mathbb{N}$ there exists $\tau_0 > 0$ such that for all $0 < \tau < \tau_0$

$$\mathcal{L}^3(E_{\varepsilon,\tau}) := \mathcal{L}^3\left(\left\{\left|\phi\left((\nabla y)^{-\top}(t)\nabla \underline{z}_\tau(t)\right) - \phi\left((\nabla \bar{y}_\tau)^{-\top}(t)\nabla \underline{z}_\tau(t)\right)\right| \ge \varepsilon\right\}\right) < \frac{1}{n}.$$

Let then $\varepsilon > 0$ and $n \in \mathbb{N}$. By the Markov's inequality and the uniform bound on $\|\nabla \underline{z}_\tau(t)\|_\alpha$ given by (3.77), there exists $C_n > 0$ such that for all $\tau > 0$

$$\mathcal{L}^3(E_\tau) := \mathcal{L}^3(\{|\nabla \underline{z}_\tau(t)| \ge C_n\}) < \frac{1}{n}.$$

Since $\{\nabla \bar{y}_\tau(t)\}$ is bounded in $L^\infty(\Omega)$ by (3.92), we have that in the set $\Omega \setminus E_\tau$ both $\{(\nabla y)^{-\top}(t)\nabla \underline{z}_\tau(t)\}$ and $\{(\nabla \bar{y}_\tau(t))^{-\top}(t)\nabla \underline{z}_\tau(t)\}$ take value in a bounded, and hence compact, subset K of $\mathbb{R}^3$. On the one hand, the continuous function ϕ is uniformly continuous on K, and there exists $\delta > 0$ such that for every $x_1, x_2 \in K$ with $|x_1 - x_2| < \delta$ there holds $|\phi(x_1) - \phi(x_2)| < \varepsilon$. On the other hand, by (3.92), there exists $\tau_0 > 0$ dependent on n and such that for all $0 < \tau < \tau_0$

$$|(\nabla \bar{y}_\tau(t))^{-\top}(t) - (\nabla y(t))^{-\top}(t)||\nabla \underline{z}_\tau(t)| < \delta$$

on $\Omega \setminus E_\tau$. For these τ we therefore have $E_{\varepsilon,\tau} \subset E_\tau$ and hence $\mathcal{L}^3(E_{\varepsilon,\tau}) \le \mathcal{L}^3(E_\tau) < 1/n$. This in turn yields (3.102).

Finally, the loading by the assumptions satisfy

$$\limsup_{\tau\to 0} \left(-\ell(k\tau, y(t), \underline{z}_\tau(t)) + \ell(k\tau, \bar{y}_\tau(t), \underline{z}_\tau(t))\right) \le 0.$$

Altogether, we have

$$\limsup_{\tau\to 0} \int_\Omega \gamma(\underline{z}_\tau(t)) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) - \gamma(\underline{z}(t)) W(\nabla y(t), \nabla^2 y(t))\,\mathrm{d}x \le 0. \tag{3.103}$$

Combining (3.101) with (3.103) we deduce (3.97). By Lemma 3.4, we infer (3.98). The convergence in (3.99) follows by (3.98), Corollary 3.4, and by (3.77), which in turn guarantees the uniform convergence of $\gamma(\bar{z}_\tau(t)) \to \gamma(z(t))$. □

3.5.7 Passage to Limit

The next lemma shows semistability of the limiting pair (y, z). We point out that, in comparison with the previous lemmata, the result holds under slightly more general lower-semicontinuity assumptions on the loading.

Lemma 3.17 (Semi-Stability)**.** *Let the hypothesis of Lemma 3.16 hold, and let the loading functional $\ell : \mathbb{R} \times \mathcal{Y} \times Z \to \mathbb{R}$ be such that the map $(t, y, z, \tilde{z}) \mapsto \ell(t, y, \tilde{z}) - \ell(t, y, z)$ is lower semi-continuous on sequences in $\mathbb{R} \times W^{2,p}(\Omega) \times W^{1,\alpha}(\Omega) \times W^{1,\alpha}(\Omega)$ that have uniformly bounded $(\det \nabla y)^{-1}$ in $L^s(\Omega)$ and converge in the strong product topology. Then,*

$$\forall t \in [0,T],\ \forall \tilde{z} \in Z: \qquad \mathcal{E}(t, y(t), z(t)) \le \mathcal{E}(t, y(t), \tilde{z}) + \mathcal{R}(\tilde{z} - z(t)). \tag{3.104}$$

Proof. Let $t \in [0,T]$ and $\tilde{z} \in Z$. *Let $\tau(t)$ be the t-dependent subsequence extracted in Lemma 3.16. With a slight abuse of notation throughout the proof we omit the explicit t-dependence and* **simply write $\boldsymbol{\tau}$**. As in Lemma 3.13, we cannot use $\tilde{z} \in Z$ directly as a competitor in the discrete semi-stability (3.56), because it may not lie in $W^{1,\beta}(\Omega)$. Thus, we work instead with its Lipschitz truncation $\tilde{z}_\tau := (\tilde{z})_{\lambda(\tau)}$. The dependence of the truncation parameter λ on the time step τ is again chosen so that $\mathcal{H}_\tau(\tilde{z}_\tau) \to 0$ (see (3.79) and (3.86)). Hence we obtain, after moving the loading to the right-hand side,

$$\begin{aligned}
&\int_\Omega \gamma(\bar{z}_\tau(t)) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) + \phi\left((\nabla \bar{y}_\tau)^{-\top}(t) \nabla \bar{z}_\tau(t)\right) \mathrm{d}x \\
&\quad + \mathcal{H}_\tau(\bar{z}_\tau(t)) \\
&\quad \le \int_\Omega \gamma(\tilde{z}_\tau) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) + \phi\left((\nabla \bar{y}_\tau)^{-\top}(t) \nabla \tilde{z}_\tau\right) \mathrm{d}x \\
&\quad - \ell(k\tau, \bar{y}_\tau(t), \tilde{z}_\tau) + \ell(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t)) + \mathcal{R}(\tilde{z}_\tau - \bar{z}_\tau(t)) + \mathcal{H}_\tau(\tilde{z}_\tau).
\end{aligned}$$

On the left-hand side, the regularization $\mathcal{H}_\tau(\bar{z}_\tau(t))$ converges to zero owing to Lemma 3.13 whereas the remaining energy terms are lower semi-continuous with respect to (3.91) - (3.93). The first two terms on the right-hand side are continuous with respect to the strong convergence by Lemma 3.13, 3.16, Corollary 3.4, and standard result on Nemytskii operators. Finally, by the strengthened lower-semi continuity of the loading functional we have

$$\limsup_{\tau\to 0} \left(-\ell(k\tau, \bar{y}_\tau(t), \tilde{z}_\tau) + \ell(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t))\right) \le -\ell(t, y(t), \tilde{z}) + \ell(t, y(t), z(t)).$$

This completes the proof of (3.104). □

The proof of the stability condition follows by similar arguments.

Lemma 3.18 (Stability)**.** *Let the hypothesis of Lemma 3.16 hold and let the loading functional $\ell : \mathbb{R} \times \mathcal{Y} \times Z \to \mathbb{R}$ be such that for each $\tilde{y} \in \mathcal{Y}$ the map $(t, y, z) \mapsto \ell(t, \tilde{y}, z) - \ell(t, y, z)$ is lower semi-continuous on $\mathbb{R} \times W^{2,p}(\Omega) \times W^{1,\alpha}(\Omega)$ with respect to the strong product topology. Then,*

$$\forall_{a.e.} t \in [0,T],\ \forall \tilde{y} \in \mathcal{Y}: \qquad \mathcal{E}(t, y(t), z(t)) \le \mathcal{E}(t, \tilde{y}, z(t)) \tag{3.105}$$

Proof. In proving stability we have to restrict ourselves to points $t \in [0,T]$ for which $z(t) = \underline{z}(t)$ and the strengthened convergence (3.77) holds. *In what follows, we will directly work with the subsequence $\tau(t)$ identified in Lemma 3.16, and for ease of notation we will omit the t-dependence simply* **denoting it $\boldsymbol{\tau}$**. Fix $\tilde{y} \in \mathcal{Y}$. By using it as a competitor in the discrete stability (3.55) we obtain, after moving the loading to the right-hand side,

$$\begin{aligned}
&\int_\Omega \gamma(\underline{z}_\tau(t)) W(\nabla \bar{y}_\tau(t), \nabla^2 \bar{y}_\tau(t)) + \phi\left((\nabla \bar{y}_\tau)^{-\top}(t) \nabla \underline{z}_\tau(t)\right) \mathrm{d}x \\
&\quad \le \int_\Omega \gamma(\underline{z}_\tau(t)) W(\nabla \tilde{y}, \nabla^2 \tilde{y}) + \phi\left((\nabla \tilde{y})^{-\top} \nabla \underline{z}_\tau(t)\right) \mathrm{d}x \\
&\qquad - \ell(k\tau, \tilde{y}, \underline{z}_\tau(t)) + \ell(k\tau, \bar{y}_\tau(t), \underline{z}_\tau(t)).
\end{aligned}$$

By Lemmas 3.13 and 3.16, we pass to the limit in the left-hand side by standard lower-semicontinuity arguments. By the continuity of γ, the convergence in (3.77), and the fact that $\gamma(\underline{z}_\tau(t)) W(\nabla \tilde{y}, \nabla^2 \tilde{y}) \le (\max_{[0,1]} \gamma) W(\nabla \tilde{y}, \nabla^2 \tilde{y})$, the first term on the right-hand side satisfies

$$\int_\Omega \gamma(\underline{z}_\tau(t)) W(\nabla \tilde{y}, \nabla^2 \tilde{y}) \,\mathrm{d}x \to \int_\Omega \gamma(z(t)) W(\nabla \tilde{y}, \nabla^2 \tilde{y}) \,\mathrm{d}x.$$

By the lower-semicontinuity assumptions on the loading with respect to the given convergences, we have, up to a countable subset $J \subset [0,T]$

$$\limsup_{\tau \to 0} \left(-\ell(k\tau, \tilde{y}, \underline{z}_\tau(t)) + \ell(k\tau, \bar{y}_\tau(t), \underline{z}_\tau(t))\right) \le -\ell(t, \tilde{y}, z(t)) + \ell(t, y(t), z(t)).$$

The passage to the limit in the ϕ term follows by the strong convergence (3.92) and (3.77) and the growth condition (3.31).

□

Remark. *As opposed to Lemma 3.13, where the strong convergence of elastic variable is proven for all times $t \in [0,T]$, here the stability holds only almost everywhere in $(0,T)$. The difference between the two proof strategies consists in the fact that here we needed to prevent both concentrations and oscillations of $\{\nabla \underline{z}_\tau(t)\}$, while in Lemma 3.13 the possible oscillations have been suppressed* for every $t \in [0,T]$ *owing to the uniform convergence of $\nabla \bar{y}_\tau(t)$. Consequently, we can prove the semi-stability and energy inequality for all times.*

We proceed by identifying the limiting reduced power, where the continuity of $-\partial \ell$ is needed.

Lemma 3.19 (Identification of the limiting reduced power)**.** *Let the hypothesis of Lemmas 3.17 and 3.18 hold. Let the reduced power $-\partial_t \ell : [0,T] \times \mathcal{Y} \times Z \to \mathbb{R}$ be continuous on strongly converging sequences in $\mathbb{R} \times W^{2,p}(\Omega) \times W^{1,\alpha}(\Omega)$ that have uniformly bounded $(\det \nabla y)^{-1}$ in $L^s(\Omega)$. Then,*

$$\underline{\theta} = \bar{\theta} \quad \textit{in } L^1(0,T) \quad \textit{and} \quad \forall t \in [0,T]: \quad \bar{\theta}^{sup}(t) = \partial_t \mathcal{E}(t, y(t), z(t)).$$

Proof. Fix $t \in [0,T]$. *Let $\tau(t)$ be the t-dependent subsequence identified in Lemma 3.16, which is, however, for simplicity* **henceforth denoted by $\boldsymbol{\tau}$**. Choose $\{k(\tau)\} \subset \mathbb{N}$, also just denoted by $\{k\}$ for simplicity, such that $t \in ((k-1)\tau, k\tau] \subset [0,T]$ and $k\tau \searrow t$. On the one hand, by (3.90) we have

$$-\partial_t \ell(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t)) = \partial_t \mathcal{E}(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t)) = \bar{\theta}_\tau(t) \to \bar{\theta}^{\,\sup}(t).$$

On the other hand, by the improved convergences (3.98) and (3.76) and by the continuity assumptions on the loading,

$$-\partial_t \ell(k\tau, \bar{y}_\tau(t), \bar{z}_\tau(t)) \to -\partial_t \ell(t, y(t), z(t)) = \partial_t \mathcal{E}(t, y(t), z(t)).$$

This yields the second part of the statement. For proving the equality of $\bar{\theta}$ and $\underline{\theta}$ we show that $\underline{\theta}_\tau - \bar{\theta}_\tau \rightharpoonup 0$ in $L^1(0,T)$, using a modified argument from [Roubíček, 2013, proof of Thm. 8.9]. We first observe that by a density argument it is enough to consider test functions of the form

$$\varphi(t) := c\chi_{[k_1\tau_0, k_2\tau_0]}(t),$$

where τ_0 is some fixed time step from the discretization, $k_1, k_2 \in \mathbb{N}$ are such that $0 < k_1\tau_0 < k_2\tau_0 < T$, and $c \in \mathbb{R}$.

Thanks to the equiintegrability of $\bar{\theta}_\tau$ and $\underline{\theta}_\tau$ (see Lemma 3.12), we may suppose without loss of generality that $\frac{\tau_0}{\tau}$ is an integer number. Then for all $\tau < \tau_0$ we have

$$\begin{aligned}
&\int_0^T (\underline{\theta}_\tau(t) - \bar{\theta}_\tau(t))\varphi(t)\,\mathrm{d}t \\
&\quad = \int_{k_1\tau_0}^{k_2\tau_0} (\underline{\theta}_\tau(t) - \bar{\theta}_\tau(t))c\,\mathrm{d}t \qquad (3.106)\\
&\quad = c \sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, y_\tau^{k-1}, z_\tau^{k-1}) - \partial_t \mathcal{E}(t, y_\tau^k, z_\tau^k)\,\mathrm{d}t \\
&\quad = c \sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, y_\tau^{k-1}, z_\tau^{k-1}) - \partial_t \mathcal{E}(t+\tau, y_\tau^k, z_\tau^k)\,\mathrm{d}t \\
&\qquad + c \sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t+\tau, y_\tau^k, z_\tau^k) - \partial_t \mathcal{E}(t, y_\tau^k, z_\tau^k)\,\mathrm{d}t \\
&\quad = c \sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t)) - \partial_t \mathcal{E}(t+\tau, \underline{y}_\tau(t+\tau), \underline{z}_\tau(t+\tau))\,\mathrm{d}t \\
&\qquad + c \int_{k_1\tau_0}^{k_2\tau_0} \partial_t \mathcal{E}(t+\tau, \bar{y}_\tau(t), \bar{z}_\tau(t)) - \partial_t \mathcal{E}(t, \bar{y}_\tau(t), \bar{z}_\tau(t))\,\mathrm{d}t. \qquad (3.107)
\end{aligned}$$

For the first term on the right-hand side of (3.107), we infer that

$$\begin{aligned}
&\sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t)) - \partial_t \mathcal{E}(t+\tau, \underline{y}_\tau(t+\tau), \underline{z}_\tau(t+\tau))\,\mathrm{d}t \\
&= \sum_{k=k_1\frac{\tau_0}{\tau}+1}^{k_2\frac{\tau_0}{\tau}} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t))\,\mathrm{d}t - \sum_{k=k_1\frac{\tau_0}{\tau}+2}^{k_2\frac{\tau_0}{\tau}+1} \int_{(k-1)\tau}^{k\tau} \partial_t \mathcal{E}(t, \underline{y}_\tau(t), \underline{z}_\tau(t))\,\mathrm{d}t \\
&= \int_{k_1\tau_0}^{k_1\tau_0+\tau} \underline{\theta}_\tau(t)\,\mathrm{d}t - \int_{k_2\tau_0}^{k_2\tau_0+\tau} \underline{\theta}_\tau(t)\,\mathrm{d}t.
\end{aligned}$$

Thanks to the equi-integrability of $\underline{\theta}_\tau$ these two integrals can be made arbitrarily small as $\tau \to 0$. Eventually, the second term on the right-hand side of (3.107) converges to zero by the Dominated Convergence Theorem. Indeed, the pointwise convergence follows by the strong continuity of $\partial_t \ell$, as well as by the convergences (3.98) and (3.76), and by the uniform bound of $(\det \nabla \bar{y}_\tau(t))^{-1}$ in $L^s(\Omega)$ provided by the growth conditions in (3.32) and by (3.99). The integrable majorant is obtained arguing exactly as in Step 1 of proof of Lemma 3.12. □

The next lemma shows that the limiting pair (y, z) satisfies an energy inequality. We point out that in proving the (semi)-stability condition lower semicontinuity of the loading with respect to the weak topology was needed, whereas for obtaining the energy inequality we need to enforce continuity with respect to the strong product topology.

Lemma 3.20 (Energy Inequality)**.** *Let the hypothesis of Lemma 3.19 hold and let the loading $\ell : [0,T] \times \mathcal{Y} \times Z \to \mathbb{R}$ be continuous on sequences in $\mathbb{R} \times W^{2,p}(\Omega) \times W^{1,\alpha}(\Omega)$ that have uniformly bounded $(\det \nabla y)^{-1} \in L^s(\Omega)$ and converges in the strong product topology. Then,*

$$\forall t_1, t_2 \in I,\ t_1 < t_2 : \mathcal{E}(t_2, y(t_2), z(t_2)) + \mathrm{Diss}_{\mathcal{R}}(z; [t_1, t_2]) \le \mathcal{E}(t_1, y(t_1), z(t_1)) + \int_{t_1}^{t_2} \partial_t \mathcal{E}(t, y(t), z(t)) \,\mathrm{d}t.$$

Proof. Fix $t_1, t_2 \in [0,T]$ with $t_1 < t_2$, and let $\tau(t_1)$ be the subsequence from Lemma 3.15 for which the convergences (3.99) and (3.98) for $\bar{y}_{\tau(t_1)}(t_1)$ hold at time t_1. Let us, for a moment, extract a further subsequence $\tau'(t_1)$ such that we have also convergence of $\bar{y}_{\tau'(t_1)}(t_2)$, namely

$$\bar{y}_{\tau'(t_1)}(t_2) \rightharpoonup \xi(t_2) \qquad \text{in } W^{2,p}(\Omega), \tag{3.108}$$

$$(\nabla \bar{y}_{\tau'(t_1)})^{-\top}(t_2) \nabla \bar{z}_{\tau'(t_1)}(t_2) \to (\nabla \xi)^{-\top}(t_2) \nabla z(t_2) \qquad \text{in } L^\alpha(\Omega), \tag{3.109}$$

where the second, strong convergence follows by the compact Sobolev embedding for $p > 3$ and the strong convergence of $\nabla \bar{z}_{\tau'(t_1)}(t_2)$, proven in Lemma 3.13 even for the original sequence. Since the result we are going to prove will not depend on the particular choice of the subsequence, i.e. on ξ, it will hold for the original sequence $\tau(t_1)$. *For ease of notation we omit the explicit dependence of the subsequences on time t_1 and* **denote them by $\boldsymbol{\tau}$ and $\boldsymbol{\tau'}$** *in the following.* Let also $\{k_1(\tau')\}$, $\{k_2(\tau')\} \subset \mathbb{N}$, also denoted simply by $\{k_1\}$ and $\{k_2\}$, be such that $t_1 \in ((k_1-1)\tau', k_1\tau'] \subset [0,T]$ and $t_2 \in ((k_2-1)\tau', k_2\tau'] \subset [0,T]$ with $k_1\tau' \searrow t_1$ and $k_2\tau' \searrow t_2$. Using the definition of the discrete dissipation, the absolute continuity of the energy (3.39), and the discrete energy inequality (3.49), we obtain

$$\begin{aligned}
&\mathcal{E}(t_2, \bar{y}_{\tau'}(t_2), \bar{z}_{\tau'}(t_2)) + \mathrm{Diss}_{\mathcal{R}}(\bar{z}_{\tau'}; [t_1, t_2]) \\
&= \mathcal{E}(k_2\tau', \bar{y}_{\tau'}(k_2\tau'), \bar{z}_{\tau'}(k_2\tau')) + \mathrm{Diss}_{\mathcal{R}}(\bar{z}_{\tau'}; [k_1\tau', k_2\tau']) - \int_{t_2}^{k_2\tau'} \bar{\theta}_{\tau'}(t) \,\mathrm{d}t \\
&\le \mathcal{E}(k_1\tau', \bar{y}_{\tau'}(k_1\tau'), \bar{z}_{\tau'}(k_1\tau')) + \int_{k_1\tau'}^{k_2\tau'} \underline{\theta}_{\tau'}(t) \,\mathrm{d}t - \int_{t_2}^{k_2\tau'} \bar{\theta}_{\tau'}(t) \,\mathrm{d}t \\
&\quad + \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(k_1\tau')) - \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(k_2\tau')) \\
&= \mathcal{E}(t_1, \bar{y}_{\tau'}(t_1), \bar{z}_{\tau'}(t_1)) + \int_{t_1}^{t_2} \underline{\theta}_{\tau'}(t) \,\mathrm{d}t - \int_{t_1}^{k_1\tau'} \underline{\theta}_{\tau'}(t) \,\mathrm{d}t - \int_{t_2}^{k_2\tau'} \bar{\theta}_{\tau'}(t) - \underline{\theta}_{\tau'}(t) \,\mathrm{d}t \\
&\quad + \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(k_1\tau')) - \mathcal{H}_{\tau'}(\bar{z}_{\tau'}(k_2\tau')).
\end{aligned}$$

For the first term on the right-hand side we apply the convergence of elastic energies in (3.99), as well as the continuity of the phase field energy ϕ and of the loading ℓ with respect to the strong convergence (3.98) and (3.76) of $\bar{y}_{\tau'}(t_1)$ and $\bar{z}_{\tau'}(t_1)$. For the second term we exploit the convergence of the reduced power (3.74), whereas the third and fourth ones converge to zero owing to the equiintegrability of $\{\bar{\theta}_{\tau'}\}$ and $\{\underline{\theta}_{\tau'}\}$. Eventually, the regularization terms converge to zero owing to (3.78).

On the left hand side we proceed by lower semi-continuity of the energy $\mathcal{E}$ with respect to the strong convergence (3.76) of the internal variable $\bar{z}_{\tau'}(t_2)$, the strong convergence (3.109) of the coupled term, and the weak convergence (3.108) of the elastic variable $\bar{y}_{\tau'}(t_2)$. The lower-semicontinuity of the dissipation $\mathrm{Diss}_{\mathcal{R}}(\bar{z}_{\tau'};[0,t])$ is a consequence of (3.70) and (3.71). Thus, using in addition the stability condition (3.105), we obtain

$$\begin{aligned}\mathcal{E}(t_2,y(t_2),z(t_2))+\mathrm{Diss}_{\mathcal{R}}(z;[t_1,t_2]) &\le \mathcal{E}(t_2,\xi(t_2),z(t_2))+\mathrm{Diss}_{\mathcal{R}}(z;[t_1,t_2])\\ &\le \mathcal{E}(t_1,y(t_1),z(t_1))+\int_{t_1}^{t_2}\underline{\theta}(t)\,\mathrm{d}t.\end{aligned}$$

Since this inequality holds for any ξ, it holds even for the original sequence $\tau\to 0$ and hence for the solution $t\mapsto(y(t),z(t))$; supposing the opposite would lead to a contradiction. To conclude we recall that by Lemma 3.19 we have $\underline{\theta}=\bar{\theta}\le\bar{\theta}^{\,\mathrm{sup}}$ a.e. in $(0,T)$ and that $\bar{\theta}^{\,\mathrm{sup}}(t)=\partial_t\mathcal{E}(t,y(t),z(t))$ even everywhere in $[0,T]$. □

Remark. *When analyzing the proof we see that* ***energy equality*** *is bound to break not only when the weak limit of $\partial_t\mathcal{E}(t,\bar{y}_\tau(t),\bar{z}_\tau(t))$ is strictly less than the maximal power $\partial_t\mathcal{E}(t,y(t),z(t))$, but also whenever $\mathcal{E}(t_2,y(t_2),z(t_2))$ $<\mathcal{E}(t_2,\xi(t_2),z(t_2))$, i.e. all the cluster points of $\bar{y}_\tau(t_2)$ maximizing the reduced power at time t_2 have strictly less energy than any limit $\xi(t_2)$ which maximizes the reduced power at time t_1.*

3.6 Existence Theorem

Let us now summarize all the steps above into a single statement.

Theorem 3.21 (Existence Result)**.** *Let $\Omega\subset\mathbb{R}^3$ be a bounded Lipschitz domain. Assume that the damage function $\gamma:\mathbb{R}\to(0,+\infty)$ is continuous and satisfies* (3.30)*, and that the stored energy density $W:\mathbb{R}^{3\times3}\times\mathbb{R}^{3\times3\times3}\to[0,+\infty)$ is continuous in its first argument, is convex in its second argument, and satisfies the coercivity condition* (3.32) *with $s\ge\frac{3p}{p-3}$, with $p>3$. Assume also that $\phi:\mathbb{R}^{3\times3}\to\mathbb{R}$ is strictly convex and fulfills the polynomial growth conditions in* (3.31) *with $\alpha>3$. Let the dissipation potential $\mathcal{R}:L^1(\Omega)\to[0,+\infty]$ be convex, positively 1-homogeneous, lower semi-continuous with respect to the weak $L^1(\Omega)$ topology, and satisfying* (3.42)*,* (3.43)*, and* (3.44)*. Let $\partial\Omega=\Gamma_D\cup\Gamma_N$ be a measurable partition, with Γ_D having a positive two dimensional Hausdorff measure. Assume that the coercivity condition* (3.33) *is satisfied, that* (3.34)*,* (3.35)*, and* (3.36) *hold true, and that both the reduced power $-\partial_t\ell$ and the loading ℓ are strongly continuous on sequences in $\mathbb{R}\times W^{2,p}(\Omega)\times W^{1,\alpha}(\Omega)$ that have uniformly bounded $(\det\nabla y)^{-1}$ in $L^s(\Omega)$. Then, the problem* (3.14) *poses a separately global solution*

in the sense of Definition 3.1, where in addition the deformation $y(t)$ is for all times $t \in [0,T]$ injective everywhere *in the domain* Ω.

Proof. Vast majority of the statement has been proven in Lemmata 3.5–3.7 and 3.12–3.20. The injectivity follows directly from the definition of the space $\mathcal{Y}$ in (3.22), the Ciarlet–Nečas condition (3.25), and the integrability of the distortion (3.26), to be proven by Hölder inequality. Due to the regularization $\mathcal{H}_\tau$ we also have to show the internal parameter satisfies the initial condition, which follows by the equalities $\bar{z}_\tau(0) = \underline{z}_\tau(0) = z_\tau^0 = (z^0)_{\lambda(\tau)}$ and convergences

$$\bar{z}_\tau(0) \rightharpoonup^* z(0) \quad \text{in } L^\infty(\Omega),$$

from (3.67) and by

$$(z^0)_{\lambda(\tau)} \to z^0 \quad \text{in } W^{1,\alpha},$$

from the propertie of the Lipschitz truncation; see Lemma A.4. □

4. Towards Anisotropic Continua within GENERIC

GENERIC stands for General Equation for Non-Equilibrium Reversible-Irreversible Coupling, which aims at 'governing time evolution of macroscopic systems on mesoscopic levels of description'; Grmela [2010]. Classical examples would include field theory of hydrodynamics or complex fluids. Although having a longer history, the framework was first coined GENERIC in Grmela and Öttinger [1997], Öttinger and Grmela [1997] and was later summarized in two monographs Öttinger [2005], Pavelka et al. [2018a]. The GENERIC formulation involves elements which are sufficiently abstract to have a clear meaning on any level of description. Namely, it builds on

- state variables,
- reversible evolution, which is supposed to be Hamiltonian,
- irreversible evolution generated by a (generalized) gradient flow,
- energy, and
- entropy.

Quoting again from Grmela [2010], the question 'Why GENERIC?' can be answered as follows:

- 'because of the guaranteed agreement of solutions with certain results of experimental observations,
- because of its usefulness in constructing new time evolution equations (especially in the context of complex fluids),
- because it arises as a natural extension of equilibrium thermodynamics.'

The first answer points mainly to the first and second law of thermodynamics and to Onsager-Casimir reciprocal relations, which according to the presentation speech at Nobel Prize Ceremony Nobel Media [2020] 'represent a further law making a thermodynamic study of irreversible processes possible'; see e.g. de Groot and Mazur [1984] or the original works Onsager [1931a,b], Casimir [1945] for further explanations of this phenomenon, or Pavelka et al. [2018a] for its treatment in GENERIC. The second answer address successful attempts to derive the field equations, i.e. both the reversible and irreversible evolution as well as the dependence of energy and entropy on the state variables, from statistical mechanics; see Öttinger [2005], Pavelka et al. [2018a] for an overview. Elaborating the third answer is actually the ultimate mission of the article Grmela [2010] and the reader is referred there for any further details.

Apart from the multi-scale approach based on statistical mechanics mentioned above, there is another way of deriving the field equations in GENERIC, namely the phenomenological one. The general method based on differential geometry has been summarized in [Öttinger, 2005, App. B.4]. We, however, follow the

work of Edwards and Beris [1991] and Pavelka et al. [2020], since we believe they represent a simple realization of this abstract procedure, where no knowledge of differential geometry is necessary. These works take as a starting point the Hamiltonian mechanics of continuum where each point is fully described by its position $\mathbf{y}(\mathbf{X})$ and momentum $\mathbf{M}(\mathbf{X})$, both function of the Lagrangian coordinate $\mathbf{X}$ in the reference configuration; for a derivation see e.g. Goldstein [1980], Simo et al. [1988] and references therein. The Lagrangian field of entropy $s_0(\mathbf{X})$ has a role of a material parameter, as for example has also the Lagrangian density $\rho_0(\mathbf{X})$. Both the works mentioned then switch from this very detailed Lagrangian description to a coarser Eulerian one, consisting of fields of density $\rho(\mathbf{x})$, momentum $\mathbf{m}(\mathbf{x})$, and entropy $s(\mathbf{x})$, all meant as densities with respect to the volume in the current configuration and functions of spatial variable $\mathbf{x}$. In addition to these hydrodynamic fields, Edwards and Beris [1991] consider the Eulerian field of left Cauchy–Green tensor $B^{ij}(\mathbf{x}) := F^i_I(\mathbf{x})F^j_I(\mathbf{x}) := \frac{\partial y^i}{\partial X^I}(\mathbf{X})\frac{\partial y^j}{\partial X^I}(\mathbf{X})\Big|_{\mathbf{x}=\mathbf{y}(\mathbf{X})}$ as the last state variable, while Pavelka et al. [2020] chose rather the Eulerian field of distortion $A^I_i(\mathbf{x}) := (F^{-1})^I_i(\mathbf{x}) = \frac{\partial X^I}{\partial x^i}(\mathbf{x})$ instead. Both of these choices, however, cannot describe materials exhibiting any kind of spatial anisotropy.

For modeling of anisotropic, visco-elastic fluids we build on the paper Rajagopal and Srinivasa [2001], which extends the framework of *natural configuration* from Rajagopal and Srinivasa [2000a], encompassing models of visco-elastic fluids that are isotropic both in their viscous and elastic response; see also Málek and Průša [2016] for an up to date overview of the thermodynamic framework of natural configuration and Šípka [2020] for an extension and update of its anisotropic modification, reflecting the recent progress in the theory. As opposed to other theories of anisotropic fluids, this one does not build on directors; no balance laws for directors are postulated, nor is there a notion of a director body force, director (or cosserat) stress or director kinetic energy. It considers only a vector describing the fluid anisotropy as an additional state variable (only transverse isotropy is treated for simplicity), which is then, following Truesdell and Noll [2004], accompanied by the standard balance laws, which build on the notion of surface forces in the sense of Cauchy. As highlighted e.g. in dell'Isola et al. [2017], 'the Cauchy straitjacket consists in the following set of assumptions:

- on a Cauchy cut separating two subbodies in a continuous body only contact surface density of forces is exerted;
- contact forces are balanced by volume forces (i.e. forces per unit volume),'

which limits the class of materials that can be described by the theory. Apart from this restriction coming from the underlying theory of simple continua, the evolution of the new vectorial variable is not general, but rather simplified and reduced to the isotropic case by an additional assumption that the vector remains constant in the natural configuration, limiting the developed theory even further.

The first goal of this chapter is straightforward, to remove the restrictions described above because it will allow to model a broader class of materials. The second, maybe even more important one, is to make the general geometrical procedure from [Öttinger, 2005, App. B.4] accessible to a wider audience, not necessarily familiar with differential geometry and Lie groups' machinery.

This standpoint already determines the structure of the chapter, where we try first to explain the fundamentals of GENERIC on the most simple example,

damped harmonic oscillator, and than move to continuum theory of isotropic, visco-elasto-plastic materials, following mostly Pavelka et al. [2018a], and provides links to other frameworks of continuum mechanics and thermodynamics, especially to natural configuration. The generalization to anisotropic materials is presented in the very last section.

Depending on the context and balancing brevity with clarity, some equations are written with indices, using Einstein's summation convention.

4.1 Toy Model

Let us first demonstrate the GENERIC framework on a very simple example - damped harmonic oscillator (e.g. a weight on a spring). We will start by explaining how the evolution equations are derived and close the part by showing a modification suitable for a description of iso-thermal processes.

State Variables

The first step we have to make is to define the *state variables*, which describes the oscillator appropriately to our intentions. Since we aim at a very coarse *level of description*, we choose the position of the weight $\mathbf{r}$, its momentum $\mathbf{p}$ and its total energy E. This is the so called *entropic representation*, where the fundamental thermodynamic relation for entropy $S = S(\mathbf{r}, \mathbf{p}, E)$ completely specifies the 'material properties' of the weight and the spring; see e.g. Callen [1960]. On the other hand, one may use the *energetic representation*, where the state variables are $\mathbf{r}$, $\mathbf{p}$ and S. The fundamental thermodynamic relation is then $E = E(\mathbf{r}, \mathbf{p}, S)$ and can be obtained by inverting the entropic one. The energetic representation is particularly useful when formulating the *reversible evolution* using Hamiltonian formalism, while the entropic representation naturally appears in gradient dynamics, which describes the *irreversible evolution*; see Pavelka et al. [2018b] or Öttinger [2005] for an explanation of time reversibility and references therein. The evolution of every state variable consists of its reversible and irreversible part. We hence in our setting have

$$\begin{aligned}
\dot{\mathbf{r}} &= (\dot{\mathbf{r}})_{\text{rev}} + (\dot{\mathbf{r}})_{\text{irr}} \,, \\
\dot{\mathbf{p}} &= (\dot{\mathbf{p}})_{\text{rev}} + (\dot{\mathbf{p}})_{\text{irr}} \,, \\
\dot{S} &= \left(\dot{S}\right)_{\text{rev}} + \left(\dot{S}\right)_{\text{irr}} \,.
\end{aligned}$$

In what follows we will explain how the equations for $(\dot{\cdot})_{\text{rev}}$ and $(\dot{\cdot})_{\text{irr}}$ are designed. The fundamental assumption is that the reversible evolution is Hamiltonian (the opposite being true unconditionally); in a compliance, gradient dynamics which generates only irreversible evolution is considered.

Reversible Kinematics

As explained above, we will use in this part the energetic representation, i.e. the state variables are $\mathbf{r}, \mathbf{p}$ and S. Kinematics of the state variables is formulated via *Poisson bracket* $\{\cdot, \cdot\}$, an anti–symmetric bi-linear form taking functions (or functionals) of the state variables as its arguments; see e.g. Pavelka et al. [2018b].

In our case it is the *canonical* Poisson bracket, describing the kinematics of a mass point

$$\{F, G\}^{\text{can}} = \frac{\partial F}{\partial \mathbf{r}} \cdot \frac{\partial G}{\partial \mathbf{p}} - \frac{\partial G}{\partial \mathbf{r}} \cdot \frac{\partial F}{\partial \mathbf{p}}, \qquad \forall F(\mathbf{r}, \mathbf{p}, S),\, G(\mathbf{r}, \mathbf{p}, S). \tag{4.1}$$

Hamiltonian evolution of an arbitrary functional $F(\mathbf{r}, \mathbf{p}, S)$ is then given by

$$\left(\dot{F}\right)_{\text{rev}} = \{F, E\}^{\text{can}} = \frac{\partial F}{\partial \mathbf{r}} \frac{\partial E}{\partial \mathbf{p}} - \frac{\partial E}{\partial \mathbf{r}} \frac{\partial F}{\partial \mathbf{p}}, \tag{4.2}$$

where $E(\mathbf{r}, \mathbf{p}, S)$ is the total energy of the system (or Hamiltonian). Obtaining the evolution equations for the state variables is straightforward; on the left-hand side the chain rule gives

$$\left(\dot{F}\right)_{\text{rev}} = \frac{\partial F}{\partial \mathbf{r}} \cdot (\dot{\mathbf{r}})_{\text{rev}} + \frac{\partial F}{\partial \mathbf{p}} \cdot (\dot{\mathbf{p}})_{\text{rev}} + \frac{\partial F}{\partial S} \cdot \left(\dot{S}\right)_{\text{rev}},$$

and since the functional F is arbitrary, the comparison with Eq. (4.2) yields

$$\begin{aligned} (\dot{\mathbf{r}})_{\text{rev}} &= \frac{\partial E}{\partial \mathbf{p}}, \\ (\dot{\mathbf{p}})_{\text{rev}} &= -\frac{\partial E}{\partial \mathbf{r}}, \\ \left(\dot{S}\right)_{\text{rev}} &= 0. \end{aligned}$$

Note that the bracket (4.1) does not contain the partial derivatives with respect to entropy, and hence entropy does not evolve in this setting at all. This is a general principle: the reversible evolution does not change entropy. In other words, entropy is always assumed to be a so called *Casimir* of general Poisson bracket $\{\cdot, \cdot\}$, which means

$$\left(\dot{S}\right)_{\text{rev}} = \{S, E\} = 0, \qquad \forall E. \tag{4.4}$$

At the same time, the anti-symmetry of the bracket implies

$$\left(\dot{E}\right)_{\text{rev}} = \{E, E\} = 0,$$

i.e. energy is automatically conserved. This represents the *first law of thermodynamics*.

Elastic Dynamics

A very common form of energy is

$$E = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} k \mathbf{r}^2 + \epsilon(S), \tag{4.5}$$

which consists of kinetic (m denotes the mass of the weight), potential (k denotes the 'spring' constant) and internal contributions. The Hamiltonian evolution equations then become

$$\begin{aligned} (\dot{\mathbf{r}})_{\text{rev}} &= \frac{\mathbf{p}}{m}, \\ (\dot{\mathbf{p}})_{\text{rev}} &= -k\mathbf{r}, \\ (\dot{S})_{\text{rev}} &= 0. \end{aligned}$$

Let us briefly summarize the reversible kinematics. Reversible evolution in GENERIC is generated by Hamiltonian mechanics. The Poisson bracket corresponds to the choice of state variables, and once energy as a function of the state variables is specified, describing the specific physical system under consideration, the reversible evolution equations can be written down in a closed form.

Irreversible Kinematics

Let us now turn to the second law of thermodynamics, i.e. the growth of entropy. We shall here take advantage of the entropic representation with the fundamental thermodynamic relation

$$S = S(\mathbf{r}, \mathbf{p}, E). \tag{4.7}$$

Before describing the structure of the irreversible part of evolution in general, we will try to motivate it by a very simple, vague example.

Example. *As already mentioned, the goal is to fulfill the second law of thermodynamics, i.e. we want*

$$\left(\dot{S}\right)_{irr} = \frac{\partial S}{\partial \mathbf{r}} \cdot \left(\dot{\mathbf{r}}\right)_{irr} + \frac{\partial S}{\partial \mathbf{p}} \cdot \left(\dot{\mathbf{p}}\right)_{irr} + \frac{\partial S}{\partial E} \left(\dot{\mathbf{r}}\right)_{irr} \geq 0.$$

If we postulate

$$\begin{pmatrix} \left(\dot{\mathbf{r}}\right)_{irr} \\ \left(\dot{\mathbf{p}}\right)_{irr} \\ \left(\dot{E}\right)_{irr} \end{pmatrix} \sim \begin{pmatrix} \dfrac{\partial S}{\partial \mathbf{r}} \\ \dfrac{\partial S}{\partial \mathbf{p}} \\ \dfrac{\partial S}{\partial E} \end{pmatrix}$$

i.e. 'proportionality with some positive *constant', we obtain*

$$\left(\dot{S}\right)_{irr} \sim \left(\frac{\partial S}{\partial \mathbf{r}}\right)^2 + \left(\frac{\partial S}{\partial \mathbf{p}}\right)^2 + \left(\frac{\partial S}{\partial E}\right)^2 \geq 0.$$

If one wanted to be precise, the relation $\sim$ is to be replaced by a positive semi-definite matrix. This simple evolution is such that the it follows the direction of the entropy gradient, i.e. in the steepest entropy ascent (SEA).

This example shows why the gradient of entropy is suitable for designing the irreversible evolution. The generalization now consists in finding a broader mathematical structure, which could replace the linear relation and still would yield the desired inequality. Within GENERIC, this structure is the (generalized) gradient dynamics generated by a *dissipation potential* (see Pavelka et al. [2018b])

$$\Xi(\mathbf{r}, \mathbf{p}, E, \mathbf{r}^*, \mathbf{p}^*, E^*),$$

which depends on the state variables as well as on the *conjugate variables* (denoted by star), which are eventually substituted by the derivatives of entropy S with

respect to the state variables, i.e. the gradient of entropy [1]. The dissipation potential is usually assumed to be

1. positive, i.e. $\Xi \geq 0$ and $\left.\frac{\partial \Xi}{\partial \mathbf{r}^*}\right|_{\mathbf{r}^*=0} = \left.\frac{\partial \Xi}{\partial \mathbf{p}^*}\right|_{\mathbf{r}^*=0} = \left.\frac{\partial \Xi}{\partial E^*}\right|_{\mathbf{r}^*=0} = 0$,

2. convex, (although this assumption can be weakened; see Janečka and Pavelka [2018b]), and

3. even with respect to TRT.

These criteria imply that the irreversible evolution vanishes in the thermodynamic equilibrium $\mathbf{r}^* = \mathbf{p}^* = E^* = 0$, the second law of thermodynamics is satisfied (as shown below) and that the thermodynamic equilibrium is stable. The last property assures that the evolution equations generated by the dissipation potential are irreversible with respect to TRT; this makes the separation into the reversible and irreversible part unambiguous.

Irreversible evolution is then postulated as follows:

$$(\dot{\mathbf{r}})_{\text{irr}} = \left.\frac{\partial \Xi}{\partial \mathbf{r}^*}\right|_{\mathbf{r}^*=\frac{\partial S}{\partial \mathbf{r}}} \tag{4.8a}$$

$$(\dot{\mathbf{p}})_{\text{irr}} = \left.\frac{\partial \Xi}{\partial \mathbf{p}^*}\right|_{\mathbf{p}^*=\frac{\partial S}{\partial \mathbf{p}}}, \tag{4.8b}$$

$$\left(\dot{E}\right)_{\text{irr}} = \left.\frac{\partial \Xi}{\partial E^*}\right|_{E^*=\frac{\partial S}{\partial E}}, \tag{4.8c}$$

where derivative of entropy are eventually substituted for the conjugate variables. The motivation for such a postulation is that the irreversible evolution of entropy (which is now not a state variable, but the functional from (4.7)) is then

$$\left(\dot{S}\right)_{\text{irr}} = \frac{\partial S}{\partial \mathbf{r}} \cdot (\dot{\mathbf{r}})_{\text{irr}} + \frac{\partial S}{\partial \mathbf{p}} \cdot (\dot{\mathbf{p}})_{\text{irr}} + \frac{\partial S}{\partial E} (\dot{\mathbf{r}})_{\text{irr}} = \mathbf{r}^* \cdot \frac{\partial \Xi}{\partial \mathbf{r}^*} + \mathbf{p}^* \cdot \frac{\partial \Xi}{\partial \mathbf{p}^*} + E^* \frac{\partial \Xi}{\partial E^*} \geq 0,$$

as follows by chain rule, positiveness, and convexity of the dissipation potential. The *second law of thermodynamics* is thus guaranteed as well.

Dissipative Dynamics

Since we want to compute in the entropic representation, we first need to invert the thermodynamic relation in Eq. (4.5), which yields

$$S = S(\mathbf{r}, \mathbf{p}, E) = \sigma\left(E - \frac{\mathbf{p}^2}{2m} - \frac{1}{2}k\mathbf{r}^2\right),$$

[1] The steepest entropy ascent (SEA), mentioned in the example above, is essentially equivalent with entropy production maximization and both these approaches are equivalent to gradient dynamics if the dissipation potential depends only on one conjugate variable or if it is k-homogeneous; see Janečka and Pavelka [2018a], Beretta [2014], Rajagopal and Srinivasa [2000a], Ziegler [1963], Rajagopal and Srinivasa [2004], Málek et al. [2015], Hron et al. [2012].

where σ is the inverse function to ϵ. The basic choice of the the dissipation potential is customary quadratic, because it usually serves as a good approximation near the thermodynamic equilibrium where $\mathbf{r}^* = \mathbf{p}^* = E^* = 0$. We choose

$$\Xi = \frac{1}{2}\zeta(\mathbf{p}^*)^2,$$

where ζ is a material constant. This choice expresses a friction proportional to the velocity. Indeed, Eqs. (4.8a) - (4.8c) become

$$\begin{aligned}
(\dot{\mathbf{r}})_{\text{irr}} &= 0, \\
(\dot{\mathbf{p}})_{\text{irr}} &= \zeta \mathbf{p}^*\Big|_{\mathbf{p}^* = \frac{\partial S}{\partial \mathbf{p}}} = -\zeta T^{-1}\frac{\mathbf{p}}{m}, \\
\left(\dot{E}\right)_{\text{irr}} &= 0,
\end{aligned}$$

where the *inverse temperature* is identified with derivative of entropy with respect to internal energy

$$T^{-1} := \frac{\partial \sigma}{\partial \epsilon} = \frac{\partial S}{\partial E} = E^*.$$

Note that total energy is conserved because Ξ is independent of E^*. Using the relation $S(\mathbf{r}, \mathbf{p}, E)$ we can now deduce the entropy production

$$\left(\dot{S}\right)_{\text{irr}} = \mathbf{p}^* \zeta \mathbf{p}^*\Big|_{\mathbf{p}^* = \frac{\partial S}{\partial \mathbf{p}}} = T^{-2}\zeta\left(\frac{\mathbf{p}}{m}\right)^2 \geq 0.$$

Final Equations

Since we have written down both the reversible and irreversible evolution explicitly for the specific energy, we are now ready to formulate the final, closed system of equations

$$\begin{aligned}
\dot{\mathbf{r}} &= \frac{\mathbf{p}}{m}, \\
\dot{\mathbf{p}} &= -k\mathbf{r} - T^{-1}\zeta\frac{\mathbf{p}}{m}, \\
\dot{S} &= T^{-2}\zeta\left(\frac{\mathbf{p}}{m}\right)^2.
\end{aligned}$$

How to formulate the complete kinematics for general energy and dissipation potential will be explained in the sequel.

We conclude this section by summarising the main points. Evolution of the state variables is the sum of the reversible Hamiltonian evolution and irreversible gradient dynamics. The Hamiltonian evolution conserves both energy and entropy while gradient dynamics conserves energy and produces entropy.

4.1.1 Energetic Conjugate Variables

When discussing this toy model, we have first declared the state variables, we saw the energetic and entropic representations, the canonical Poisson bracket and a

simple dissipation potential. Conjugate variables, which naturally appear in gradient dynamics, were eventually identified with derivatives of entropy. However, in the irreversible and reversible evolution, different state variables and thermodynamic relations are used. Hence we cannot simply add them together in order to obtain the final, total evolution; they are like sheep and goats. Another reason for introducing the energetic conjugate variables is that the formulation is sometimes easier. For example, it is better to work with velocity than minus velocity over temperature, as we will see in the section 4.2; we also refer to Pavelka et al. [2018a] for a Navier-Stokes dissipation potential.

We will overcome this difficulty by rewriting the gradient dynamics into the energetic representation, replacing the entropy conjugate variables by energetic ones, here $\mathbf{r}^\dagger$, $\mathbf{p}^\dagger$ and $s^\dagger$. Energetic conjugate variables are eventually identified with derivatives of energy with respect to the state variables,

$$\mathbf{r}^\dagger = \frac{\partial E}{\partial \mathbf{r}} = \frac{\partial V}{\partial \mathbf{r}}, \qquad \mathbf{p}^\dagger = \frac{\partial E}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m}, \qquad \text{and} \qquad S^\dagger = \frac{\partial E}{\partial S} = \frac{\partial \epsilon}{\partial S} = T.$$

Using the implicit function theorem, the energetic conjugate variables are related to the entropic conjugate variables through

$$\left(\frac{\partial S}{\partial \mathbf{r}}\right)_{\mathbf{p},E} = -\frac{\left(\frac{\partial E}{\partial \mathbf{r}}\right)_{\mathbf{p},S}}{\left(\frac{\partial E}{\partial S}\right)_{\mathbf{r},\mathbf{p}}} \quad \text{and} \quad \left(\frac{\partial E}{\partial \mathbf{p}}\right)_{\mathbf{r},E} = -\frac{\left(\frac{\partial E}{\partial \mathbf{p}}\right)_{\mathbf{r},S}}{\left(\frac{\partial E}{\partial S}\right)_{\mathbf{r},\mathbf{p}}}.$$

These transformations can be considered as generally applicable also for other sets of state variables, where the relations are analogical. The conjugate variables then transform as

$$\mathbf{r}^* = -\frac{\mathbf{r}^\dagger}{S^\dagger}, \qquad \mathbf{p}^* = -\frac{\mathbf{p}^\dagger}{S^\dagger}, \qquad \text{and} \qquad E^* = \frac{1}{S^\dagger}.$$

The dissipation potential can be thus expressed in terms of the energetic conjugate variables, in our toy model

$$\Xi = \frac{\zeta}{2}\left(\frac{\mathbf{p}^\dagger}{S^\dagger}\right)^2,$$

and derivatives of the dissipation potential are

$$\frac{\partial \Xi}{\partial \mathbf{r}^*} = \frac{\partial \Xi}{\partial \mathbf{r}^\dagger}\frac{\partial \mathbf{r}^\dagger}{\partial \mathbf{r}^*} = -S^\dagger \frac{\partial \Xi}{\partial \mathbf{r}^\dagger}, \qquad \text{and} \qquad \frac{\partial \Xi}{\partial \mathbf{p}^*} = \frac{\partial \Xi}{\partial \mathbf{p}^\dagger}\frac{\partial \mathbf{p}^\dagger}{\partial \mathbf{p}^*} = -S^\dagger \frac{\partial \Xi}{\partial \mathbf{p}^\dagger},$$

see Pavelka et al. [2018a] for a detailed calculation. In our toy model we have

$$(\dot{\mathbf{p}})_{\text{irr}} = \left.\frac{\partial \Xi}{\partial \mathbf{p}^*}\right|_{\mathbf{p}^* = \frac{\partial S}{\partial \mathbf{p}}} = -S^\dagger \left.\frac{\partial \Xi}{\partial \mathbf{p}^\dagger}\right|_{\mathbf{p}^\dagger = \frac{\partial E}{\partial \mathbf{p}}} = -\zeta \frac{\mathbf{p}^\dagger}{S^\dagger} = -\zeta T^{-1}\frac{\mathbf{p}}{m},$$

which is of course equal to the irreversible evolution for $\mathbf{p}$ obtained before. In a full generality the final system reads

$$\begin{aligned}
\dot{\mathbf{r}} &= \frac{\partial E}{\partial \mathbf{p}}, \\
\dot{\mathbf{p}} &= -\frac{\partial E}{\partial \mathbf{r}} - \frac{1}{\frac{\partial E}{\partial S}} \left.\frac{\partial \Xi}{\partial \mathbf{p}^\dagger}\right|_{\mathbf{p}^\dagger = \frac{\partial E}{\partial \mathbf{p}}} \\
\dot{S} &= \frac{1}{\left(\frac{\partial E}{\partial S}\right)^2} \mathbf{p}^\dagger \cdot \left.\frac{\partial \Xi}{\partial \mathbf{p}^\dagger}\right|_{\mathbf{p}^\dagger = \frac{\partial E}{\partial \mathbf{p}}}.
\end{aligned}$$

4.1.2 Dissipative Matrix

We will mention another possibility how to design the irreversible evolution, i.e. via *dissipation matrix*; see Öttinger [2005]. Let us assume that the dissipation potential is quadratic,

$$\Xi = \frac{1}{2} x_i^* M^{ij} x_j^*,$$

where $(x_1^*, \ldots, x_n^*)$ are the coordinates of the conjugate variable $\mathbf{x}^*$. Evolution of an arbitrary functional then reads

$$\dot{A} = \{A, E\} + \left\langle \frac{\delta A}{\delta x^i}, \left. \frac{\delta \Xi}{\delta x_i^*} \right|_{x_i^* = \frac{\delta S}{\delta x^i}} \right\rangle = \{A, E\} + \underbrace{\left\langle \frac{\delta A}{\delta x^i}, M^{ij} \frac{\delta S}{\delta x^j} \right\rangle}_{=[A,S]}, \tag{4.11}$$

and the latter term is often referred to as the dissipative bracket, operator M^{ij} being a dissipative matrix. The dissipative matrix is symmetric by definition (although this condition is sometimes intentionally violated, see Öttinger [2005], which leads to a different version of GENERIC), and positive definite (from convexity of Ξ). The requirement the irreversible evolution does not change total energy then reads

$$\frac{\delta E}{\delta x^i} M^{ij} = 0. \tag{4.12}$$

Note that the quadratic dissipation potential is positively homogeneous of degree 2 and hence the entropy rate is

$$\dot{S} = \{S, E\} + \left\langle \frac{\delta S}{\delta x^i}, \left. \frac{\delta \Xi}{\delta x_i^*} \right|_{x_i^* = \frac{\delta S}{\delta x^i}} \right\rangle = 2\Xi = [S, S] \geq 0,$$

providing the relation between the dissipation bracket and the dissipation potential.

4.1.3 Isothermal Case

Assume now that the temperature has the same constant value everywhere in the system. Assume, moreover, that the dissipation potential is quadratic. Then we can use a single functional $F(\mathbf{x})$ ($\mathbf{x}$ denotes a general state variable) playing the role of Helmholtz free energy,

$$F(\mathbf{x}) = E(\mathbf{x}) - TS(\mathbf{x}),$$

to generate the evolution equations. Indeed, Eq. (4.11) can be rewritten as

$$\dot{A} = \{A, F\} - T \underbrace{\{A, S\}}_{=0} - \frac{1}{T}[A, F] + \frac{1}{T} \underbrace{[A, E]}_{=0} = \{A, F\} - \frac{1}{T}[A, F], \tag{4.13}$$

where the degeneracies (4.4) and (4.12) were employed. In the isothermal case it is enough to have the free energy of the system, which then generates both reversible and irreversible evolution.

Note that energy is no longer conserved; it actually cannot be, because the iso-thermal setting means the body is in a heat bath with its surrounding and

hence interchanges energy. The rate by which the free energy is being dissipated is then

$$\dot{F} = \{F, F\} - \frac{1}{T}[F, F] = -\frac{1}{T}[F, F] \leq 0.$$

The evolution equation for temperature could be obtained from the evolution equation for entropy. Since the temperature is constant, the evolution equation of entropy density is effectively suppressed in the isothermal case.

Summary

Let us now summarize the construction of GENERIC. One first needs the set of state variables $\mathbf{x}$. Once they are chosen, the Poisson bracket expressing their kinematics is usually known (typically by a geometric argument, see e.g. Simo et al. [1988] and reference therein). For a given energy functional, one can write the reversible equations in a closed form. Irreversible evolution is generated by (generalized) gradient dynamics. The dissipation potential is typically convex in the conjugate variables and has a minimum at the origin. After conjugate variables are identified with derivatives of entropy, also the irreversible evolution gets a closed form. Complete evolution equations of the state variables $\mathbf{x}$ are the sum of the reversible and irreversible contribution, and the evolution of any functional $F(\mathbf{x})$ is given by the General Equation for Non-Equilibrium Reversible and Irreversible Coupling (GENERIC)

$$\dot{F} = \{F, E\} + \left\langle \frac{\delta F}{\delta \mathbf{x}}, \frac{\delta \Xi}{\delta \mathbf{x}^*}\Big|_{\mathbf{x}^* = \frac{\delta S}{\delta \mathbf{x}}} \right\rangle.$$

Remark 4.1 (State variables as coordinates)**.** *This formulation is written in a coordinate-less form. When we were dealing with reversible kinematics, entropy, momentum and position were suitable coordinates in the state space, while for irreversible it was energy, momentum and position. Since we wanted to express the equation as a whole in one coordinate system, namely entropy, momentum and density, we defined the energy conjugate variables. The irreversible part then had to be transformed appropriately.*

4.2 Isotropic Model

After explaining the basic principles on the toy model, let us move to a full continuum setting. We briefly describe the derivation of field equations for distortion based on Pavelka et al. [2018a] and show how the irreversible evolution is written in the entropic and energetic representation. In our examples, however, we focus on iso-thermal processes only, including a variant of a Giesekus model; possible modifications leading to Maxwell or Oldroyd-B model are discussed. At the end of the section we demonstrate how the kinematics of the natural configuration was recovered within GENERIC.

State Variables

Since we have moved from finite dimensional setting to continuum, the state variables are no longer elements of $\mathbb{R}^n$ for a degree of freedom $n \in \mathbb{N}$; we will

work with Lagrangian or Eulerian fields instead. First, we will derive its reversible kinematics in Lagrangian and subsequently in the Eulerian frame. The advantage of such a general approach is that the kinematics and dynamics still remain independent. Namely, energy can depend on the state variable in whatever way, while keeping the evolution equations still valid. We will conclude by prescribing a specific energy and dissipation potential, leading to the well known Oldroyd-B model.

Lagrangian Reversible Kinematics

Let us start in the Lagrangian frame, where each material point of the continuum has its own label $\mathbf{X}$ (Lagrangian position). The actual Eulerian position of the material point in an laboratory frame is denoted by mapping $\mathbf{y}(\mathbf{X})$. Compared with the setting of particle mechanics in the Sec. 4.1, this mapping is a continuum analogue of position $\mathbf{r}$ of the i-th particle, just the index is now continuous. Therefore, one may anticipate a momentum density field $\mathbf{M}(\mathbf{X})$ being the analogue of $\mathbf{p}$. The analogical Poisson bracket is

$$\{F, G\}^{\text{Lagrange}} = \int_{\mathbb{R}^3} \left(\frac{\delta F}{\delta y^i} \frac{\delta G}{\delta M_i} - \frac{\delta G}{\delta y^i} \frac{\delta F}{\delta M_i} \right) \mathrm{d}\mathbf{X}, \tag{4.14}$$

see e.g. Goldstein [1980], Simo et al. [1988], Pavelka et al. [2020] for the definition of the bracket and Morrison [1998] for an explanation of the functional derivative $\frac{\delta F}{\delta \mathbf{y}}$ and the related calculus. The sum is replaced by an integral (or a suitable inner product), the partial derivatives by functional ones. This bracket can be alternatively derived from the principle of least action, having Lagrangian dependent on the fields $\mathbf{y}$ and $\dot{\mathbf{y}}$.

As in the finite dimensional case, by comparing the both sides of $\dot{F} = \{F, E\}$ we see that the evolution equations implied by bracket (4.14) are

$$\left(\frac{\partial y^i}{\partial t} \right)_{\text{rev}} = \frac{\delta E}{\delta M_i} \tag{4.15a}$$

$$\left(\frac{\partial M_i}{\partial t} \right)_{\text{rev}} = -\frac{\delta E}{\delta y^i}, \tag{4.15b}$$

$$\left(\frac{\partial s}{\partial t} \right)_{\text{rev}} = 0. \tag{4.15c}$$

By s we denote the entropy density with respect to the volume in the reference configuration. For the same reason as in the Section 4.1, it is constant at every material point. The second equation expresses how momentum of the points is changed and the first one equation describes how the material points move.

Lagrangian Elastic Dynmaics

Typical dependence of energy on fields $\mathbf{y}$ and $\mathbf{M}$ is

$$E = \int_{\mathbb{R}^3} \frac{|\mathbf{M}|^2}{2\rho_0(\mathbf{X})} + \rho_0(\mathbf{X}) W \left(\frac{\partial \mathbf{y}}{\partial \mathbf{X}} \right) \mathrm{d}\mathbf{X} \tag{4.16}$$

where $\rho_0(\mathbf{X})$ is the field of density and $W(\mathbb{F})$ is the stored elastic energy. Equations (4.15) then become

$$\left(\frac{\partial \mathbf{y}}{\partial t}\right)_{\text{rev}} = \frac{\mathbf{M}}{\rho_0}, \tag{4.17a}$$

$$\left(\frac{\partial \mathbf{M}}{\partial t}\right)_{\text{rev}} = \text{Div}\left(\rho_0 \frac{\partial W}{\partial \mathbb{F}}\right), \tag{4.17b}$$

where Div stands for the divergence with respect to the Lagrangian position $\mathbf{X}$. By differentiating (4.17a) and substituting to the right-hand side from (4.17b) we would obtain a second order equation, the standard balance of momentum in hyperelasticity.

Reversible Kinematics of Distortion

The Lagrangian description is very detailed, we know the position and momentum of every point of the continuum. We aim, however, at Eulerian description of systems for which more rough state variables are appropriate. We hence switch from the state variables $(\mathbf{y}, \mathbf{M})$ to $(\rho, \mathbf{m}, s, \mathbb{A})$, the Eulerian fields of density, momentum, entropy and distortion defined as the inverse deformation gradient

$$(\mathbb{A})^I_i = A^I_i := \frac{\partial X^I}{\partial y^i} = \left(\frac{\partial y^i}{\partial X^i}\right)^{-1}.$$

The reason for taking the inverse deformation gradient as a new state variable, and not the deformation gradient itself, is simple. Since on the Eulerian description the current configuration is known, it is more natural to consider a tensor which takes the spatial vectors as an argument.

The idea of projection is very simple, just a mere substitution and a chain rule; however, not every projection is possible, simply because it may happen the Poisson bracket cannot be expressed solely in terms of the new variables [2]. Since in this case the arguments are fields and their gradients, and the new Eulerian fields depend on one of the old state variables, namely the position, the calculations are slightly more involved. We refer to Pavelka et al. [2020] for the complete derivation. The bracket for the state variables $(\rho, \mathbf{m}, s, \mathbb{A})$ consists of the 'fluid mechanics' part, i.e. the bracket for density, momentum and entropy,

[2] The most simple example of a failure would be the projection from the field of deformation gradient to the right Cauchy–Green tensor. In the Eulerian description the material derivative is given by $\dot{\mathbb{C}} = \mathbb{F}^\top \mathbb{L}^\top \mathbb{L}\mathbb{F}$, where $\mathbb{L} := \nabla \mathbf{v}$ is the Eulerian gradient of the Eulerian velocity field. One can choose $\mathbb{C}$ as the new state variable, but has to switch from the Eulerian velocity field $\mathbf{v}$ to the Lagrangian field of its pull-back to the reference configuration; see Simo et al. [1988] for a detailed derivation and explanation. We also refer to Pavelka et al. [2019] for a general method applicable when the projection fails.

plus two new terms for the distortion, namely

$$\begin{aligned}\{F,G\}^{\text{Euler}} = &\int_{\mathbb{R}^3} \rho \left(\frac{\partial}{\partial x^i}\frac{\delta F}{\delta \rho}\frac{\delta G}{\delta m_i} - \frac{\partial}{\partial x^i}\frac{\delta G}{\delta \rho}\frac{\delta F}{\delta m_i} \right) \mathrm{d}\mathbf{x} \\ &+ \int_{\mathbb{R}^3} m_i \left(\frac{\partial}{\partial x^j}\frac{\delta F}{\delta m_i}\frac{\delta G}{\delta m_j} - \frac{\partial}{\partial x^j}\frac{\delta G}{\delta m_i}\frac{\delta F}{\delta m_j} \right) \mathrm{d}\mathbf{x} \\ &+ \int_{\mathbb{R}^3} s \left(\frac{\partial}{\partial x^i}\frac{\delta F}{\delta s}\frac{\delta G}{\delta m_i} - \frac{\partial}{\partial x^i}\frac{\delta G}{\delta s}\frac{\delta F}{\delta m_i} \right) \mathrm{d}\mathbf{x} \\ &+ \int_{\mathbb{R}^3} A^I_i \left(\frac{\partial}{\partial x^j}\frac{\delta F}{\delta A^I_j}\frac{\delta G}{\delta m_i} - \frac{\partial}{\partial x^j}\frac{\delta G}{\delta A^I_j}\frac{\delta F}{\delta m_i} \right) \mathrm{d}\mathbf{x} \\ &+ \int_{\mathbb{R}^3} \left(\frac{\partial A^I_i}{\partial x^j} - \frac{\partial A^I_j}{\partial x^i} \right) \left(\frac{\delta F}{\delta A^I_j}\frac{\delta G}{\delta m_i} - \frac{\delta G}{\delta A^I_j}\frac{\delta F}{\delta m_i} \right) \mathrm{d}\mathbf{x}.\end{aligned}$$

The same localisation procedure as for the Lagrange bracket, though more integration by parts has to be carried out, leads (after a suitable re-arrangement) to evolution equations

$$\begin{aligned}\left(\frac{\partial \rho}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^i}\left(\rho \frac{\delta E}{\delta m_i}\right), \\ \left(\frac{\partial m_i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^j}\left(m_i \frac{\delta E}{\delta m_j}\right) - \rho \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \rho} - m_j \frac{\partial}{\partial x^i}\frac{\delta E}{\delta m_j} - s\frac{\partial}{\partial x^i}\frac{\delta E}{\delta s} - A^J_j \frac{\partial}{\partial x^i}\frac{\delta E}{\delta A^J_j} \\ &\quad + \frac{\partial}{\partial x^i}\left(A^J_j \frac{\delta E}{\delta A^J_j}\right) + \frac{\partial}{\partial x^j}\left(-A^J_i \frac{\delta E}{\delta A^J_j}\right), \\ \left(\frac{\partial s}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^i}\left(s \frac{\delta E}{\delta m_i}\right), \\ \left(\frac{\partial A^I_i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^i}\left(A^I_j \frac{\delta E}{\delta m_j}\right) + \left(\frac{\partial A^I_j}{\partial x^i} - \frac{\partial A^I_i}{\partial x^j}\right)\frac{\delta E}{\delta m_j} = -\frac{\partial A^I_i}{\partial x^j}\frac{\delta E}{\delta m_j} - A^I_j \frac{\partial}{\partial x^i}\frac{\delta E}{\delta m_j}.\end{aligned}$$

As already mentioned, the equations are valid for any energy functional, be it one for standard simple fluids, Korteweg, or other non-simple continua. The equations for density and entropy are nothing but a mere convection, corresponding to a balance equation with zero flux and source. For the equation for distortion we recall (4.15a) by which $\frac{\delta E}{\delta m_j}$ is nothing but the velocity and hence the equation agrees with the standard formula for material derivative of the deformation gradient $\dot{\mathbb{F}} = \mathbb{L}\mathbb{F}$. It is only the equation for momentum which does not resemble any standard formulation of continuum mechanics, but it will be shown in the following subsection that for a suitable class of energy functionals the standard structure is indeed recovered.

Elastic Dynamics of Distortion

For the sake of simplicity we stick to the iso-thermal setting. As can be seen from the equation (4.13), for the reversible kinematics it just means to replace the total energy E by its Legendre transform, the free energy F. We will suppose

it takes the form

$$F(\rho, \mathbf{m}, T, \mathbb{A}) = \int_{\mathbb{R}^3} f(\rho, \mathbf{m}, T, \mathbb{A}) \, \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \frac{|\mathbf{m}|^2}{2\rho} + \phi(T, \rho) + \rho\psi(T, \mathbb{A}) \, \mathrm{d}\mathbf{x}. \tag{4.18}$$

Using the special structure of the free energy functional, we now rewrite the evolution equation for momentum to a more standard form. Since the density f depends on the fields only in an algebraic manner, the functional derivatives of F are represented by the partial derivatives of f. If we further use

$$s = -\frac{\partial f}{\partial T}, \qquad T = \frac{\partial e}{\partial s}, \qquad \frac{\partial T}{\partial x^i} = 0,$$

a direct computation leads to

$$\begin{aligned}
\left(\frac{\partial m_i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \rho \frac{\partial}{\partial x^i}\frac{\partial f}{\partial \rho} - m_j \frac{\partial}{\partial x^i}\frac{\partial f}{\partial m_j} + \frac{\partial f}{\partial T}\frac{\partial T}{\partial x^i} - A_j^J \frac{\partial}{\partial x^i}\frac{\partial f}{\partial A_j^J} \\
&\quad + \frac{\partial}{\partial x^i}\left(A_j^J \frac{\partial f}{\partial A_j^J}\right) + \frac{\partial}{\partial x^j}\left(-A_i^J \frac{\partial f}{\partial A_j^J}\right) \\
&= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \frac{\partial}{\partial x^i}\left(-f + \rho\frac{\partial f}{\partial \rho} + m_j \frac{\partial f}{\partial m_j}\right) + \frac{\partial}{\partial x^j}\left(-A_i^J \frac{\partial f}{\partial A_j^J}\right) \\
&= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \frac{\partial}{\partial x^i}\left(-\phi + \rho\frac{\partial \phi}{\partial \rho}\right) + \frac{\partial}{\partial x^j}\left(-\rho A_i^J \frac{\partial \psi}{\partial A_j^J}\right).
\end{aligned}$$

Simplyfying the other equations for this specific free energy ansatz leads to the final system (note that the equation for entropy has been dropped)

$$\begin{aligned}
\left(\frac{\partial \rho}{\partial t}\right)_{\text{rev}} &= -\operatorname{div}(\rho \mathbf{v}), \\
\left(\frac{\partial \mathbf{m}}{\partial t}\right)_{\text{rev}} &= -\operatorname{div}(\mathbf{m} \otimes \mathbf{v}) + \operatorname{div} \mathbb{T}, \\
\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{rev}} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L},
\end{aligned}$$

where we defined

$$\begin{aligned}
\mathbf{v} &:= \frac{\delta F}{\delta \mathbf{m}} = \frac{\partial f}{\partial \mathbf{m}} = \frac{\mathbf{m}}{\rho}, & \mathbb{L} &:= \nabla \mathbf{v}, \\
\mathbb{T} &:= -p_{th}\mathbb{I} - \rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}}, & p_{th} &:= -\phi + \rho \frac{\partial \phi}{\partial \rho},
\end{aligned}$$

i.e. the evolution equations for $\mathbf{m}$ now have the standard form of balance of momentum.

If one were to specify ψ, a good choice for a viscoelastic fluid would be

$$\psi(T, \mathbb{A}) = \frac{G(T)}{2}(|\mathbb{A}^{-1}|^2 - 3) - k_B T \ln \det(\mathbb{A}^{-1}\mathbb{A}^{-\top}), \tag{4.19}$$

since it can be derived from a more detailed level of description; see e.g. Pavelka et al. [2018b] where they use as a state parameter $\mathbb{B} := \mathbb{A}^{-1}\mathbb{A}^{-\top}$ satisfying $\operatorname{Tr}\mathbb{B} = |\mathbb{A}^{-1}|^2$.

Remark. *We stress that there is no material or phenomenological constant in front of the logarithm, only the universal Boltzmann constant k_B. The only freedom is then in specifying the dependence of the elastic parameter G on temperature T. The reason for such a restriction lies in the origin of the two terms in the energy. While the first comes from internal energy where it express a phenomenological stiffness, e.g of a polymer chain, the second appears due to the Legendre transform and comes from entropy, which is derived from theoretical considerations and contains no phenomenology at all.*

For this very specific choice of energy we find that

$$\mathbb{T} = -p_{th}\mathbb{I} + \rho G(T)\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{2k_BT}{G(T)}\mathbb{I}\right),$$

which is nothing but the standard compressible Neo-Hook model with $\mathbb{B} := \mathbb{A}^{-1}\mathbb{A}^{-\top}$.

Irreversible Kinematics of Distortion

As in the finite dimensional setting we consider the entropic representation, having therefore $(\rho, \mathbf{m}, e, \mathbb{A})$ as the state variables. Note that here e denotes the field of total energy *per volume*. The thermodynamic relation then take the form

$$S = S(\rho, \mathbf{m}, e, \mathbb{A}),$$

i.e. entropy is now a functional of the state variables. Irreversible evolution of any functional F is a gradient flow driven by the dissipation potential $\Xi(\rho, \mathbf{m}, e, \mathbb{A}, \rho^*, \mathbf{m}^*, e^*, \mathbb{A}^*)$

$$\begin{aligned}\left(\dot{F}\right)_{\text{irr}} &= \left\langle \frac{\delta F}{\delta \mathbf{x}}, \left.\frac{\delta \Xi}{\delta \mathbf{x}^*}\right|_{\mathbf{x}^*=\frac{\delta S}{\delta \mathbf{x}}} \right\rangle \\ &= \left\langle \frac{\delta F}{\delta \rho}, \left.\frac{\delta \Xi}{\delta \rho^*}\right|_{\rho^*=\frac{\delta S}{\delta \rho}} \right\rangle + \left\langle \frac{\delta F}{\delta \mathbf{m}}, \left.\frac{\delta \Xi}{\delta \mathbf{m}^*}\right|_{\mathbf{m}^*=\frac{\delta S}{\delta \mathbf{m}}} \right\rangle \\ &\quad + \left\langle \frac{\delta F}{\delta e}, \left.\frac{\delta \Xi}{\delta e^*}\right|_{e^*=\frac{\delta S}{\delta e}} \right\rangle + \left\langle \frac{\delta F}{\delta \mathbb{A}}, \left.\frac{\delta \Xi}{\delta \mathbb{A}^*}\right|_{\mathbb{A}^*=\frac{\delta S}{\delta \mathbb{A}}} \right\rangle,\end{aligned}$$

or in the localized form

$$\begin{aligned}\left(\frac{\partial \rho}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta \Xi}{\delta \rho^*}\right|_{\rho^*=\frac{\delta S}{\delta \rho}}, \\ \left(\frac{\partial m_i}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta \Xi}{\delta (m^*)^i}\right|_{(m^*)^i=\frac{\delta S}{\delta m_i}}, \\ \left(\frac{\partial e}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta \Xi}{\delta e^*}\right|_{e^*=\frac{\delta S}{\delta e}}, \\ \left(\frac{\partial A_i^I}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta \Xi}{\delta (A^*)_I^i}\right|_{(A^*)_I^i=\frac{\delta S}{\delta A_i^I}}.\end{aligned} \tag{4.20}$$

Apart from the standard properties of Ξ summarized in the section 4.1, the dissipation potential has to be such that:

1. The total mass $M := \int_{\mathbb{R}^3} \rho \, \mathrm{d}\mathbf{x}$ is conserved.

2. The total energy $E := \int_{\mathbb{R}^3} e \, \mathrm{d}\mathbf{x}$ is conserved.

These conditions are for example satisfied when Ξ depends merely on gradients of ρ^* and e^*. If we wanted also momentum to be conserved, the same would hold also for $\mathbf{m}^*$.

As before, we would like to switch to state variables $(\rho, \mathbf{m}, s, \mathbb{A})$, where s is the volume density of the entropy functional. For simplicity we assume that

$$S = \int_{\mathbb{R}^3} s(e(\mathbf{x}), \rho(\mathbf{x}), \mathbf{m}(\mathbf{x}), \mathbb{A}(\mathbf{x})) \, \mathrm{d}\mathbf{x},$$

i.e. the dependence is purely algebraic, not involving e.g. gradients of the fields ρ, $\mathbf{m}$ or $\mathbb{A}$. The energy functional then rerads

$$E = \int_{\mathbb{R}^3} e(s(\mathbf{x}), \rho(\mathbf{x}), \mathbf{m}(\mathbf{x}), \mathbb{A}(\mathbf{x})) \, \mathrm{d}\mathbf{x},$$

where $e = s^{-1}$ is the total energy *per volume*, and hence we have simple relations between conjugate variables

$$s^\dagger := \left(\frac{\delta E}{\delta s}\right) = \frac{1}{e^*} =: \left(\frac{\delta S}{\delta e}\right)^{-1}, \quad \rho^\dagger = -s^\dagger \rho^* \quad \mathbf{m}^\dagger = -s^\dagger \mathbf{m}^*, \quad \mathbb{A}^\dagger = -s^\dagger \mathbb{A}^*.$$

Note that $s^\dagger$ is nothing but the temperature. We also do not consider dissipation potentials involving gradients of the conjugate fields. The procedure would be analogical, but far more technical. For more general entropies and dissipation potentials it is better to proceed case to case, always with the specific form at disposal. In the next section we will show how to add viscous dissipation in an iso-thermal setting. Non-isothermal cases and other examples, e.g. heat transfer, can be found in [Pavelka et al., 2018b, sec. 4.5].

Under these assumptions on S and Ξ we are now ready to transform the equations. For a detailed description we refer to [Pavelka et al., 2018b, sec. 4.5], here we mention only the main steps. First, one needs to rewrite $\frac{\delta \Xi}{\delta \mathbf{x}^*}$ in terms of $\frac{\delta \Xi}{\delta \mathbf{x}^\dagger}$ and $s^\dagger$. Then the irreversible evolution of entropy is found by chain rule, plugging from the evolution equations of other state variables. After doing so, one arrives at

$$\left(\frac{\partial A_i^I}{\partial t}\right)_{\text{irr}} = -s^\dagger \left.\frac{\delta \Xi}{\delta (A_I^i)^\dagger}\right|_{(A_I^i)^\dagger = \frac{\delta E}{\delta A_i^I}},$$

$$\left(\frac{\partial s}{\partial t}\right)_{\text{irr}} = (A_I^i)^\dagger \left.\frac{\delta \Xi}{\delta (A_I^i)^\dagger}\right|_{(A_I^i)^\dagger = \frac{\delta E}{\delta A_i^I}} \geq 0.$$

Note that since we want to conserve mass, momentum and energy, the algebraic dissipation potential cannot depend on the corresponding conjugate variables at all. Hence the irreversible evolution of other variables is zero and the evolution equation for entropy contains no flux term. Finally, since the dissipation potential does not depend on e^*, its dependence on the energetic conjugate variables cannot be arbitrary. One possible way how to comply with this restriction is to suppose that

- the dissipation potential Ξ is a function of fractions $\frac{(A_I^i)^\dagger}{s^\dagger}$.

Dissipative Dynamics of Distortion

Let us now show how one can derive a variant of an isothermal Giesekus model of visco-elastic fluids. As in the elastic case, we will specify the Helmholtz free energy, which is more suitable for isothermal processes. Using the same ansatz (4.18) we obtain the specific form of the conjugate variables that will be needed

$$\begin{aligned}\mathbf{v} := \mathbf{m}^\dagger = \frac{\delta E}{\delta \mathbf{m}} = \frac{\partial e}{\partial \mathbf{m}} = \frac{\partial f}{\partial \mathbf{m}} = \frac{\mathbf{m}}{\rho},\\ \mathbb{A}^\dagger = \frac{\delta E}{\delta \mathbb{A}} = \frac{\partial e}{\partial \mathbb{A}} = \frac{\partial f}{\partial \mathbb{A}} = \rho\frac{\partial \psi}{\partial \mathbb{A}}.\end{aligned}$$

In iso-thermal setting the choice of the dissipation bracket is simply

$$[F,G] = \int_{\mathbb{R}^3} 2\mu \left(\nabla \frac{\delta F}{\delta \mathbf{m}}\right)_{\text{sym}} : \left(\nabla \frac{\delta G}{\delta \mathbf{m}}\right)_{\text{sym}} + \Lambda \left(\mathbb{A}^\top \frac{\delta F}{\delta \mathbb{A}}\right) : \left(\mathbb{A}^\top \frac{\delta G}{\delta \mathbb{A}}\right) \mathrm{d}\mathbf{x}, \quad (4.21)$$

where $(\nabla\cdot)_{\text{sym}}$ stands for the symmetric gradient, because it leads to a dissipation rate

$$\dot{F} = -\frac{1}{T}[F,F] = -\frac{1}{T}\int_{\mathbb{R}^3} 2\mu\,|\mathbb{D}|^2 + \Lambda \left|\rho\mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}}\right|^2 \mathrm{d}\mathbf{x},$$

where $\mathbb{D}$ stands for the symmetric velocity gradient. In general, the coefficients may be temperature dependent. For a non-isothermal variant the reader is referred to Pavelka et al. [2018b]. The first term yields the standard viscous dissipation, the second is chosen since it is a multiple of the partial Cauchy stress. Localizing the bracket (4.21) yields the irreversible evolution

$$\begin{aligned}\left(\frac{\partial \mathbf{m}}{\partial t}\right)_{\text{irr}} &= \frac{1}{T}\operatorname{div}(2\mu\mathbb{D}),\\ \left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{irr}} &= \frac{\Lambda}{T}\mathbb{A}\left(-\rho\mathbb{A}^\top\frac{\partial\psi}{\partial\mathbb{A}}\right).\end{aligned} \quad (4.22)$$

If we choose ψ as in (4.19) we obtain

$$\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{irr}} = \frac{\Lambda}{T}G(T)\rho\mathbb{A}\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{k_BT}{G(T)}\mathbb{I}\right).$$

For the sake of simpler comparison, we would like to rewrite the irreversible evolution in terms of

$$\mathbb{F}_\kappa := \mathbb{A}^{-1}, \quad \text{and} \quad \mathbb{B}_\kappa := \mathbb{F}_\kappa\mathbb{F}_\kappa^\top = \mathbb{A}^{-1}\mathbb{A}^{-\top}.$$

Since we have

$$\mathbb{A}^\dagger = \frac{\delta E}{\delta \mathbb{A}} = -\mathbb{F}_\kappa^\top\mathbb{F}_\kappa^\dagger\mathbb{F}_\kappa^\top, \qquad \text{and} \qquad \mathbb{F}_\kappa^\dagger = 2\mathbb{B}_\kappa^\dagger\mathbb{F}_\kappa,$$

rewriting the dissipation bracket in terms of $\mathbb{F}_\kappa$ and $\mathbb{B}_\kappa$ leads to an irreversible evolution

$$\begin{aligned}\left(\frac{\partial \mathbb{F}_\kappa}{\partial t}\right)_{\text{irr}} &= -\frac{\Lambda}{T}\left(\rho\frac{\partial\psi}{\partial\mathbb{F}_\kappa}\mathbb{F}_\kappa^\top\right)\mathbb{F}_\kappa,\\ \left(\frac{\partial \mathbb{B}_\kappa}{\partial t}\right)_{\text{irr}} &= -\frac{\Lambda}{T}\left(2\rho\frac{\partial\psi}{\partial\mathbb{B}_\kappa}\mathbb{B}_\kappa\right)\mathbb{B}_\kappa.\end{aligned}$$

Final Equations

Once the energy functional and the dissipation bracket are specified in (4.18) and (4.21) respectively, we can formulate the final equations

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0,\\ \frac{\partial \mathbf{m}}{\partial t} + \operatorname{div}(\mathbf{m} \otimes \mathbf{v}) &= \operatorname{div}\left(-p_{th}\mathbb{I} - \rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + 2\mu \mathbb{D}\right),\\ \frac{\partial \mathbb{A}}{\partial t} + [\nabla \mathbb{A}]\mathbf{v} &= -\mathbb{A}\mathbb{L} + \frac{\Lambda}{T}\mathbb{A}\left(-\rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}}\right).\end{aligned}$$

When rewritten in terms of $\mathbb{F}_\kappa := \mathbb{A}^{-1}$ they become

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0,\\ \frac{\partial \mathbf{m}}{\partial t} + \operatorname{div}(\mathbf{m} \otimes \mathbf{v}) &= \operatorname{div}\left(-p_{th}\mathbb{I} + \rho \frac{\partial \psi}{\partial \mathbb{F}_\kappa}\mathbb{F}_\kappa^\top + 2\mu \mathbb{D}\right),\\ \frac{\partial \mathbb{F}_\kappa}{\partial t} + [\nabla \mathbb{F}_\kappa]\mathbf{v} &= \mathbb{L}\mathbb{F}_\kappa - \frac{\Lambda}{T}\left(\rho \frac{\partial \psi}{\partial \mathbb{F}_\kappa}\mathbb{F}_\kappa^\top\right)\mathbb{F}_\kappa,\end{aligned}$$

and for $\mathbb{B} := \mathbb{A}^{-1}\mathbb{A}^{-\top} = \mathbb{F}_\kappa \mathbb{F}_\kappa^\top$ they are

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0,\\ \frac{\partial \mathbf{m}}{\partial t} + \operatorname{div}(\mathbf{m} \otimes \mathbf{v}) &= \operatorname{div}\left(-p_{th}\mathbb{I} + 2\rho \frac{\partial \psi}{\partial \mathbb{B}_\kappa}\mathbb{B}_\kappa + 2\mu \mathbb{D}\right),\\ \frac{\partial \mathbb{B}_\kappa}{\partial t} + [\nabla \mathbb{B}_\kappa]\mathbf{v} &= \mathbb{L}\mathbb{B}_\kappa + \mathbb{B}_\kappa \mathbb{L}^\top - \frac{\Lambda}{T}\left(2\rho \frac{\partial \psi}{\partial \mathbb{B}_\kappa}\mathbb{B}_\kappa\right)\mathbb{B}_\kappa.\end{aligned}$$

If we even use the specific energy (4.19), now written in terms of $\mathbb{B}_\kappa$ as

$$\psi(T, \mathbb{B}_\kappa) = \frac{G(T)}{2}(\operatorname{Tr}\mathbb{B}_\kappa - 3) - k_B T \ln \det(\mathbb{B}_\kappa),$$

we recover the standard compressible Giesekus model

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) &= 0,\\ \frac{\partial \mathbf{m}}{\partial t} + \operatorname{div}(\mathbf{m} \otimes \mathbf{v}) &= \operatorname{div}\left(-p_{th}\mathbb{I} + \rho G(T)\left(\mathbb{B}_\kappa - \frac{2k_B T}{G(T)}\mathbb{I}\right) + 2\mu \mathbb{D}\right),\\ \frac{\partial \mathbb{B}_\kappa}{\partial t} + [\nabla \mathbb{B}_\kappa]\mathbf{v} &= \mathbb{L}\mathbb{B}_\kappa + \mathbb{B}_\kappa \mathbb{L}^\top - \frac{\Lambda G(T)}{T}\rho\left(\mathbb{B}_\kappa - \frac{2k_B T}{G(T)}\mathbb{I}\right)\mathbb{B}_\kappa.\end{aligned}$$

In all of these systems, the irreversible part of the evolution equation for $\mathbb{A}$, $\mathbb{F}_\kappa$ or $\mathbb{B}_\kappa$, respectively, represents a '*slip*', by which these variables differ if they were merely advected by the velocity field.

Remark (Maxwell and Oldroyd-B models)**.** *If we choose the dissipation bracket such that the dissipation rate is*

$$\begin{aligned}\dot{F} &= -\frac{1}{T}[F, F] = -\frac{1}{T}\int_{\mathbb{R}^3} 2\Lambda \mathbb{B}_\kappa^\dagger \mathbb{B}_\kappa : \mathbb{B}_\kappa^\dagger \,\mathrm{d}\mathbf{x}\\ &= -\frac{1}{T}\int_{\mathbb{R}^3} 2\Lambda(\mathbb{B}_\kappa^\dagger \mathbb{B}_\kappa) : (\mathbb{B}_\kappa^\dagger \mathbb{B}_\kappa)\mathbb{B}_\kappa^{-1} \,\mathrm{d}\mathbf{x} = -\frac{1}{T}\int_{\mathbb{R}^3} \frac{\Lambda}{2}\left|2\mathbb{B}_\kappa^\dagger \mathbb{B}_\kappa\right|^2_{\mathbb{B}_\kappa^{-1}} \,\mathrm{d}\mathbf{x},\end{aligned}$$

i.e. with no viscosity and with a different norm of the Cauchy stress, the equation for $\mathbb{B}_\kappa$ *becomes*

$$\frac{\partial \mathbb{B}_\kappa}{\partial t} + [\nabla \mathbb{B}_\kappa]\mathbf{v} = \mathbb{L}\mathbb{B}_\kappa + \mathbb{B}_\kappa \mathbb{L}^\top - \frac{\Lambda}{T} 2\rho \frac{\partial \psi}{\partial \mathbb{B}_\kappa}\mathbb{B}_\kappa$$

which leads to the Maxwell model. Adding the viscosity part as before would yield the Oldroyd-B model.

Summary

We started with a canonical bracket describing the kinematics of standard continua. Since this description was to detailed for our purposes, we derived the bracket for hydromechanics fields supplemented by distortion. When restricted to energies of simple continua (i.e. not depending on gradients of the fields), we recovered the standard, reversible equations of elastic materials. Then we formulated the irreversible evolution using the dissipation potential and show how it can be rewritten using the energetic conjugate variables, which is needed for a unified formulation of the final equations in the energetic representation. Nevertheless in the example we restrict ourselves to iso-thermal processes where the total evolution is generated by a single potential, the Helmholtz free energy. The entropic representation is then not necessary and both the reversible and irreversible evolutions are formulated in the energetic representation directly. The chosen dissipation bracket then lead to a dissipation rate quadratic in the symmetric velocity gradient and the partial Cauchy stress corresponding to the distortion. In general, the dissipation rate in the distortion can be expressed as a suitable norm of a chosen stress measure, where both choices should reflect the underlying physics. This choice then affects how evolution differs from a mere advection. Finally, for the Neo-Hook free energy we obtained a closed system of equations, a variant of the Giesekus model.

Remark (Plastic Distortion)**.** *Switching from deformation* $\mathbf{y}$ *and momentum* $\mathbf{M}$ *to hydromechanic variables and distortion has also another reason. In the former description, we could add dissipation only to the equation for momentum, i.e. viscosity, which would lead to a Kelvin-Voight like rheology. For recovering the irreversible kinematics of distortion, the original two state variables* $(\mathbf{y}, \mathbf{M})$ *need to be supplemented by a new one, namely by the plastic distortion* $\mathbb{G}$*, whose evolution would be purely irreversible. These descriptions are then related by* $\nabla \mathbf{y} = \mathbb{A}^{-1}\mathbb{G}$*.*

Remark (Structural Space and Natural Configuration)**.** *Let us highlight that the kinematics of distortion*

$$\frac{\partial \mathbb{A}}{\partial t} + [\nabla \mathbb{A}]\mathbf{v} = -\mathbb{A}\mathbb{L} - T\frac{\delta \Xi}{\delta \mathbb{A}^\dagger}, \tag{4.23}$$

is nothing but the kinematics of the structural space *defined by the Kröner decomposition (see e.g. Gurtin et al. [2010]) or* the kinematics of the natural configuration *(see Rajagopal and Srinivasa [2000b], Málek and Průša [2016]), where the choice of* $E = E(\mathbb{A})$ *and* $\Xi = \Xi(\mathbb{A}, \mathbb{A}^\dagger)$ *(or the dissipative bracket* $[\cdot, \cdot]$*) specifies respectively its elastic and dissipative dynamics. The reasons are the following:*

- *The reference configuration (which is by definition obtained by tracking the particles' trajectories) can be reconstructed by the integration of a tensor field, which is a solution to the evolution equations*

$$\frac{\partial \mathbb{A}}{\partial t} + [\nabla \mathbb{A}]\mathbf{v} = -\mathbb{A}\mathbb{L}.$$

The complete GENERIC equation for distortion, containing also the irreversible part, yields, in general, a different solution. This justify the standard illustrative splitting of the reference, local natural, and current configuration. Moreover, if the tensor field $\mathbb{A}$ satisfies the integrability condition, the natural configuration exists globally.

- *Energy depends on the distortion $\mathbb{A}$, i.e. the deformation from the natural configuration to the current one is elastic. The Helmholtz free energy typically satisfies*

$$\frac{\partial \psi}{\partial \mathbb{A}}(\mathbb{I}) = 0,$$

i.e. when the material occupies the natural configuration (the natural and current configuration coincides), it is in a (partial-)stress-free state. In general, as e.g. for (4.19)*, the natural configuration defined by $\mathbb{A}$ is stress-free up to a homogeneous compression/expansion, which is due to the spherical part of stress only.*

- *The dissipation potential Ξ is a function of $\mathbb{A}$ and*

$$\mathbb{A}^\dagger = \rho \frac{\partial \psi}{\partial \mathbb{A}},$$

i.e. the dissipation rate depends on some specific stress measure. This might be seen as an analogue to [Málek and Průša, 2016, Fig. 4], where the dissipation is due to the 'dashpot' pulled by the 'elastic spring'. As explained in the following remark, the dissipation potential, and hence the dissipation rate, can be evenly expressed in terms of the 'rate of the dashpot' rather than in the 'stress of the elastic spring'.

Remark 4.2 (Forces, Fluxes and Affinities)**.** *Entropy production can be equivalently expressed in rates, i.e. as a function of $(\dot{\mathbf{x}})_{irr} = \dot{\mathbf{x}} - (\dot{\mathbf{x}})_{rev}$, using the conjugate dissipation potential Ξ^*; see [Pavelka et al., 2018b, sec. 4.4.3] or Janečka and Pavelka [2018a]. Hence, when written in the inverse of distortion $\mathbb{F}_\kappa$, it depends on*

$$\frac{\partial \mathbb{F}_\kappa}{\partial t} + [\nabla \mathbb{F}_\kappa]\mathbf{v} - \mathbb{L}\mathbb{F}_\kappa =: -\mathbb{F}_\kappa \mathbb{L}_\kappa.$$

Under special circumstances, e.g. for concentration, working with Ξ or Ξ^* corresponds respectively to a description of the dissipation either by thermodynamic fluxes or forces. In some cases, like in the following section, it is beneficial to work with the dual dissipation potential Ξ^* instead.

Remark (Incompressible Inelastic Response)**.** *Were the trace of the irreversible evolution of distortion zero, the determinants of distortion and of deformation gradient have the same evolution equation. In other words, the irreversible evolution of the determinant of distortion is zero.*

4.3 An-isotropic Model

After having established the connections to other thermodynamic frameworks and well established models of isotropic, visco-elastic fluids, we are now ready to move to anisotropy. Materials can exhibit anisotropy with regard to mechanical response in several ways. For instance, in crystal plasticity, we can have anisotropy with respect to the elastic response, described by the stored energy function. We can also have anisotropy associated with the yield surface and this is captured by the properties of the dissipation potential. If we were to model liquid crystals, regarded as a rod like suspension in an isotropic fluid, we would also observe two kinds of anisotropic response, both of a different nature. Elastic rods lead to an anisotropy in the elastic response, while the movement of the rods in the viscous fluid, itself isotropic, causes that the rate of dissipation is different for motions along different directions. The last example of anisotropy is related to temperature expansion, which may occur for example in a steel reinforced concrete.

The procedure of deriving the field equations is the same as for the isotropic model, only more information from the Lagrangian description by $(\mathbf{y}, \mathbf{M})$ is extracted. Keeping the same structure as in the previous sections, we first choose the state variables and show an example of free energy. When explaining the irreversible kinematics we profit from the dual formulation using the conjugate dissipation potential Ξ^* and characterize a class of models for which the symmetry is constant in the structural space, or the natural configuration. Let us recall that this is the restriction imposed in Rajagopal and Srinivasa [2001], which we now overcome. We close the section by two simple models following this distinction; one having anisotropic vector constant in the structural space, which is for example common in crystal plasticity (see e.g. Gurtin et al. [2010], Kratochvíl et al. [2016]), the other one describing visco-elastic fibers immersed in a visco-elastic fluids, where additional dissipation originates in the slip between the fiber and the fluid, serving as a prototype of models describing e.g. for highly concentrated polymeric fluids or liquid crystals, as suggested also in Rajagopal and Srinivasa [2001].

State Variables

While the description by $(\mathbf{y}, \mathbf{M})$ is still far too detailed for many applications, mainly because it allows only for trivial entropies, the fields $(\rho, \mathbf{m}, s, \mathbb{A})$ alone are not sufficient for describing anisotropic materials. Hence we will cast a projection from $(\mathbf{y}, \mathbf{M})$ to a richer class of state variables. Following Rajagopal and Srinivasa [2001], we choose for simplicity $(\rho, \mathbf{m}, s, \mathbb{A}, \mathbf{b})$ as the target set, where $\mathbf{b}$ is the vector describing the anisotropy, observed in the current, spatial configuration, which is suitable for describing materials with transverse isotropy. For other anisotropies more vectors may be considered, see e.g. Kratochvíl et al. [2016] where three vectors (or co-vectors) are used to describe crystal lattice. A general approach to anisotropy can be based on the structural tensors described e.g. in Zhang and Rychlewski [1990] and an application of the general procedure described in [Öttinger, 2005, App. B.4].

The forthcoming derivation of the mechanics for $(\rho, \mathbf{m}, s, \mathbb{A}, \mathbf{b})$ relies com-

pletely on our understanding of the nature of $\mathbf{b}$. We suppose that the anisotropy in the reference configuration is described by a *vector* field $\mathbf{B}(\mathbf{X})$ and hence we define

$$\mathbf{b}(\mathbf{x})|_{\mathbf{x}=\mathbf{y}(\mathbf{X})} := \frac{\partial \mathbf{y}}{\partial \mathbf{X}}(\mathbf{X})\mathbf{B}(\mathbf{X}). \tag{4.24}$$

Although strictly speaking the anisotropy is rather described by the structural tensors $\mathbf{b}\otimes\mathbf{b}$ and $\mathbf{B}\otimes\mathbf{B}$, since they do not carry the information about orientation, only about the one-dimensional subspace (they are invariant under changing the direction of the vector), we choose for simplicity rather $\mathbf{b}$ as the additional state variable.

Reversible Kinematics

As already mention in the precedent section 4.2, the projection of $(\mathbf{y}, \mathbf{M})$ on $(\rho, \mathbf{m}, s, \mathbb{A})$ is carried out in [Pavelka et al., 2020, App. B] [3] . Here we therefore highlight just how the new field $\mathbf{b}$ enters the procedure. We hence consider a projection from $(\mathbf{y}, \mathbf{M})$ to $(\rho, \mathbf{m}, s, \mathbb{A}, \mathbf{b})$. Recalling the definition (4.24) we have

$$b^i(\mathbf{x}) := F^i_I(\mathbf{x})B^I(\mathbf{x}),$$

where F^i_I stands for the deformation gradient (i.e. the inverse of the distortion A^J_j) and

$$\mathbf{B}(\mathbf{x})|_{\mathbf{x}=\mathbf{y}(\mathbf{X})} := \mathbf{B}(\mathbf{X})$$

is the Eulerian field derived from the Lagrangian field $\mathbf{B}(\mathbf{X})$.

Since by the Leibniz rule we have

$$\frac{\delta b^i(\mathbf{x})}{\delta y^k(\mathbf{X})} = \frac{\delta F^i_I(\mathbf{x})}{\delta y^k(\mathbf{X})}B^I(\mathbf{x}) + F^i_I(\mathbf{x})\frac{\delta B^I(\mathbf{x})}{\delta y^k(\mathbf{X})},$$

we can use the formulas from [Pavelka et al., 2020, App. B] expressing the derivative with respect to arbitrary Eulerian field

$$\frac{\delta B^I(\mathbf{x})}{\delta y^k(\mathbf{X})} = -\frac{\partial B^I}{\partial x^k}(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x})),$$

and the derivative of the Eulerian field of the deformation gradient

$$\frac{\delta F^i_I(\mathbf{x})}{\delta y^k(\mathbf{X})} = -\frac{\partial \delta}{\partial X^I}(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\delta^i_k - \frac{\partial F^i_I}{\partial x^k}(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x})).$$

[3] We rely fully on the formalism used in Pavelka et al. [2020], which skips completely the analytical aspects. The same formalism is used e.g. in Öttinger [2005] or Simo et al. [1988] and the reader is encourage to consult Morrison [1998] for a thorough explanation of its practical aspects. All these works refer to [Courant and Hilbert, 1989, Gelfand and Fomin, 1963, Chap. IV] for the rigor mathematical treatment of infinite dimensional spaces. Nevertheless, the calculations carried out are purely formal, which is, however, a common practice in continuum mechanics when it is customary to assume the fields are regular enough such that the computations are valid.

Hence we obtain

$$\frac{\delta b^i(\mathbf{x})}{\delta y^k(\mathbf{x})} = -\frac{\partial \delta}{\partial X^I}(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\delta^i_k B^I(\mathbf{x}) - \frac{\partial F^i_I}{\partial x^k}(\mathbf{x})B^I(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x})) \tag{4.25}$$

$$- F^i_I(\mathbf{x})\frac{\partial B^I}{\partial x^k}(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x})) \tag{4.26}$$

$$= -\frac{\partial \delta}{\partial X^I}(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\delta^i_k B^I(\mathbf{x}) - \frac{\partial b^i}{\partial x^k}(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x})). \tag{4.27}$$

Now we can proceed with rewriting of the Poisson bracket

$$\{F, G\}^{\text{Lagrange}} = \int_{\mathbb{R}^3} \frac{\delta F}{\delta y^k(\mathbf{X})}\frac{\delta G}{\delta M_k(\mathbf{X})} - \frac{\delta G}{\delta y^k(\mathbf{X})}\frac{\delta F}{\delta M_k(\mathbf{X})}\,\mathrm{d}\mathbf{X}.$$

Again by [Pavelka et al., 2020, App. B] we have

$$\frac{\delta G}{\delta M_k(\mathbf{X})} = \left.\frac{\delta G}{\delta m_k(\mathbf{x})}\right|_{\mathbf{x}=\mathbf{y}^{-1}(\mathbf{x})}, \tag{4.28}$$

while by the chain rule

$$\frac{\delta F}{\delta y^k(\mathbf{X})} = \int_{\mathbb{R}^3} \frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\delta b^i(\mathbf{x})}{\delta y^k(\mathbf{X})}\,\mathrm{d}\mathbf{x}. \tag{4.29}$$

Here we intentionally dropped the derivatives of F with respect to the fields ρ, $\mathbf{m}$, s, and $\mathbb{A}$. Putting (4.28), (4.29) and (4.27) together we obtain [4]

$$\begin{aligned}
&\int_{\mathbb{R}^3} \frac{\delta F}{\delta y^k(\mathbf{X})}\frac{\delta G}{\delta M_k(\mathbf{X})}\,\mathrm{d}\mathbf{X} \\
&\quad= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\delta F}{\delta b^i(\mathbf{x})} \\
&\qquad\qquad \left(-\frac{\partial \delta}{\partial X^I}(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\delta^i_k B^I(\mathbf{x}) - \frac{\partial b^i}{\partial x^k}(\mathbf{x})\delta(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\right) \\
&\qquad\qquad\qquad\qquad \left.\frac{\delta G}{\delta m_k(\mathbf{x})}\right|_{\mathbf{x}=\mathbf{y}^{-1}(\mathbf{x})}\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{X} \\
&\quad= -\int_{\mathbb{R}^3} \frac{\delta F}{\delta b^i(\mathbf{x})}B^I(\mathbf{x})\int_{\mathbb{R}^3} \frac{\partial \delta}{\partial X^I}(\mathbf{X} - \mathbf{y}^{-1}(\mathbf{x}))\left.\frac{\delta G}{\delta m_i(\mathbf{x})}\right|_{\mathbf{x}=\mathbf{y}^{-1}(\mathbf{x})}\,\mathrm{d}\mathbf{X}\,\mathrm{d}\mathbf{x} \\
&\qquad - \int_{\mathbb{R}^3} \frac{\partial b^i}{\partial x^k}(\mathbf{x})\frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\delta G}{\delta m_k(\mathbf{x})}\,\mathrm{d}\mathbf{x} \\
&\quad= \int_{\mathbb{R}^3} \frac{\delta F}{\delta b^i(\mathbf{x})}B^I(\mathbf{x})\frac{\partial}{\partial X^I}\frac{\delta G}{\delta m_i(\mathbf{x})}\,\mathrm{d}\mathbf{x} - \int_{\mathbb{R}^3} \frac{\partial b^i}{\partial x^k}(\mathbf{x})\frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\delta G}{\delta m_k(\mathbf{x})}\,\mathrm{d}\mathbf{x} \\
&\quad= \int_{\mathbb{R}^3} \frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\partial x^j}{\partial X^I}B^I(\mathbf{x})\frac{\partial}{\partial x^j}\frac{\delta G}{\delta m_i(\mathbf{x})}\,\mathrm{d}\mathbf{x} - \int_{\mathbb{R}^3} \frac{\partial b^i}{\partial x^k}(\mathbf{x})\frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\delta G}{\delta m_k(\mathbf{x})}\,\mathrm{d}\mathbf{x} \\
&\quad= \int_{\mathbb{R}^3} b^j(\mathbf{x})\frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\partial}{\partial x^j}\frac{\delta G}{\delta m_i(\mathbf{x})}\,\mathrm{d}\mathbf{x} - \int_{\mathbb{R}^3} \frac{\partial b^i}{\partial x^k}(\mathbf{x})\frac{\delta F}{\delta b^i(\mathbf{x})}\frac{\delta G}{\delta m_k(\mathbf{x})}\,\mathrm{d}\mathbf{x}.
\end{aligned}$$

[4] In the sense of Morrison [1998], the integration represents a scalar product, the derivative of one field with respect to other an operator from one tangent space to another, and the Fubini theorem to an adjoint operation in the scalar product.

Since the right-hand side depends solely on the new state variables, the projection was successful.

The Poisson bracket, from now on including also the fields ρ, $\mathbf{m}$, s, and $\mathbb{A}$, becomes (note the interchange of indexes)

$$\begin{aligned}\{F,G\}^{(B\&b)} = \{F,G\}^{\text{Euler}} &\\ + \int_{\mathbb{R}^3} b^i \left(\frac{\delta F}{\delta b^j} \frac{\partial}{\partial x^i} \frac{\delta G}{\delta m_j} - \frac{\delta G}{\delta b^j} \frac{\partial}{\partial x^i} \frac{\delta F}{\delta m_j} \right) \mathrm{d}\mathbf{x} &\\ - \int_{\mathbb{R}^3} \frac{\partial b^j}{\partial x^i} \left(\frac{\delta F}{\delta b^j} \frac{\delta G}{\delta m_i} - \frac{\delta G}{\delta b^j} \frac{\delta F}{\delta m_i} \right) \mathrm{d}\mathbf{x}.&\end{aligned} \tag{4.30}$$

The standard localization procedure, the same used for isotropic material, leads to field equations

$$\begin{aligned}
\left(\frac{\partial \rho}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^i}\left(\rho \frac{\delta E}{\delta m_i}\right), \\
\left(\frac{\partial m_i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^j}\left(m_i \frac{\delta E}{\delta m_j}\right) - \rho \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \rho} - m_j \frac{\partial}{\partial x^i}\frac{\delta E}{\delta m_j} - s\frac{\partial}{\partial x^i}\frac{\delta E}{\delta s} - A_j^J \frac{\partial}{\partial x^i}\frac{\delta E}{\delta A_j^J} \\
&\quad - b^j \frac{\partial}{\partial x^i}\frac{\delta E}{\delta b^j} + \frac{\partial}{\partial x^i}\left(A_j^J \frac{\delta E}{\delta A_j^J} + \frac{\delta E}{\delta b^j} b^j\right) + \frac{\partial}{\partial x^j}\left(-A_i^J \frac{\delta E}{\delta A_j^J} + \frac{\delta E}{\delta b^i} b^j\right) \\
\left(\frac{\partial s}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^i}\left(s \frac{\delta E}{\delta m_i}\right), \\
\left(\frac{\partial A_i^I}{\partial t}\right)_{\text{rev}} &= -\frac{\partial A_i^I}{\partial x^j}\frac{\delta E}{\delta m_j} - A_j^I \frac{\partial}{\partial x^i}\frac{\delta E}{\delta m_j}, \\
\left(\frac{\partial b^i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial b^i}{\partial x^j}\frac{\delta E}{\delta m_j} + \frac{\partial}{\partial x^j}\frac{\delta E}{\delta m_i} b^j.
\end{aligned}$$

Since the evolution equation for $\mathbf{b}$ is also compatible with the equation $\dot{F} = \mathbb{L}\mathbb{F}$, it is again the equation of momentum which is not in the standard form and, at the same time, contains the main advantage of this approach, i.e. its validity for any energy functional. In order to highlight the resemblance with the other models as before, we stick in the next section to an energy ansatz, similar to the one for the isotropic model.

Remark 4.3 (Equations versus Brackets)**.** *Were one interested solely in the fields equations, it would be enough to rewrite* (4.15) *using the very same arguments while reducing the complexity of the whole calculation; the main advantage, i.e. the validity of the equations for an arbitrary energy functional, would remain. Nevertheless in some situations, like the stability analysis in Morrison [1998] or the exact geometry equations for rods and plates in Simo et al. [1988], it is beneficial to have the Poisson structure at hand, and since the bracket* (4.30) *has been obtained by a projection from the canonical bracket, it indeed a Poisson bracket and no proof, especially of the Jacobi identity (usually very tedious), is not necessary. In addition, the formulation using Poisson and dissipation bracket does not use coordinates; see Remark 4.1 and can be regarded also as a weak formulation, testing the evolution with a selected class of functionals.*

Elastic Dynamics

As in the preceding section we stick to isothermal processes, using a modification of the free energy ansatz (4.18)

$$F(\rho, \mathbf{m}, T, \mathbb{A}, \mathbf{b}) = \int_{\mathbb{R}^3} f(\rho, \mathbf{m}, T, \mathbb{A}, \mathbf{b}) \, \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \frac{|\mathbf{m}|^2}{2\rho} + \phi(T, \rho) + \rho\psi(T, \mathbb{A}, \mathbf{b}) \, \mathrm{d}\mathbf{x}, \tag{4.31}$$

for which the equation for momentum simplifies to

$$\begin{aligned}
\left(\frac{\partial m_i}{\partial t}\right)_{\text{rev}} &= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \rho \frac{\partial}{\partial x^i}\frac{\partial f}{\partial \rho} - m_j \frac{\partial}{\partial x^i}\frac{\partial f}{\partial m_j} + \frac{\partial f}{\partial T}\frac{\partial T}{\partial x^i} \\
&\quad - A_j^J \frac{\partial}{\partial x^i}\frac{\partial f}{\partial A_j^J} - b^j \frac{\partial}{\partial x^i}\frac{\partial f}{\partial b^j} \\
&\quad + \frac{\partial}{\partial x^i}\left(A_j^J \frac{\partial f}{\partial A_j^J} + \frac{\partial f}{\partial b^j} b^j\right) + \frac{\partial}{\partial x^j}\left(-A_i^J \frac{\partial f}{\partial A_j^J} + \frac{\partial f}{\partial b^i} b^j\right) \\
&= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \frac{\partial}{\partial x^i}\left(-f + \rho\frac{\partial f}{\partial \rho} + m_j \frac{\partial f}{\partial m_j}\right) \\
&\quad + \frac{\partial}{\partial x^j}\left(-A_i^J \frac{\partial f}{\partial A_j^J} + \frac{\partial f}{\partial b^i} b^j\right) \\
&= -\frac{\partial}{\partial x^j}\left(m_i \frac{m_j}{\rho}\right) - \frac{\partial}{\partial x^i}\left(-\phi + \rho\frac{\partial \phi}{\partial \rho}\right) + \frac{\partial}{\partial x^j}\left(-\rho A_i^J \frac{\partial \psi}{\partial A_j^J} + \rho \frac{\partial \psi}{\partial b^i} b^j\right).
\end{aligned}$$

Hence we arrive at the system

$$\begin{aligned}
\left(\frac{\partial \rho}{\partial t}\right)_{\text{rev}} &= -\operatorname{div}(\rho \mathbf{v}), \\
\left(\frac{\partial \mathbf{m}}{\partial t}\right)_{\text{rev}} &= -\operatorname{div}(\mathbf{m} \otimes \mathbf{v}) + \operatorname{div} \mathbb{T}, \\
\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{rev}} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L}, \\
\left(\frac{\partial \mathbf{b}}{\partial t}\right)_{\text{rev}} &= -[\nabla \mathbf{b}]\mathbf{v} + \mathbb{L}\mathbf{b}
\end{aligned}$$

where again we use the same notation as for the isotropic material

$$\mathbf{v} := \frac{\delta F}{\delta \mathbf{m}} = \frac{\partial f}{\partial \mathbf{m}} = \frac{\mathbf{m}}{\rho}, \qquad \mathbb{L} := \nabla \mathbf{v}, \qquad p_{th} := -\phi + \rho\frac{\partial \phi}{\partial \rho},$$

the only difference being in the Cauchy stress

$$\mathbb{T} := -p_{th}\mathbb{I} - \rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b},$$

which now contains the anisotropic elastic response.

If one were to describe an anisotropic material, where $\mathbf{b}$ describes the orientation of elastic fibers, a suitable candidate for ψ, based on the former one in

(4.19), would be

$$\begin{aligned}\psi(T,\mathbb{A},\mathbf{b}) = \frac{G(T)}{2}(|\mathbb{A}^{-1}|^2-3) - k_BT\ln\det(\mathbb{A}^{-1}\mathbb{A}^{-\top}) \\ + \frac{H(T)}{2}\left(\frac{|\mathbf{b}|^2}{L^2(T)}-1\right) - k_BT\ln\frac{|\mathbf{b}|^2}{L^2(T)},\end{aligned} \tag{4.32}$$

where the material constant $L(T)$ is introduced for a dimensional reasons and represents the fiber's stress-free length. Indeed, for this particular ψ we have

$$\mathbb{T} = -p_{th}\mathbb{I} + \rho G(T)\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{2k_BT}{G(T)}\mathbb{I}\right) + \rho H(T)\left(\frac{|\mathbf{b}|^2}{L^2(T)} - \frac{2k_BT}{H(T)}\right)\frac{\mathbf{b}\otimes\mathbf{b}}{|\mathbf{b}^2|}.$$

Remark (Anisotropic Energy)**.** *The motivation for such an energy comes from [Pavelka et al., 2018b, Sec. 5.5], where the isotropic part of energy is obtained in terms of the left Cauchy-Green tensor $\mathbb{B} = \mathbb{A}^{-1}\mathbb{A}^{-\top}$. If one supposes that each fiber is described by its own $\tilde{\mathbb{B}}$, whose two eigenvalues corresponds to its constant width, the resulting one is nothing but its length squared, i.e. $|\mathbf{b}|^2$. Hence*

$$\operatorname{Tr}\tilde{\mathbb{B}} = \frac{|\mathbf{b}|^2}{L^2(T)} + const, \qquad and \qquad \ln\det\tilde{\mathbb{B}} = \ln\frac{|\mathbf{b}|^2}{L^2(T)},$$

which leads to the anisotropic contribution. Both the logarithmic terms are again derived from entropy rather than energy storage.

Irreversible Kinematics

As in the previous section, we will start to design the irreversible evolution in the entropic representation, where the state variables are $(\rho, \mathbf{m}, e, \mathbb{A}, \mathbf{b})$, e being the field of total energy *per volume*. For the sake of brevity we will consider only

$$\Xi = \Xi(\mathbb{A}, \mathbf{b}, \mathbb{A}^*, \mathbf{b}^*),$$

since the viscous dissipation in isothermal setting can be added in the very same way as in the preceding section. The equations of irreversible evolution then reads

$$\begin{aligned}\left(\frac{\partial A_i^I}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta\Xi}{\delta(A^*)_I^i}\right|_{(A^*)_I^i=\frac{\delta S}{\delta A_i^I}}, \\ \left(\frac{\partial b^i}{\partial t}\right)_{\text{irr}} &= \left.\frac{\delta\Xi}{\delta(b^*)_i}\right|_{(b^*)_i=\frac{\delta S}{\delta b^i}}.\end{aligned} \tag{4.33}$$

As already adumbrated in Remark 4.2, it will be convenient for the modeling reasons to reformulate these equations via the Legendre–Fenchel conjugate

$$\Xi^*(\mathbb{A},\mathbf{b},\mathbb{A}^\circ,\mathbf{b}^\circ) := \sup_{(\mathbb{A}^*,\mathbf{b}^*)}\left(\mathbb{A}^\circ : \mathbb{A}^* + \mathbf{b}^\circ\cdot\mathbf{b}^* - \Xi(\mathbb{A},\mathbf{b},\mathbb{A}^*,\mathbf{b}^*)\right),$$

i.e. prescribing the dissipation in rather in rates rather than fluxes. Formally the dual dissipation potential is

$$\Xi^*(\mathbb{A},\mathbf{b},\mathbb{A}^\circ,\mathbf{b}^\circ) = \mathbb{A}^\circ : \bar{\mathbb{A}}^* + \mathbf{b}^\circ\cdot\bar{\mathbf{b}}^* - \Xi(\mathbb{A},\mathbf{b},\bar{\mathbb{A}}^*,\bar{\mathbf{b}}^*),$$

where $(\bar{\mathbb{A}}^*, \bar{\mathbf{b}}^*)$ is the solution of the equations

$$\frac{\delta \Xi}{\delta \mathbb{A}^*} = \mathbb{A}^\circ, \qquad \frac{\delta \Xi}{\delta \mathbf{b}^*} = \mathbf{b}^\circ,$$

where $(\mathbb{A}^*, \mathbf{b}^*)$ play the role of the unknown and $(\mathbb{A}^\circ, \mathbf{b}^\circ)$ is the right-hand side. Therefore $(\bar{\mathbb{A}}^*, \bar{\mathbf{b}}^*)$ are functions of $\mathbb{A}^\circ, \mathbf{b}^\circ$, and so the potential Ξ^* is.

Using the properties of the Legendre–Fenchel transform, we obtain from (4.33) the dual representation of the irreversible evolution

$$\begin{aligned} \frac{\delta S}{\delta A_i^I} &= \left.\frac{\delta \Xi^*}{\delta (A^\circ)_i^I}\right|_{(A^\circ)_i^I = \left(\frac{\partial A_i^I}{\partial t}\right)_{\text{irr}}}, \\ \frac{\delta S}{\delta b^i} &= \left.\frac{\delta \Xi^*}{\delta (b^\circ)^i}\right|_{(b^\circ)^i = \left(\frac{\partial b^i}{\partial t}\right)_{\text{irr}}}. \end{aligned} \tag{4.34}$$

The dissipative dynamics is then formulated via Ξ^* in terms of 'irreversible rates' of the state variables.

Before we specify Ξ and rewrite the equations to the energetic representation, we characterize a distinguished class of models, for which the symmetry in the structural space, or natural configuration, is not evolving. Let us suppose that

$$\Xi(\mathbb{A}, \mathbf{b}, \mathbb{A}^*, \mathbf{b}^*) = \hat{\Xi}(\mathbb{A}, \mathbf{b}, \mathbb{A}^\top \mathbb{A}^* - \mathbf{b}^* \otimes \mathbf{b}),$$

i.e. the dissipation potential depends only on the conjugate variables only through

$$\sigma := \mathbb{A}^\top \mathbb{A}^* - \mathbf{b}^* \otimes \mathbf{b}$$

which is up to the temperature the partial stress due to $\mathbb{A}$ and $\mathbf{b}$ in the equation for momentum. Then the conjugate dissipation potential Ξ^* is given by

$$\begin{aligned} \Xi^*(\mathbb{A}, \mathbf{b}, \mathbb{A}^\circ, \mathbf{b}^\circ) &= \sup_{(\mathbb{A}^*, \mathbf{b}^*)} \left(\mathbb{A}^\circ : \mathbb{A}^* + \mathbf{b}^\circ \cdot \mathbf{b}^* - \Xi(\mathbb{A}, \mathbf{b}, \mathbb{A}^*, \mathbf{b}^*)\right) \\ &= \sup_{(\sigma, \mathbf{b}^*)} \left(\mathbb{A}^{-1}\mathbb{A}^\circ : \sigma + (\mathbb{A}^{-1}\mathbb{A}^\circ \mathbf{b} + \mathbf{b}^\circ) \cdot \mathbf{b}^* - \hat{\Xi}(\mathbb{A}, \mathbf{b}, \sigma)\right) \\ &= \hat{\Xi}^*(\mathbb{A}, \mathbf{b}, \mathbb{A}^{-1}\mathbb{A}^\circ) + I_{K(\mathbb{A}, \mathbf{b})}(\mathbb{A}^\circ, \mathbf{b}^\circ), \end{aligned}$$

where $\hat{\Xi}^*(\mathbb{A}, \mathbf{b}, \sigma^\circ)$ is the conjugate potential to $\hat{\Xi}(\mathbb{A}, \mathbf{b}, \sigma)$ and

$$I_{K(\mathbb{A}, \mathbf{b})}(\mathbb{A}^\circ, \mathbf{b}^\circ) := \begin{cases} 0 & \text{if } (\mathbb{A}^\circ, \mathbf{b}^\circ) \in K(\mathbb{A}, \mathbf{b}), \\ +\infty & \text{else,} \end{cases}$$

is the indicator function of the convex set

$$K(\mathbb{A}, \mathbf{b}) = \left\{ (\mathbb{A}^\circ, \mathbf{b}^\circ) \,\middle|\, \mathbb{A}^\circ \mathbf{b} + \mathbb{A} \mathbf{b}^\circ = 0 \right\}. \tag{4.35}$$

The corresponding equations then read

$$\begin{pmatrix} \dfrac{\delta S}{\delta \mathbb{A}} \\ \dfrac{\delta S}{\delta \mathbf{b}} \end{pmatrix} \in \begin{pmatrix} \mathbb{A}^{-\top} \left.\dfrac{\delta \hat{\Xi}^*}{\delta \sigma^\circ}\right|_{\sigma^\circ = \mathbb{A}^{-1}\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{irr}}} \\ 0 \end{pmatrix} + \left. \partial_{\mathbf{x}^\circ} I_{K(\mathbb{A}, \mathbf{b})} \right|_{\mathbf{x}^\circ = \left(\frac{\partial \mathbf{x}}{\partial t}\right)_{\text{irr}}},$$

where $\mathbf{x} = (\mathbb{A}, \mathbf{b})$ and $\mathbf{x}^\circ = (\mathbb{A}^\circ, \mathbf{b}^\circ)$. Since the sub-differential of the indicator function $I_{K(\mathbb{A},\mathbf{b})}$ is nothing but the normal cone $N_{K(\mathbb{A},\mathbf{b})}$ of the set $K(\mathbb{A}, \mathbf{b})$, given by

$$N_{K(\mathbb{A},\mathbf{b})} = \left\{ \left(\mathbf{d} \otimes \mathbf{b},\, \mathbb{A}^\top \mathbf{d} \right)^\top \mid \mathbf{d} \in \mathbb{R}^3 \right\},$$

we can rewrite the equations to

$$\begin{aligned} \frac{\delta S}{\delta \mathbb{A}} &= \mathbb{A}^{-\top} \left. \frac{\delta \hat{\Xi}^*}{\delta \sigma^\circ} \right|_{\sigma^\circ = \mathbb{A}^{-1} \left(\frac{\partial \mathbb{A}}{\partial t} \right)_{\text{irr}}} + \mathbf{d} \otimes \mathbf{b}, \\ \frac{\delta S}{\delta \mathbf{b}} &= \mathbb{A}^\top \mathbf{d}, \end{aligned}$$

where $\mathbf{d}$ is the Lagrange multiplier assuring that the constraint

$$\left(\frac{\partial (\mathbb{A}\mathbf{b})}{\partial t} \right)_{\text{irr}} = \left(\frac{\partial \mathbb{A}}{\partial t} \right)_{\text{irr}} \mathbf{b} + \mathbb{A} \left(\frac{\partial \mathbf{b}}{\partial t} \right)_{\text{irr}} = 0, \tag{4.36}$$

coming from the definition of $K(\mathbb{A}, \mathbf{b})$ in (4.35), is satisfied. Putting these equations together we have

$$\begin{aligned} \sigma = \mathbb{A}^\top \frac{\delta S}{\delta \mathbb{A}} - \frac{\delta S}{\delta \mathbf{b}} \otimes \mathbf{b} = \left. \frac{\delta \hat{\Xi}^*}{\delta \sigma^\circ} \right|_{\sigma^\circ = \mathbb{A}^{-1} \left(\frac{\partial \mathbb{A}}{\partial t} \right)_{\text{irr}}}, \\ -\mathbb{A}^{-1} \left(\frac{\partial \mathbb{A}}{\partial t} \right)_{\text{irr}} \mathbf{b} = \left(\frac{\partial \mathbf{b}}{\partial t} \right)_{\text{irr}}. \end{aligned}$$

By performing the Legendre transformation once more we obtain the primer formulation. Hence we have established the following equivalence. The materials whose symmetry is not affected by irreversible evolution are exactly those, whose dissipation depends on the partial stress σ (and eventually the state variables $\mathbb{A}$ and $\mathbf{b}$).

Dissipative Dynmaics

As in the isotropic case, only isothermal processes will be considered. We will introduce two models - one decoupled in $\mathbb{A}^\dagger$ and $\mathbf{b}^\dagger$ and incorporating anisotropic viscosity, the other with no viscosity, but keeping the material symmetry in the natural configuration (or structural space) constant. The former is addressed as the *Needles Model*, since it describes visco-elastic fluid with dissolved fibers, each of them also visco-elastic. The letter is called *Crystlicity*, referring to a continuum description of crystal plasticity, where the lattice vectors in the structural space remains invariant under the plastic deformation, see e.g. [Gurtin et al., 2010, Chap. 91], but since all the other aspects of plasticity are disregarded, the explicit use of the term is therefore avoided. It should be noted that there the vector $\mathbf{b}$ corresponds to the observed lattice vector, i.e. mapped from the structural space by $\mathbb{A}^{-1}$, and it should *not* be interchanged with the Burgers vector,

usually denoted also by the same letter. For both of the models we will use the relations for conjugate variables, which are valid for the ansatz (4.31)

$$\begin{aligned}\mathbf{v} := -T\mathbf{m}^* = \mathbf{m}^\dagger = \frac{\delta E}{\delta \mathbf{m}} = \frac{\partial e}{\partial \mathbf{m}} = \frac{\partial f}{\partial \mathbf{m}} = \frac{\mathbf{m}}{\rho},\\ -T\mathbb{A}^* = \mathbb{A}^\dagger = \frac{\delta E}{\delta \mathbb{A}} = \frac{\partial e}{\partial \mathbb{A}} = \frac{\partial f}{\partial \mathbb{A}} = \rho\frac{\partial \psi}{\partial \mathbb{A}},\\ -T\mathbf{b}^* = \mathbf{b}^\dagger = \frac{\delta E}{\delta \mathbf{b}} = \frac{\partial e}{\partial \mathbf{b}} = \frac{\partial f}{\partial \mathbf{b}} = \rho\frac{\partial \psi}{\partial \mathbf{b}}.\end{aligned}$$

Needles Model

In isothermal setting we can choose the dissipation bracket

$$[F,G] = \int_{\mathbb{R}^3} 2\mu \left(\nabla\frac{\delta F}{\delta \mathbf{m}}\right)_{\text{sym}} : \left(\nabla\frac{\delta G}{\delta \mathbf{m}}\right)_{\text{sym}} \tag{4.37}$$

$$+ 2\nu \left(\frac{\mathbf{b}}{|\mathbf{b}|}\cdot\left(\nabla\frac{\delta F}{\delta \mathbf{m}}\right)\frac{\mathbf{b}}{|\mathbf{b}|}\right)\left(\frac{\mathbf{b}}{|\mathbf{b}|}\cdot\left(\nabla\frac{\delta G}{\delta \mathbf{m}}\right)\frac{\mathbf{b}}{|\mathbf{b}|}\right) \tag{4.38}$$

$$+ \Lambda\left(\mathbb{A}^\top\frac{\delta F}{\delta \mathbb{A}}\right) : \left(\mathbb{A}^\top\frac{\delta G}{\delta \mathbb{A}}\right) + \lambda\left(\frac{\delta F}{\delta \mathbf{b}}\otimes\mathbf{b}\right) : \left(\frac{\delta G}{\delta \mathbf{b}}\otimes\mathbf{b}\right)\,\mathrm{d}\mathbf{x}, \tag{4.39}$$

because for the ansatz (4.31) it leads to the dissipation rate

$$\dot{F} = -\frac{1}{T}\int_{\mathbb{R}^3} 2\mu\,|\mathbb{D}|^2 + 2\nu\frac{(\mathbf{b}\cdot\mathbb{D}\mathbf{b})^2}{|\mathbf{b}|^4} + \Lambda\left|\rho\mathbb{A}^\top\frac{\partial\psi}{\partial\mathbb{A}}\right|^2 + \lambda\left|\rho\frac{\partial\psi}{\partial\mathbf{b}}\otimes\mathbf{b}\right|^2\,\mathrm{d}\mathbf{x}, \tag{4.40}$$

where ν and λ are material parameters whose meaning is analogical to the standard viscosity μ and relaxation parameter Λ, and can also depend on the temperature. Since the dissipation in $\mathbb{A}$ is the same as in the isotropic model, we do not calculate it further. Localizing the dissipation bracket gives the irreversible evolution

$$\begin{aligned}\left(\frac{\partial\mathbf{m}}{\partial t}\right)_{\text{irr}} &= \frac{1}{T}\operatorname{div}\left(2\mu\mathbb{D} + 2\nu\frac{(\mathbf{b}\cdot\mathbb{D}\mathbf{b})}{|\mathbf{b}|^4}\mathbf{b}\otimes\mathbf{b}\right),\\ \left(\frac{\partial\mathbf{b}}{\partial t}\right)_{\text{irr}} &= -\frac{\lambda}{T}|\mathbf{b}|^2\left(\rho\frac{\partial\psi}{\partial\mathbf{b}}\right),\end{aligned}$$

where only the equations differing from (4.22) are given, i.e. the equation for $\mathbb{A}$ remains the same. The equation of momentum contains additional viscosity in the direction of $\mathbf{b}$, whose irreversible evolution is zero in the stress-free state and decoupled with the equation for $\mathbb{A}$.

If we specify ψ as in (4.32), the equation for $\mathbf{b}$ becomes

$$\left(\frac{\partial\mathbf{b}}{\partial t}\right)_{\text{irr}} = -\frac{\lambda}{T}H(T)\rho\left(\frac{|\mathbf{b}|^2}{L^2} - \frac{2k_BT}{H(T)}\right)\mathbf{b}.$$

Crystlicity Model

A simple model falling to this class is given by a dissipation bracket

$$[F,G] = \int_{\mathbb{R}^3}\Lambda\left(-\mathbb{A}^\top\frac{\delta F}{\delta\mathbb{A}} + \frac{\delta F}{\delta\mathbf{b}}\otimes\mathbf{b}\right) : \left(-\mathbb{A}^\top\frac{\delta G}{\delta\mathbb{A}} + \frac{\delta G}{\delta\mathbf{b}}\otimes\mathbf{b}\right)\,\mathrm{d}\mathbf{x}, \tag{4.41}$$

yielding for the free energy ansatz (4.32) the dissipation rate

$$\dot{F} = -\frac{1}{T}[F,F] = -\frac{1}{T}\int_{\mathbb{R}^3} \Lambda \left| -\rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b} \right|^2 \mathrm{d}\mathbf{x}, \tag{4.42}$$

and the following equations for $\mathbb{A}$ and $\mathbf{b}$

$$\begin{aligned}
\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{irr}} &= \frac{\Lambda}{T}\mathbb{A}\left(-\rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b}\right), \\
\left(\frac{\partial \mathbf{b}}{\partial t}\right)_{\text{irr}} &= -\frac{\Lambda}{T}\left(-\rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b}\right)\mathbf{b},
\end{aligned}$$

which indeed satisfy the constraint (4.36). The irreversible evolution is therefore vanishes when the partial Cauchy stress σ is zero. For ψ in (4.32), we obtain

$$\begin{aligned}
\left(\frac{\partial \mathbb{A}}{\partial t}\right)_{\text{irr}} &= \frac{\Lambda}{T} G(T) \rho \mathbb{A}\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{k_B T}{G(T)}\mathbb{I}\right) \\
&\quad + \frac{\Lambda}{T}\frac{H(T)}{|\mathbf{b}|^2}\rho \mathbb{A}\left(\frac{|\mathbf{b}|^2}{L^2} - \frac{2k_B T}{H(T)}\right)\mathbf{b}\otimes\mathbf{b} \\
&= \frac{\Lambda}{T}\rho\mathbb{A}\left(G(T)\mathbb{A}^{-1}\mathbb{A}^{-\top} + H(T)\frac{\mathbf{b}\otimes\mathbf{b}}{L^2} - k_B T\mathbb{I} - 2k_B T\frac{\mathbf{b}\otimes\mathbf{b}}{|\mathbf{b}|^2}\right), \\
\left(\frac{\partial \mathbf{b}}{\partial t}\right)_{\text{irr}} &= -\frac{\Lambda}{T}G(T)\rho\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{k_B T}{G(T)}\mathbb{I}\right)\mathbf{b} - \frac{\Lambda}{T}H(T)\rho\left(\frac{|\mathbf{b}|^2}{L^2} - \frac{2k_B T}{H(T)}\right)\mathbf{b} \\
&= -\frac{\Lambda}{T}\rho\left(G(T)\mathbb{A}^{-1}\mathbb{A}^{-\top}\mathbf{b} + H(T)\frac{|\mathbf{b}|^2}{L^2}\mathbf{b} - 3k_B T\mathbf{b}\right).
\end{aligned}$$

Remark. *The model can be relaxed by enhancing the bracket*

$$[F,F] = \int_{\mathbb{R}^3} \Lambda \left| -\rho \mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b} \right|^2 + \lambda \left| \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b} \right|^2,$$

where $\lambda \searrow 0$ is the relaxation parameter for the evolutionary constraint.

Final Equations

Since in the isothermal setting both the reversible and irreversible evolution can be expressed directly in the (free) energetic representation, using the Helmholtz free energy F instead the total energy E, we can easily formulate the total evolution of $(\rho, \mathbf{m}, \mathbb{A}, \mathbf{b})$.

Needles Model

In the 'Needles Model' the evolution is driven by the free energy (4.31) and the dissipation bracket (4.37) determining the dissipation rate (4.40), which yields

the following equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\operatorname{div}(\rho \mathbf{v}), \\
\frac{\partial \mathbf{m}}{\partial t} &= -\operatorname{div}(\mathbf{m} \otimes \mathbf{v}) + \operatorname{div}\left(\mathbb{T} + \frac{2\mu}{T}\mathbb{D} + \frac{2\nu}{T}\frac{(\mathbf{b}\cdot\mathbb{D}\mathbf{b})}{|\mathbf{b}|^4}\mathbf{b}\otimes\mathbf{b}\right), \\
\frac{\partial \mathbb{A}}{\partial t} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L} + \frac{\Lambda}{T}\mathbb{A}\left(-\rho\mathbb{A}^\top\frac{\partial \psi}{\partial \mathbb{A}}\right), \\
\frac{\partial \mathbf{b}}{\partial t} &= -[\nabla \mathbf{b}]\mathbf{v} + \mathbb{L}\mathbf{b} - \frac{\lambda}{T}\left(\rho\frac{\partial \psi}{\partial \mathbf{b}}\otimes\mathbf{b}\right)\mathbf{b}
\end{aligned}$$

where we denote

$$\mathbb{T} := -p_{th}\mathbb{I} - \rho\mathbb{A}^\top\frac{\partial \psi}{\partial \mathbb{A}} + \rho\frac{\partial \psi}{\partial \mathbf{b}}\otimes\mathbf{b}, \qquad p_{th} := -\phi + \rho\frac{\partial \phi}{\partial \rho}.$$

If we use ψ from (4.32), the equations for $\mathbb{A}$ and $\mathbf{b}$ become

$$\begin{aligned}
\frac{\partial \mathbb{A}}{\partial t} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L} + \frac{\Lambda}{T}G(T)\rho\mathbb{A}\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{k_BT}{G(T)}\mathbb{I}\right), \\
\frac{\partial \mathbf{b}}{\partial t} &= -[\nabla \mathbf{b}]\mathbf{v} + \mathbb{L}\mathbf{b} - \frac{\lambda}{T}H(T)\rho\left(\frac{|\mathbf{b}|^2}{L^2} - \frac{2k_BT}{H(T)}\right)\mathbf{b},
\end{aligned}$$

while in the equation for momentum $\mathbf{m}$ we have

$$\mathbb{T} = -p_{th}\mathbb{I} + \rho G(T)\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{2k_BT}{G(T)}\mathbb{I}\right) + \rho H(T)\left(\frac{|\mathbf{b}|^2}{L^2(T)} - \frac{2k_BT}{H(T)}\right)\frac{\mathbf{b}\otimes\mathbf{b}}{|\mathbf{b}^2|}.$$

As already suggested at the beginning of this subsection about isotropic materials, this model may describes a rod like visco-elastic structures immersed in a visco-elastic fluid (e.g. liquid crystals or highly concentrated polymeric fluids), provided the inertia of the rods is negligible (i.e. it is not a director continuum). The anisotropy vector is mapped by the plastic distortion $\mathbb{G}$ from the reference configuration to the natural configuration, i.e. it does not remain constant there, and the dissipation comes from the fluid viscosity, the rods viscosity, and the slip rate of the fluid on the rods' surface.

Crystlicity Model

In the 'Crystlicity Model' the evolution is driven by the free energy (4.31) and the dissipation bracket (4.41) determining the dissipation rate (4.42), which yields the following equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\operatorname{div}(\rho \mathbf{v}), \\
\frac{\partial \mathbf{m}}{\partial t} &= -\operatorname{div}(\mathbf{m} \otimes \mathbf{v}) + \operatorname{div}\mathbb{T}, \\
\frac{\partial \mathbb{A}}{\partial t} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L} + \frac{\Lambda}{T}\mathbb{A}\left(-\rho\mathbb{A}^\top\frac{\partial \psi}{\partial \mathbb{A}} + \rho\frac{\partial \psi}{\partial \mathbf{b}}\otimes\mathbf{b}\right), \\
\frac{\partial \mathbf{b}}{\partial t} &= -[\nabla \mathbf{b}]\mathbf{v} + \mathbb{L}\mathbf{b} - \frac{\Lambda}{T}\left(-\rho\mathbb{A}^\top\frac{\partial \psi}{\partial \mathbb{A}} + \rho\frac{\partial \psi}{\partial \mathbf{b}}\otimes\mathbf{b}\right)\mathbf{b}
\end{aligned}$$

where we denote

$$\mathbb{T} := -p_{th}\mathbb{I} - \rho\mathbb{A}^\top \frac{\partial \psi}{\partial \mathbb{A}} + \rho \frac{\partial \psi}{\partial \mathbf{b}} \otimes \mathbf{b}, \qquad p_{th} := -\phi + \rho \frac{\partial \phi}{\partial \rho}.$$

If we use ψ from (4.32), the equations for $\mathbb{A}$ and $\mathbf{b}$ become

$$\begin{aligned}
\frac{\partial \mathbb{A}}{\partial t} &= -[\nabla \mathbb{A}]\mathbf{v} - \mathbb{A}\mathbb{L} \\
&\quad + \frac{\Lambda}{T}\rho\mathbb{A}\left(G(T)\mathbb{A}^{-1}\mathbb{A}^{-\top} + H(T)\frac{\mathbf{b}\otimes\mathbf{b}}{L^2} - k_BT\mathbb{I} - 2k_BT\frac{\mathbf{b}\otimes\mathbf{b}}{|\mathbf{b}|^2}\right), \\
\frac{\partial \mathbf{b}}{\partial t} &= -[\nabla \mathbf{b}]\mathbf{v} + \mathbb{L}\mathbf{b} - \frac{\Lambda}{T}\rho\left(G(T)\mathbb{A}^{-1}\mathbb{A}^{-\top}\mathbf{b} + H(T)\frac{|\mathbf{b}|^2}{L^2}\mathbf{b} - 3k_BT\mathbf{b}\right),
\end{aligned}$$

while in the equation for momentum $\mathbf{m}$ we have as for the 'Needles Model'

$$\mathbb{T} = -p_{th}\mathbb{I} + \rho G(T)\left(\mathbb{A}^{-1}\mathbb{A}^{-\top} - \frac{2k_BT}{G(T)}\mathbb{I}\right) + \rho H(T)\left(\frac{|\mathbf{b}|^2}{L^2(T)} - \frac{2k_BT}{H(T)}\right)\frac{\mathbf{b}\otimes\mathbf{b}}{|\mathbf{b}^2|}.$$

This model goes into the direction of continuum models of crystal plasticity, where the crystal lattice (defining the slip planes and crystal symmetry) is invariant under under the plastic slip, i.e. the lattice vectors are constant in the structural space. The dissipation comes from the plastic slip and if it were prescribed as rate-independent, it would directly lead to a yield stress criterion. Relaxed models that only approximates rate-independence, as the one in Kratochvíl et al. [2016], are also possible.

Summary

Let us recapitulate how the derivation in GENERIC was performed. We first had to decide what the state variables are. Since we wanted to work with a continuum that is sufficiently described by a position $\mathbf{y}$ of each point and its momentum $\mathbf{M}$ (the points have no internal structure, unlike e.g. cosserat continuum), we took the canonical bracket (4.14), or just the equations (4.15a), as the starting point. The second step than was too choose a more coarse set of variables, carrying less information than $(\mathbf{y}, \mathbf{M})$, but still more than $(\rho, \mathbf{m}, s, \mathbb{A})$.

Once the definition of the additional field $\mathbf{b}$ in terms of the original state variables $(\mathbf{y}, \mathbf{M})$ was clear, the reversible evolution equations for $(\rho, \mathbf{m}, s, \mathbb{A}, \mathbf{b})$ followed and since the new bracket did not involve derivatives with respect to the old variables, the projection was successful. As explained in Remark 4.3, the computation of the bracket is not necessary, but may be advantageous in some situations. For any state variables the choice of the energy can be in principle purely phenomenological, but we rather built on formulas backed by a microscopic derivation.

The irreversible evolution was again a generalized gradient flow. Using the convex analysis we characterized a class of models for which the vector $\mathbf{b}$ pulled back to the natural configuration remains constant. Such an evolution is typical e.g. for lattice vectors in crystal plasticity, while we do not expect it is valid for other applications, for example flows of liquid crystals or highly concentrated polymeric fluids, where the dissipation emanates from the slip between the fluid

and the additive. For both of these classes we provided an example of a dissipation bracket, trying to highlight the most important features of these models. In both cases the choice of the dissipation potential was purely phenomenological.

Conclusion

We first address all the chapters separately and discuss their connections at the end.

Peridynamics

In our opinion, the biggest advantage of our approach is the use of the substitution formula (1.10) which provides a better insight into the problem. It leads to an expression (1.18) for the non-local force flux which is subsequently helpful for proving that the peridynamic interaction cannot be described by a tensor in general; however, when only interactions through planes are considered, the formula can be simplified to (1.12) and the flux has a tensorial character.

Based upon this simplified formula we defined the peridynamic tensor $\mathbf{P}$, whose divergence turned out to be of the correct form (1.15). Moreover, thanks to this mechanical interpretation (i.e. a force flux through a plane), the derived peridynamic tensor $\mathbf{P}$ seems to be more convenient than the peridynamic tensor ν which has only the correct divergence. The defect of the tensor ν, as shown in the Example 1.2, is that it is computed in the reference configuration disregarding the non-local transformation of the geometry due to the deformation. This example also shows that the two tensors ν and $\mathbf{P}$ differ, though some kind of uniqueness result for the former was presented in Silling and Lehoucq [2008].

As was already mentioned, the formula (1.18) for the non-local force flux shows that the peridynamic tensor $\mathbf{P}$ can not be considered as the 1st Piola-Kirchhoff stress tensor. On the other hand, the same formula may be used for proving that in the limit of vanishing non-locality the collapsed tensor $\mathbf{P}_0$ indeed is the 1st Piola-Kirchhoff stress tensor. Fortunately it also holds that this tensor coincides with the collapsed peridynamic tensor ν_0 computed in Silling and Lehoucq [2008]. This provides the so far missing explanation why the tensor ν_0 may provide a relevant description of the limiting model in local elasticity.

The last thing to be discussed is the question of symmetry, related to the balance of angular momentum. There is no ambiguity left in bond-based peridynamic since the peridynamic tensor $\mathbf{P}^{\mathbf{y}}$ is symmetric. In the state based peridynamic, the question of symmetry still remains open. We conjecture that for non-polar materials the tensor $\mathbf{P}^{\mathbf{y}}$ might be also symmetric. Nevertheless, since this tensors is no longer supposed to coincide strictly with the Cauchy stress tensor, its symmetry is perhaps no longer relevant. What is of true importance is the symmetry of its collapsed counterpart $\mathbf{P}_0^{\mathbf{y}}$. Since it holds that the tensors $\mathbf{P}_0$ and ν_0 are equal, one can use the result for the latter which was proved in Silling and Lehoucq [2008]. It says that the tensor ν_0 complies with the balance of angular momentum provided the balance of angular momentum in state-based peridynamic is satisfied.

Concerning further research, the possible next step could be the incorporation of boundary conditions, both for finite horizon and the limiting case. It would be also worthy to specify the sufficient regularity under which the identification of the collapsed tensor $\mathbf{P}_0$ and the 1st Piola-Kirchhoff tensor may be proved rigorously. The main difficulty is to select a family of sufficiently regular control volumes which is at the same time preserved by the deformation. Despite a lot

of effort (c.f. Noll [1974] or Ziemer [1983]) no such a selection is still perfect (see Noll [2010]).

Rate-Independent Systems in Continuum Mechanics

In the second chapter we showed in Theorem 2.9 the existence of a solution to an evolutionary rate-independent model allowing for non-convex energies, suitable e.g. for predicting the mechanical response of shape memory alloys at large strains. Compared to the previous works we weaken the assumptions on the energy functional, using the notion of gradient polyconvexity (GPC) from Definition 2.3. GPC is a natural extension of Ball's polyconvexity since it exploits weak continuity of nonlinear minors of deformation gradients not only in Lebesgue but also in Sobolev spaces, and it brings additional spatial smoothness of volume and area element changes. Our model hence encompasses a broader range of materials, including those with energies of the type shown in Example (2.20).

In the third chapter we generalized the concept of local solutions, developed in Toader and Zanini [2009], Roubíček [2015] only for separately convex energies, by introducing the notion of separately global solutions in Definition 3.1. Unlike energetic solutions, this concept does not force 'too early jumps' and has therefore a broader range of application. We established an existence Theorem 3.21 for separately global solutions to a wide class of problems arising in large strain mechanics, e.g. the gradient bulk damage; see Section 3.2. In particular, the deformation is proven to be injective everywhere in the domain, the energies are non convex and are allowed to blow up for extreme compression, and, last but not least, the dependence on the Eulerian gradient of the Eulerian field of internal variables is covered. This dependence is important from the modelling point of view and in terms of analysis it introduces a coupling between the Lagrangian gradients of the deformation and internal variables contained in the term $\phi\left((\nabla y)^{-\top}\nabla z\right)$ of the total energy (3.29).

To overcome the difficulties caused by this non-linear coupling we use the regularisation by the second gradient of deformation $\nabla^2 y$, which is usually used in so-called non-simple materials (see the Remark 3.2), and also the notable Healey-Krömer Corollary 3.4 adopted from Healey and Krömer [2009]. This allowed us to prove that both ∇y and $(\nabla y)^{-1}$ are bounded in $L^\infty(\Omega)$, even uniformly for the whole sequence of discrete solutions, which in turn makes the problem of integrability and compactness of the term $\phi\left((\nabla y)^{-\top}\nabla z\right)$ partially decoupled, underlying hence the assumed product structure of the state space (3.21).

This kind of regularization was necessary for passing to the limit with the discrete solutions, but it is not necessary for proving their existence. In Lemmata 3.8 and 3.10 polyconvex energies coercive solely in the first gradient ∇y are satisfactory. This is caused by the alternating minimization scheme (3.46) which makes the discrete problem effectively decoupled.

On the other hand, the discrete solutions obtained by this scheme satisfy discrete stability (3.55) and semi-stability (3.56) with different time interpolants of the internal variable. This complicates improving their convergence and hence different techniques, not based on error estimates between the right- and left-continuous piece-wise constant interpolants, had to be used in Lemmata 3.16 and 3.13.

The strong convergence of the variables was needed for passing to the limit in the (semi-)stability in Lemmata 3.18 and (3.17) and for proving energy inequality in Lemma 3.20, which has energy evaluated at arbitrary time on its right-hand side. As opposed to energy *equality* where the energy at final time appears on the left hand side and hence mere lower semi-continuity suffices.

For proving the energy inequality, apart selecting deformations that maximize the reduced power in the sense of (3.90), we also strongly relied on the separate global minimization in the elastic variable (3.105). Both these issues are connected to non-uniqueness of deformations (caused by the lack of convexity) which makes the selection of t-dependent subsequences in Lemma 3.15 more subtle, as already mentioned in Francfort and Mielke [2006].

Although the ansatz for the stored energy density in (3.29) is rather specific, the fully general loading functional illuminates the general strategy. All the (weak lower semi-)continuity properties can be shown in the same way as far as the energy separates the highest order terms of the elastic and internal variable, following hence the product structure of the state space. A possible generalization then includes e.g. phase transformation or plasticity. For the latter the convexity in the internal variable would be lost and hence the connection with the local stability (3.3a) broken. Nevertheless the existence theory based on global semistability, replacing the dissipation potential with a dissipation distance, would be in principle feasible. It would be only restricted to energies that comply with the assumption of splitting the highest order terms.

Future work on separately global solutions may include removing the selectivity gap, already present in the concept of local solutions, either by moving to BV-solutions or to the vanishing viscosity solutions. The latter can be now tackled at least heuristically in numerics by supplying an additional viscous dissipation on the discrete level, although the rigorous convergence analysis is of course still to be done. The numerical computations of separately global solutions are challenging due to the non-convex minimization and also the selection of deformations satisfying the condition (3.90), crucial for obtaining the energy inequality, represents, up to our knowledge, still an open problem.

Another aspect of the separately global solutions, that could be addressed, is their consistency with the concept of local solutions used in the small-strain regime; see Roubíček [2015]. The objective would be to analyze the limiting behavior of the separately global solutions under the assumption that the strain converges to zero and prove whether they converge to the local solutions at small strains; and if, in which sense the convergence is to be understood.

The last comment concerning further generalization concerns the regularization of the energy by the second gradient of deformations $\nabla^2 y$. If one chooses rather the ansatz (3.16) depending on $\mathrm{Cof}\,\nabla y \nabla z$, one has to ask whether the regularization by the gradient polyconvexity (GPC), depending on gradients of nonlinear minors, cannot be used; see Benešová et al. [2018]. It is known that GPC allows for the existence of minimizers under weaker regularity assumptions on the deformation. However, when the boundedness of $\det \nabla y$ from zero is assumed, which was the key ingredient of our analysis, GPC still implies in some cases integrability of the second gradient. It remains an open question, whether the existence theory is possible merely using GPC.

GENERIC

In the last chapter devoted to GENERIC, we first explained the fundamentals on the very simple example of damped harmonic oscillator and continued by derivation of standard visco-elastic models of Giesekus, Maxwell or Oldroyd-B. We used the phenomenological approach, which enhances the standard hydromechanic fields of density, momentum, and entropy by additional structural parameters, making the resulting models able to capture more complex phenomena. Instead of relying on the machinery of differential geometry, c.f. [Öttinger, 2005, App. B.4], we derived the kinematics of the new state variables from the continuum counterpart of the Hamilton's canonical equations, following the earlier works Edwards and Beris [1991], Pavelka et al. [2020]. The difficulty hence consists in realizing what the state parameters of the new system should be and how they are defined in terms of a more detailed system, whose evolution is known. In this spirit we derived the reversible evolution of the anisotropic model, keeping the advantage of the continuum canonical equations, i.e. the full generality of the energy functional. The irreversible evolution was prescribed as a generalized gradient flow, removing hence the kinematic restriction present in Rajagopal and Srinivasa [2001], which supposed the vector describing the anisotropy is constant in the natural configuration. Using the dual dissipation potential we then characterized materials complying with this constraint, which is typical e.g. for crystal plasticity. We then closed the chapter by two models, one mimicking the crystal plasticity, the other one rather liquid crystals or highly concentrated polymeric fluids. In both models the choice of dissipation potential and energy was purely phenomenological, although the latter was inspired by energies backed by microscopic derivation.

One of the main goals of this chapter was to show that it is not necessary to abandon the variational principles (least action or Hamiltonian mechanics), because they lead to reversible, non-dissipative systems; instead they can be successfully modified, yielding then an evolution that dissipates energy and which is compatible with the laws of thermodynamics. The GENERIC framework aims directly at obtaining the most important parts of every model:

- Reversible evolution: $\left(\dot{F}\right)_{\text{rev}} = \{F, E\}$,
  derived from Hamiltonian mechanics,
  does *not* build on *surface forces* and works for *general energy* E,
- Irreversible evolution: $\left(\dot{F}\right)_{\text{rev}} = [F, S]$,
  based on entropy production,
  does *not* use *inelastic stress tensors* and works for *general entropy* S,
- 1st law: $\dot{E} = \{E, E\} + [E, S] = 0$,
  assured by antisymmetry of $\{\cdot, \cdot\}$ and degeneracy of $[\cdot, \cdot]$,
  no heat flux or power of forces are necessary to introduce,
- 2nd law: $\dot{S} = \{S, E\} + [S, S] = [S, S] \geq 0$,
  implied by degeneracy of $\{\cdot, \cdot\}$ and monotonicity of $[\cdot, \cdot]$,
  no entropy flux or net entropy production has to be identified,
- '4th law': Onsager-Casimir Reciprocal Relations,
  guaranteed by the transformation properties of the dissipation potential Ξ

with respect to the Time Reversal Transformation,
no further structural assumptions are necessary.

GENERIC gives structure, which is elegant and suitable for theoretical considerations. It also says what the key steps one should focus on are:

- to choose the state variables which describes the system appropriately,
- to derive their mechanics, describing processes fully under control,
- to specify the energy determining the materials' 'elastic' properties,
- to derive the dissipation potential which determines the entropy production, caused by processes on a more detailed level of description which are no more under control.

GENERIC does not make these steps necessarily easier; however, having a unified framework is advantageous when one wants to derive all the GENERIC's building blocks from a more detailed level of description; for state variables one uses the chain rule [5], the entropy (and hence energy) can be computed using the static MaxEnt (max entropy) method (see Pavelka et al. [2019, 2018a]), and the dissipation potential can be inferred from statistical mechanics, for example by large deviations principle; see Touchette [2009], Mielke et al. [2014], Öttinger [2005]. Apart from this multi-scale approach, there is also the phenomenological one. The reversible mechanics may be derived by geometric arguments or by the principle of least action (see e.g. Simo et al. [1988], Öttinger [2005] and references therein), and is determined solely by the set of the state variables, which has to be selected by experimentalists. The dissipation potential is chosen by the entropy production it yields. Finally, energy, or equivalently entropy, may be chosen by the very same techniques as in other theories of continuum mechanics, e.g. it can be based on different strain measures, theory of invariants, representation theorems, etc; see e.g. Gurtin et al. [2010], Hutter and Jöhnk [2004], Ciarlet [1988].

It should be stressed that many of the key ideas in GENERIC are also a vital part of other theories. In particular, the framework of the natural configuration follows the presented guideline as it extends the set of hydromechanic variables by an additional tensor field defining the natural configuration. Moreover, its elastic response is determined by energy, while the inelastic by the dissipation function prescribing the dissipation rate. The only difference is that either the evolution is such that the entropy rate is maximized, or the constitutive relations are given by closures leading to the prescribed entropy production. In some cases, the former procedure can be proven to be equivalent to GENERIC; Janečka and Pavelka [2018a]. On the other hand, the latter procedure may yield various constitutive relations and requires identification of the entropy flux and the net entropy production, itself also non-unique, whereas in GENERIC the irreversible evolution is fully specified by the entropy production. Therefore, the only restriction of this framework comes from the underlying theory of simple materials; see e.g. Truesdell and Noll [2004], Gurtin et al. [2010], Ciarlet [1988].

[5] See e.g. Pavelka et al. [2019] for derivations where the projection of the Poisson bracket fails.

Regarding this so-called 'Cauchy straitjacket' we would like to compare GENERIC with another approach to continuum mechanics and thermodynamics, namely the Principle of Virtual Power (PVP), which removes the Cauchy restriction of surface forces in an elegant way; see dell'Isola et al. [2017], Frémond [2002], Gurtin et al. [2010]. Instead of energy, it builds on the functional of virtual power, which determines the equation of motion, valid also for dissipative systems. The functional of virtual power is defined on the field of virtual velocities, and hence its structure is given by the Schwartz general representation theorems for distributions; see dell'Isola et al. [2017]. On the other hand, the incorporation of the first and second law of thermodynamics into the framework is still based on the existence of heat flux and entropy flux, their relation, and identification of the net entropy production; see Frémond [2002]. In total, the Cauchy straitjacket might be still present in the considered form of the entropy or energy flux, and even if the standard relation between the heat and entropy flux is abandoned, the identification of the net internal entropy production is again ambiguous.

Afterword

Let us finish by two remarks which link the chapters together. First, in GENERIC there is a procedure for deriving effective models, called *dynamic* MaxEnt reduction, which is based on the relaxation of the state variables towards the thermodynamic equilibrium; see Pavelka et al. [2018a], Klika et al. [2019]. Roughly speaking, the variable which relaxes the fastest is replaced by its equilibrium value, others variables being fixed. The set of state variables is reduced and an effective evolution, having again the GENERIC structure, is obtained. The explicit example in Pavelka et al. [2018a], Klika et al. [2019] demonstrates the method on harmonic oscillator, adumbrating a hierarchy of models of continuum mechanics, starting with a full description, continuing by viscous gradient flow, rate-independent processes coupled with temperature, and ending with a fully rate-independent system.

The second remark concerns the generality of the five building blocks of GENERIC, energy in particular, and the limit of peridynamics for vanishing nonlocality, anticipated to be the standard local theory. Computation of the limiting free energy functional is trivial (on the formal level, see e.g. Silling [2000]) or at least straightforward when convergence of solution(s) is also addressed (see Bellido et al. [2015], Pelech [2016] for computation of the Γ-limit); in contrast to the definition of traction or stress tensor, which requires long lines of reasoning and even though it is not consistent and definitely not unique. The problem of computing the stress tensor from microscopic or atomic theories is definitely not new and has been addressed in many works; see Schofield and Henderson [1982] or Murdoch [2007] just to mention a few.

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A. Attachments

A.1 Analytical Tools

Lemma A.1 (Healey-Krömer). *Let $p > 3$, $s \geq \frac{3p}{p-3}$, Then for every $y \in \mathcal{Y}$ there exists $\varepsilon_y > 0$ s.t.*

$$\det \nabla y \geq \varepsilon_y > 0 \quad \text{in } \overline{\Omega}. \tag{A.1}$$

Moreover, if a sequence $\{y_\tau\} \subset \mathcal{Y}$ is uniformly bounded in $W^{2,p}(\Omega)$, and the sequence $\{(\det \nabla y_\tau)^{-1}\}$ is uniformly bounded in $L^s(\Omega)$, then the bound on the determinant in (A.1) *is uniform.*

Proof. As $p > 3$, $y \in \mathcal{Y}$ can be considered continuous. Assume without loss of generality that $0 \in \Omega$, and assume by contradiction that $\det \nabla y(0) = 0$. Then we have for every $x \in \Omega$ that

$$|\det \nabla y(x)| \leq C(1 + |\nabla y(x)|^2 + |\nabla y(0)|^2)|\nabla y(x) - \nabla y(0)| \leq \tilde{C}|x|^\alpha \ ,$$

where $\alpha = 1 - 3/p$ is given by the continuous embedding $W^{2,p}(\Omega) \hookrightarrow C^{0,\alpha}(\Omega)$, and where the first inequality follows from the local Lipschitz property of $F \mapsto \det F$, see also [Dacorogna, 2008, Prop. 2.32]. Hence,

$$\begin{aligned}\int_\Omega \frac{\mathrm{d}x}{(\det \nabla y)^s}\,\mathrm{d}x \geq \int_{B(0,r)} \frac{\mathrm{d}x}{(\det \nabla y)^s}\,\mathrm{d}x \geq \int_{B(0,r)} \frac{\mathrm{d}x}{\tilde{C}^s|x|^{\alpha s}} \\ \geq \frac{4}{3}\pi r^3 \frac{1}{\tilde{C}^s r^{\alpha s}} \ .\end{aligned}$$

However, the last expression diverges for $r \to 0$ if $3 - \alpha s < 0$, i.e., if $s > 3p/(p-3)$. If $s = 3p/(p-3)$ then we have that for every $r > 0$ small enough

$$\int_{B(0,r)} \frac{\mathrm{d}x}{(\det \nabla y)^s} \geq \frac{4\pi}{3\tilde{C}^s} \ ,$$

which is not possible if $(\det \nabla y)^{-1} \in L^s(\Omega)$, because the Lebesgue integral is absolutely continuous. Altogether, we proved that $y \notin \mathcal{Y}$. If $0 \in \partial\Omega$ then we proceed in a similar way. Namely, as Ω is Lipschitz, it has the cone property. This implies that $\mathcal{L}^3((B(0,r) \cap \Omega) \geq \tilde{C}r^3$ for $r > 0$ small and some $\tilde{C} > 0$ independent of r. Hence $\det \nabla y > 0$ in $\bar{\Omega}$ and it is a continuous function. Inevitably, it is bounded from below by a positive constant in $\bar{\Omega}$.

For the proof of the uniform bound we refer to [Benešová et al., 2018, Proof of Prop. 5.1], from which we can apply the procedure for an infinite number of minimizers. □

Lemma A.2. *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Assume that $C, c > 0$ and $h : \Omega \times \mathbb{R} \times \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3\times3} \to \mathbb{R}$ is a Carathéodory integrand such that for all $(x, z, F, G) \in \Omega \times \mathbb{R} \times \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3\times3}$ and some $p, q \in [1, +\infty)$*

$$c(|z|^q + |F|^{p*} + |G|^p) - C \leq h(x, z, F, G) \leq C(1 + |z|^q + |F|^{p^*} + |G|^p) \ ,$$

where $h(x,z,F,\cdot)$ is strictly convex and

$$p^* := \begin{cases} pn/(n-p) & \text{if } 1<p<n, \\ +\infty & \text{otherwise.} \end{cases}$$

If $y_k \rightharpoonup y$ in $W^{2,p}(\Omega;\mathbb{R}^n)$, $z_k \to z$ in L^q, and

$$\int_\Omega h(x,z_k(x),\nabla y_k(x),\nabla^2 y_k(x))\,\mathrm{d}x \to \int_\Omega h(x,z(x),\nabla y(x),\nabla^2 y(x))\,\mathrm{d}x, \qquad \text{(A.2)}$$

then $y_k \to y$ in $W^{2,p}(\Omega;\mathbb{R}^n)$.

Proof. Consider the sequence $\{(z_k,\nabla y_k,\nabla^2 y_k)\}$. By the fundamental theorem on Young measures, see [Pedregal, 1997, Thm. 6.2] or Ball [1989], there is a subsequence generating a Young measure ν. Thanks to [Pedregal, 1997, Prop. 6.13] the strong convergence of z_τ and ∇y_τ implies

$$\nu_x = \delta_{z(x)} \otimes \delta_{\nabla y(x)} \otimes \mu_x \quad \text{for a.e. } x \in \Omega$$

where $\mu = \mu_x$ is the Young measure generated by $(\nabla^2 y_k)_{k\in\mathbb{N}}$. In view of (A.2) and [Pedregal, 1997, Thm. 6.11] applied to $\tilde{h} := h + c$ we get

$$\begin{aligned}\int_\Omega \tilde{h}(x,z(x),\nabla y(x),\nabla^2 y(x))\,\mathrm{d}x &= \liminf_{k\to\infty} \int_\Omega \tilde{h}(x,z_k(x),\nabla y_k(x),\nabla^2 y_k(x))\,\mathrm{d}x \\ &\geq \int_\Omega \int_{\mathbb{R}^{3\times3\times3}} \tilde{h}(x,z(x),\nabla y(x),G)\mu_x(\mathrm{d}G)\,\mathrm{d}x\ .\end{aligned}$$

The strict convexity of $\tilde{h}$ in in the last variable together with Jensen's inequality imply that $\mu_x = \delta_{\nabla^2 y(x)}$ for almost every $x \in \Omega$. This further implies that $\nabla^2 y_k$ converges to $\nabla^2 y$ in measure; see [Müller, 1999, Cor.3.2]. Finally, (A.2) with [Pedregal, 1997, Corollary 6.10] yields the strong convergence of $y_k \to y$ in $W^{1,p}(\Omega;\mathbb{R}^3)$. □

Remark. *For a reader not familiar with Young measures we sketch different proof, which, however, still relies on coercivity and growth of the energy and its equiintegrability, and resembles in many aspects original proof. The key idea is to use the old Visintin result, allowing x-dependence, for the convergence*

$$\int_\Omega h(x,z(x),\nabla y(x),\nabla^2 y_k(x))\,\mathrm{d}x \to \int_\Omega h(x,z(x),\nabla y(x),\nabla^2 y(x))\,\mathrm{d}x.$$

To prove this we first need to show

$$\int_\Omega h(x,z_k(x),\nabla y_k(x),\nabla^2 y_k(x)) - h(x,z(x),\nabla y(x),\nabla^2 y_k(x))\,\mathrm{d}x \to 0.$$

Proving that the integrand convergences in measure is standard, while the integrability question is reduced, thanks to coercivity and growth, to equiintegrability of $h(x,z_k(x),\nabla y_k(x),\nabla^2 y_k(x))$. The latter follows by the convergence (A.2)*. Indeed, the lower semi-continuity of the functional implies convergence on all measurable subset of Ω. Hence the biting limit coincides with $h(x,z(x),\nabla y(x),\nabla^2 y(x))$ and since* (A.2) *holds we have by [Pedregal, 1997, Lemma 6.9] the biting convergence is actually a weak one, by which the equiintegrability follows.*

Lemma A.3 (Decomposition Lemma; Fonseca et al. [1998]). *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain and let $\{w_i\} \subset W^{1,\alpha}(\Omega)$, $\alpha > 1$, be bounded. Then there exists a subsequence $\{w_j\}$ and a sequence $\{v_j\} \subset W^{1,\alpha}(\Omega)$ such that*

$$\begin{aligned} \|v_j\|_{1,\infty} &\leq C(\alpha, \Omega) j, \\ \mathcal{L}^3(M_j) &\leq \frac{C}{j^\alpha}, \\ \{|\nabla v_j|^\alpha\} &\text{ is equiintegrable,} \end{aligned}$$

where $M_j := \{x \in \Omega : w_j(x) \neq v_j(x) \text{ or } \nabla w_j(x) \neq \nabla v_j(x)\}$.

Lemma A.4 (Lipschitz Truncation; Ziemer [1989]). *Let $\Omega \subset \mathbb{R}^3$ be a Lipschitz domain, $1 < \alpha < +\infty$, and $u \in W^{1,\alpha}(\Omega)$. Then for every $\lambda > 0$ there exists $u^\lambda \in W^{1,\infty}(\Omega)$ such that*

$$\begin{aligned} \|u^\lambda\|_{1,\infty} &\leq C(\alpha, \Omega)\lambda, \\ \mathcal{L}^3(\{u \neq u^\lambda \text{ or } \nabla u \neq \nabla u^\lambda\}) &\leq \frac{C(\alpha)}{\lambda^\alpha} \int_{|\nabla u| \geq \lambda/2} |\nabla u(x)|^\alpha \, \mathrm{d}x \\ \|u^\lambda\|_{1,\alpha} &\leq C(\alpha, \Omega)\|u\|_{1,\alpha}. \end{aligned}$$

In particular, denoting $M_\lambda := \{x \in \Omega : u(x) \neq u^\lambda(x) \text{ or } \nabla u(x) \neq \nabla u^\lambda(x)\}$, we have

$$\lim_{\lambda \to \infty} \lambda^\alpha \mathcal{L}^3(M_\lambda) = 0, \quad \text{and} \quad \lim_{\lambda \to \infty} \|u^\lambda - u\|_{1,\alpha} = 0.$$