INTERNATIONAL JOURNAL OF STRUCTURAL CHANGES IN SOLIDS – Mechanics and Applications
Volume 1, Number 1, December 2009, pp. 61-72
IJSCS

Two configurational approaches on the modelling of continuum dislocation inelasticity ☆

A. Menzel[a,b,*], B. Svendsen[a]

[a] *Institute of Mechanics, Faculty of Mechanical Engineering, TU Dortmund University, Leonhard-Euler-Str. 5, D-44227 Dortmund, Germany*
[b] *Division of Solid Mechanics, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden*

Abstract

The main focus of this contribution consists in the elaboration of a continuum modelling approach accounting for dislocation-based quantities. Related deformation dependent history-variables are attached to individual material points and, moreover, are extended by means of gradients thereof so that so-called weak non-localities are captured. These gradients of internal variables may be further specified and in this regard are here reduced to particular representations of dislocation density tensors. While in this work we will make use of the concept of a material isomorphism—similarly present in the kinematic framework denoted as multiplicative decomposition—the approach itself can also be generalised, for instance with application to micromorphic continua. Apart from the non-simple kinematic framework, special emphasis is placed on the configurational mechanics perspective of the problem at hand. First, a variational strategy is discussed in detail, whereby the underlying stored energy density is assumed as an isotropic function in terms of its arguments. Later on, the configurational framework derived is compared with the configurational balance of linear momentum as based on straightforward transformation relations of its standard spatial representation. As a result, similar forms of the configurational Eshelby stresses are obtained for the two different approaches, and the related volume forces additionally incorporate contributions related to the material's hereogeneities and inhomogeneities.

Key words: Configurational mechanics, inelasticity, material isomorphism, variational formulation, non-simple material

1. Introduction

Material design constitutes a continuously increasing field of multi-disciplinary research. The rapid development of this engineering and material science area essentially rely on the elaboration and further development of the various mechanical—and in general also chemical—properties of advanced materials at their several scales of observation. In particular, it is the material's microstructure—such as defects, dislocations, texture, and so forth—and the evolution thereof that determine the overall properties of the material itself. Different approaches to incorporate such inhomogeneities into field equations and constitutive equations have been proposed in the literature; an overview is provided in the contributions by, for instance, Noll (1967), Capriz (1989), Šilhavý (1997), and Epstein and Elżanowski (2007).

The description and incorporation of the material's inhomogeneities is directly reflected by configurational modelling approaches, which date back to the pioneering works of Eshelby; see the collected papers in Markenscoff and Gupta (2006), and the reader is also referred to the monographs by Hanyga (1985), Maugin (1993), and

☆Dedicated to the occasion of the 75th birthday of Alan Wineman.

*Corresponding author
Email address: andreas.menzel@udo.edu/andreas.menzel@solid.lth.se (A. Menzel)

Gurtin (2000a) for a survey. In general, the derivation of configurational balance relations can either be based on variational strategies or on transformations of standard established balance equations. Reviews on the first type of formulations are reviewed in, for example, Ogden (1997) or Podio-Guidugli (2001), while the latter one is discussed in, for instance, Steinmann (2002b). Moreover, the transformation-based framework has been extended towards gradient continua and micromorphic continua in Kirchner and Steinmann (2007) and Hirschberger *et al.* (2007). Within the last decade, variational approaches have been developed for different fields of application in the area of computational inelasticity; see Hackl (1997), Ortiz and Repetto (1999), Miehe (2002), and Carstensen *et al.* (2002). The extension of such an incremental variational formulation to a configurational mechanics framework has been suggested in Svendsen (2005).

In this contribution we make use of the introduction of a so-called material isomorphism as elaborated by Noll (1967), Negahban and Wineman (1992), Bertram (1999), and Svendsen (1998). Extensions of this nowadays classical framework towards a configurational mechanics setting are proposed in the contributions by Epstein and Maugin (1990), and Epstein (2002), Maugin (2003), or—with emphasis on computational aspects of a configurational small strain inelasticity formulation—by Menzel *et al.* (2004, 2005). In view of theoretical investigations that in particular study the relation between configurational volume forces and the continuum theory of dislocations, we additionally refer the reader to Steinmann (2002a) and Menzel and Steinmann (2005, 2007). Alternatively, one may include dislocation-related quantities as arguments into the stored energy function; see Menzel and Steinmann (2000), Gurtin (2000b, 2002), Svendsen (2002), and Levkovitch and Svendsen (2006) for an overview on different formulations in this regard. A general framework, as based on an incremental variational formulation, is suggested in Svendsen *et al.* (2009), wherein the additional field variable is either treated as a Mindlin-type variable or kinematically coupled in the spirit of a material isomorphism.

As mentioned above, we will make use of two different frameworks to derive configurational balance relations: a variational approach and a transformation-based approach. Furthermore, the overall idea consists in elaborating formulations that in a continuum framework reflect dislocation- and inelasticity phenomena. Accordingly, the gradient of the material isomorphism is incorporated into the strain energy function in terms of a dislocation density tensor. For reasons of conceptual simplicity, we will neglect any additional hardening effects. Before we begin with reviewing some essential kinematic relations in section 2, some aspects of the Peach-Koehler force as well as general transformations of divergence and curl operations, as present in common balance relations, are briefly summarised. Based on this, section 3 discusses further constitutive restrictions in the framework of hyper-elastic forms. As a key aspect of the continuum dislocation framework, a variational formulation is developed in section 4, whereby the overall spatial motion of the body itself as well as the material isomorphism are treated as field variables. With these two balance equations in hand, section 5 elaborates the two different configurational approaches that as a result render identical flux terms, or rather Eshelby stresses, but different source terms, or rather volume forces. Finally, the relation to the Peach-Koehler force is briefly discussed in section 6.

1.1. A brief note on the Peach-Koehler force and the transformation of balance equations

The celebrated Peach-Koehler force, as introduced in Peach and Koehler (1950), has nowadays been applied in various fields of solid mechanics. The particular form of this configurational force can be based on different concepts and derivations. A classical example of this pseudo vector consists in its interpretation as the force driving a single dislocation. In addition to the literature cited above, we here give reference to the early work by Kröner (1958), where the Peach-Koehler force ($\mathrm{d}\mathbf{f}$) was derived from the principle of virtual displacements ($\mathrm{d}\boldsymbol{\xi}$). To be specific, the external (V) and internal potential (W) were related to the particular force of interest via $\mathrm{d}\mathbf{f}\cdot\mathrm{d}\boldsymbol{\xi} = -\,[\,\mathrm{d}V + \mathrm{d}W\,]$. Furthermore, let $\mathrm{d}\boldsymbol{a} = \mathrm{d}\boldsymbol{\xi}\times\mathrm{d}\boldsymbol{l}$ characterise the area element passed over by the line element $\mathrm{d}\boldsymbol{l}$ of the dislocation. With $\boldsymbol{\sigma}$ denoting the stresses acting on a 'virtual' cut along $\mathrm{d}\boldsymbol{a}$, one concludes that $\mathrm{d}V + \mathrm{d}W + \mathrm{d}\boldsymbol{a}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{b} = 0$, wherein $-\,\boldsymbol{b}$ corresponds to an infinitesimal displacement vector. Straightforward arguments of comparison then render

$$\mathrm{d}\mathbf{f} = \mathrm{d}\boldsymbol{l}\times[\,\boldsymbol{\sigma}\cdot\boldsymbol{b}\,] \tag{II.148}$$

and

> *Die weitreichende Gültigkeit der Gl. (II.148) rührt daher, dass sie allein eine Folge des sehr allgemeinen Prinzips der virtuellen Verrückungen ist.* (Kröner, 1958, p. 86)

While these investigations were based on small deformation kinematics,

> *It is a tricky matter to correctly interpret calculations of forces acting when a dislocation moves through a material. ... For linear theory, the Peach-Koehler forces are among those considered, and it is hard to know how to define these, for nonlinear theory.* (Ericksen, 1998, p. 19,20)

From the conceptual point of view, one may especially rise the question, where to introduce the dislocation itself—either in the so-called current or in a reference configuration. Apparently, the particular choice renders the related driving force to be settled in the respective configuration as well. When making use of additional modelling concepts, such as the introduction of a local material isomorphism, the dislocation-related incompatibility can be referred to these local transformations so that neither the particular reference (material) configuration chosen nor the current (spatial) configuration have to be incompatible. Nevertheless, these geometric aspects render the standard form of the Piola identity—see, for example, Ciarlet (1988)—to be no longer valid when referred to the material isomorphism mentioned. A rigorous derivation of these relations was already established in the pioneering work by Noll (1967), where he stated that

> *The usual version of Cauchy's equation of balance is very useful only when applied to bodies that are homogeneous. For applications to materially uniform but inhomogeneous bodies, a new version of Cauchy's equations is much more suitable than the usual one.* (Noll, 1967, p. 2)

By analogy with (Noll, 1967§15.) and in line with the investigations reported in Dassiso and Lindell (2001) and G. de Saxcé (2001), we briefly review the implications of non-compatible transformations of standard balance equations. In other words, the effect of the incompatible part of the second-order tensor that transforms a vectorial balance equation is discussed. In this context, consider the extension of the vectorial Helmholtz decomposition of a vector field $\boldsymbol{v}$ to a second-order tensor field $\boldsymbol{T}$, namely

$$\boldsymbol{v} = \nabla_{\boldsymbol{\Xi}}\, a + \nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times \boldsymbol{b} + \boldsymbol{v}_c \quad \text{so that} \quad \boldsymbol{T} = \nabla_{\boldsymbol{\Xi}}\, \boldsymbol{a} + \nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times \boldsymbol{B} + \boldsymbol{T}_c\,, \tag{1}$$

whereby $\boldsymbol{v}_c$ and $\boldsymbol{T}_c$ are constants. The incompatibility of both fields is directly related to the curl-terms $\nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times \bullet$ with $\boldsymbol{\Xi}$ denoting vectorial positions in space. Next, let $\boldsymbol{T}$ take the interpretation of a local isomorphism. Apparently, the related Piola-identity $\nabla_{\boldsymbol{\Xi}} \cdot \mathrm{cof}(\boldsymbol{T}) = \boldsymbol{0}$ is violated for $\nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times \boldsymbol{B} \neq \boldsymbol{0}$. In view of two second-order tensors, say $\boldsymbol{K}$ and $\boldsymbol{\kappa}$, that are Piola-related in terms of $\boldsymbol{T}$ via $\boldsymbol{K} = \boldsymbol{\kappa} \cdot \mathrm{cof}(\boldsymbol{T})$, we obtain non-standard transformation relations for the divergence and curl-operation. Based on $\mathrm{d}\boldsymbol{\xi} = \boldsymbol{T} \cdot \mathrm{d}\boldsymbol{\Xi}$, so that $\nabla_{\boldsymbol{\Xi}} \bullet = [\,\nabla_{\boldsymbol{\xi}} \bullet\,] \cdot \boldsymbol{T}$, one ends up with

$$\begin{aligned} \nabla_{\boldsymbol{\Xi}} \cdot \boldsymbol{K} \quad &= \quad \boldsymbol{\kappa} \cdot [\,\nabla_{\boldsymbol{\Xi}} \cdot \mathrm{cof}(\boldsymbol{T})\,] \quad + \quad \det(\boldsymbol{T})\, \nabla_{\boldsymbol{\xi}} \cdot \boldsymbol{\kappa}\,, \\ \nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times (\,\boldsymbol{\kappa} \cdot \boldsymbol{T}\,) \quad &= \quad \boldsymbol{\kappa} \cdot [\,\nabla^{\mathrm{t}}_{\boldsymbol{\Xi}} \times \boldsymbol{T}\,] \quad + \quad [\,\nabla^{\mathrm{t}}_{\boldsymbol{\xi}} \times \boldsymbol{\kappa}\,] \cdot \mathrm{cof}(\boldsymbol{T})\,, \end{aligned} \tag{2}$$

which determines the transformation of flux terms as present in common balance relations.

With these rather general considerations—on the Peach-Koehler force and the format of transformations of balance equations in terms of an incompatible local isomorphism—in hand, we next study the configurational mechanics of an inelastic continuum. The particular formulation considered is based on the introduction of a material isomorphism, which allows interpretation as an incompatible tensorial quantity. Its curl-term characterises this incompatibility and is referred to a dislocation density tensor. As this physically motivated object is introduced as an additional argument into the stored energy function, the balance of linear momentum relation is directly influenced by the incompatible part of the material isomorphism. In a configurational mechanics context, the Eshelby-type stresses as well as the related volume force take an extended form according to these additional contributions.

2. Basic kinematics

To set the stage and to introduce notation, this section briefly reviews basic kinematic relations essential for the subsequent elaborations. The particular framework adopted is based on the introduction of a material isomorphism, which can be related to what commonly is referred to as the multiplicative decomposition of the deformation gradient; see figure 1 for a graphical illustration.

In this regard, consider a sufficiently smooth motion of a body B, which we introduce as $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X}, t) : \mathcal{B}_0 \times \mathcal{T} \to \mathcal{B}_t$. The arguments of the mapping $\boldsymbol{\varphi}$ are referential positions of material particles, $\boldsymbol{X} \in \mathcal{B}_0$, and time, t. In addition to the motion gradient, $\boldsymbol{F} = \nabla_{\boldsymbol{X}} \boldsymbol{\varphi}$ with $J = \det(\boldsymbol{F}) > 0$, the overall constitutive response of the inelastic material considered is assumed to further depend on internal variables. Here, we adopt the concept of a material isomorphism, so that the second-order tensor $\boldsymbol{F}_{\mathrm{p}}$—with $J_{\mathrm{p}} = \det(\boldsymbol{F}_{\mathrm{p}}) > 0$—reflects the local effects of inelastic deformations. On the one hand, use of a kinematically directly coupled form of $\boldsymbol{F}_{\mathrm{p}}$ and $\boldsymbol{F}$ will be made, namely $\boldsymbol{F}_{\mathrm{e}} = \boldsymbol{F} \cdot \boldsymbol{F}_{\mathrm{p}}^{-1}$ so that $J_{\mathrm{e}} = J\, J_{\mathrm{p}}^{-1} > 0$. On the other hand, we are particularly interested in introducing weakly non-local dislocation-related quantities as supplementary arguments into the stored energy. Accordingly, gradients of $\boldsymbol{F}_{\mathrm{p}}$ are accounted for in terms of so-called dislocation density tensors. Due to the fact that the motion $\boldsymbol{\varphi}$ is assumed to be compatible, one alternatively could set up a one-to-one formulation based on gradients of $\boldsymbol{F}_{\mathrm{e}}$. In this contribution, however, we restrict ourselves to an outline in terms of $\boldsymbol{F}_{\mathrm{p}}$ and consider the curve-integral

$$\int_{\mathcal{C}_{\mathrm{p}}} \mathrm{d}\boldsymbol{x}_{\mathrm{p}} = \oint_{\mathcal{C}_0} \boldsymbol{F}_{\mathrm{p}} \cdot \mathrm{d}\boldsymbol{X} = \int_{\mathcal{A}_0} \nabla_{\boldsymbol{X}}^{\mathrm{t}} \times \boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{N} \,\mathrm{d}A_0 = \int_{\mathcal{A}_0} \boldsymbol{A}_{\mathrm{p}} \cdot \boldsymbol{N} \,\mathrm{d}A_0 \neq \boldsymbol{0}\,, \tag{3}$$

whereby use of Stoke's theorem has been made, and $\boldsymbol{N}$ characterises a referential outward surface normal unit vector. The two-point tensor $\boldsymbol{A}_{\mathrm{p}} = \nabla_{\boldsymbol{X}}^{\mathrm{t}} \times \boldsymbol{F}_{\mathrm{p}} = -\nabla_{\boldsymbol{X}} \boldsymbol{F}_{\mathrm{p}} : \boldsymbol{E}$ represents the dislocation density tensor, which, moreover, defines the continuum Burgers density vector $\boldsymbol{b}_{\mathrm{p}}^{\mathrm{bur}} = \boldsymbol{A}_{\mathrm{p}} \cdot \boldsymbol{N}$. In order to deal with a one-point tensor, as commonly used in continuum dislocation theories, we apply a formal Piola transformation, $\boldsymbol{n}_{\mathrm{p}}\, \mathrm{d}A_{\mathrm{p}} = \mathrm{cof}(\boldsymbol{F}_{\mathrm{p}}) \cdot \boldsymbol{N}\, \mathrm{d}A_0$ with $\boldsymbol{n}_{\mathrm{p}} \cdot \boldsymbol{n}_{\mathrm{p}} = 1$, which enables us to identify the one-point dislocation density tensor sought, i.e.

$$\boldsymbol{D}_{\mathrm{p}} = \boldsymbol{A}_{\mathrm{p}} \cdot \mathrm{cof}(\boldsymbol{F}_{\mathrm{p}}^{-1})\,. \tag{4}$$

3. Hyper-elastic forms

The constitutive equations for the stress-type flux terms, occurring in the balance equations considered later on, are here assumed to stem from the derivative of a potential—the stored energy function. In fact, the introduction of such an energy potential turns out to be essential for the two different configurational approaches discussed as this contribution proceeds.

As the material body is, in general, heterogeneous and inhomogeneous, we allow all arguments of the stored energy—as well as explicitly the stored energy itself—to depend on the referential positions of particles. Its density form then allows representation as

$$W(\boldsymbol{F}, \boldsymbol{F}_{\mathrm{p}}, \boldsymbol{A}_{\mathrm{p}}; \boldsymbol{X}) \tag{5}$$

Since $\boldsymbol{F}_{\mathrm{p}}$ is modelled in particular as an elastic material isomorphism, there exists a reduced form of the stored energy such that

$$W = \widetilde{W}(\boldsymbol{F} \cdot \boldsymbol{F}_{\mathrm{p}}^{-1}, \boldsymbol{A}_{\mathrm{p}} \cdot \mathrm{cof}(\boldsymbol{F}_{\mathrm{p}}^{-1}); \boldsymbol{X}) = \widetilde{W}(\boldsymbol{F}_{\mathrm{e}}, \boldsymbol{D}_{\mathrm{p}}; \boldsymbol{X})\,. \tag{6}$$

This in turn implies a direct coupling of both deformation measures as shown in figure 1. Besides these basic assumptions on the coupling of $\boldsymbol{F}$ and $\boldsymbol{F}_{\mathrm{p}}$, the stored energy function is further restricted by the principle of material frame-indifference and the material's symmetry properties. In other words, the spatial action of the orthogonal group on the arguments of W leaves the stored energy unchanged, i.e. $\widetilde{W}(\boldsymbol{F}_{\mathrm{e}}, \boldsymbol{D}_{\mathrm{p}}; \boldsymbol{X}) = \widetilde{W}(\boldsymbol{q} \cdot$

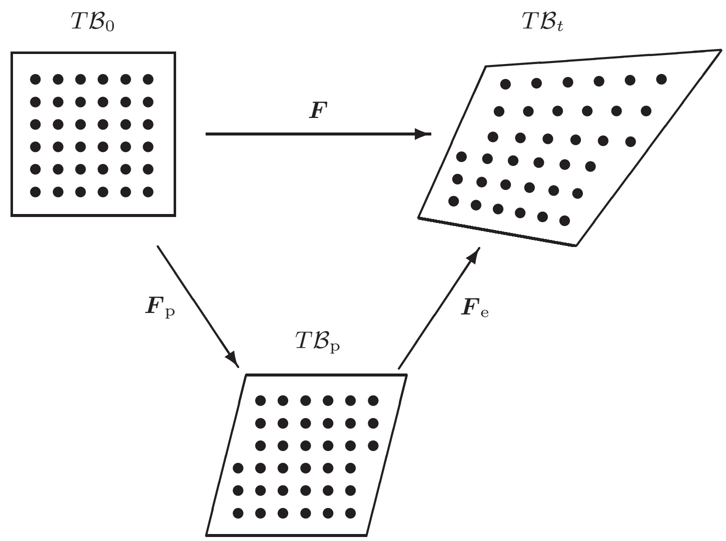

Figure 1: Basic kinematics: material isomorphism and its relation to the so-called multiplicative decomposition.

$\boldsymbol{F}_\mathrm{e}, \boldsymbol{D}_\mathrm{p}; \boldsymbol{X})$ for all $\boldsymbol{q}^\mathrm{t} = \boldsymbol{q}^{-1}$. It is then obvious that the directional derivative with respect to $\boldsymbol{q}_\varepsilon = \exp(\varepsilon\, \boldsymbol{w}) \cdot \boldsymbol{q}$ must vanish, i.e.

$$[\,\partial_{\boldsymbol{F}_\mathrm{e}} W \cdot \boldsymbol{F}_\mathrm{e}^\mathrm{t}\,] : \boldsymbol{w} = 0 \qquad \forall\, \boldsymbol{w} = -\,\boldsymbol{w}^\mathrm{t}\,. \tag{7}$$

Furthermore, we assume the material body of interest to be isotropic. As a consequence, the stored energy remains invariant under the material action of the orthogonal group on its arguments, namely $\widetilde{W}(\boldsymbol{F}_\mathrm{e}, \boldsymbol{D}_\mathrm{p}; \boldsymbol{X}) = \widetilde{W}(\boldsymbol{F}_\mathrm{e} \cdot \boldsymbol{Q}, \boldsymbol{Q}^\mathrm{t} \cdot \boldsymbol{D}_\mathrm{p} \cdot \boldsymbol{Q}; \boldsymbol{X})$ for all $\boldsymbol{Q}^\mathrm{t} = \boldsymbol{Q}^{-1}$. Similar to eq. (7), the directional derivative—now based on $\boldsymbol{Q}_\varepsilon = \exp(\varepsilon\, \boldsymbol{W}) \cdot \boldsymbol{Q}$—further constrains the stored energy,

$$[\,\boldsymbol{F}_\mathrm{e}^\mathrm{t} \cdot \partial_{\boldsymbol{F}_\mathrm{e}} W + \boldsymbol{D}_\mathrm{p}^\mathrm{t} \cdot \partial_{\boldsymbol{D}_\mathrm{p}} W - \partial_{\boldsymbol{D}_\mathrm{p}} W \cdot \boldsymbol{D}_\mathrm{p}^\mathrm{t}\,] : \boldsymbol{W} = 0 \qquad \forall\, \boldsymbol{W} = -\,\boldsymbol{W}^\mathrm{t}\,. \tag{8}$$

Practically speaking, eq. (7) and (8), together with adopting hyper-elastic stress forms, yield the Kirchhoff stresses, respectively the combination of Mandel stresses and Mandel-type back-stresses, to be symmetric.

4. Incremental variational formulation

In this section, a variational approach is reviewed, wherein the underlying incremental potential accounts for the material's inhomogeneities and heterogeneities. To set the stage, use of the balance of entropy for the isothermal and quasi static case will be made, based on which local field equations of interest can be derived. In this regard, let D denote the dissipation rate density, whereas $\boldsymbol{t}$ and $\boldsymbol{T}_\mathrm{p}$ characterise the respective traction-type quantities, so that

$$\int_{\mathcal{B}_0} \dot{W} + D \,\mathrm{d}V = \int_{\partial\mathcal{B}_0} \boldsymbol{t} \cdot \dot{\boldsymbol{\varphi}} + \boldsymbol{T}_\mathrm{p} : \dot{\boldsymbol{F}}_\mathrm{p} \,\mathrm{d}A\,. \tag{9}$$

Note that any additional contributions stemming from further volume sources as well as terms related to, for example, singular surfaces are, for conceptual simplicity but without loss of generality, not incorporated into (9). Adopting standard notation, $\dot{\bullet} = \partial_t \bullet|_{\boldsymbol{X}}$ abbreviates the material time derivative. Since the particular deformation processes considered are dissipative in general, such as plastic slip respectively dislocation activation and motion, the evolution in time of $\boldsymbol{F}_\mathrm{p}$ is derived from a rate potential

$$R = \dot{W} + P \qquad \text{with} \qquad P(\dot{\boldsymbol{F}}_\mathrm{p};\boldsymbol{X}) \tag{10}$$

being the corresponding dissipation potential. Next, we compute the variation of the bulk contribution, namely

$$\begin{aligned} \delta \int_{\mathcal{B}_0} R\,\mathrm{d}V &= \int_{\mathcal{B}_0} \partial_{\dot{\boldsymbol{F}}} R : \delta\dot{\boldsymbol{F}} + \partial_{\dot{\boldsymbol{F}}_\mathrm{p}} R : \delta\dot{\boldsymbol{F}}_\mathrm{p} + \partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R : \delta\dot{\boldsymbol{A}}_\mathrm{p}\,\mathrm{d}V \\ &= \int_{\partial\mathcal{B}_0} \boldsymbol{t}\cdot\delta\dot{\boldsymbol{\varphi}} + \boldsymbol{T}_\mathrm{p} : \delta\dot{\boldsymbol{F}}_\mathrm{p}\,\mathrm{d}A\,, \end{aligned} \tag{11}$$

and make use of the identities

$$\begin{aligned} \partial_{\dot{\boldsymbol{F}}} R : \delta\dot{\boldsymbol{F}} &= \nabla_{\boldsymbol{X}}\cdot[\,\delta\dot{\boldsymbol{\varphi}}\cdot\partial_{\dot{\boldsymbol{F}}} R\,] - [\,\nabla_{\boldsymbol{X}}\cdot\partial_{\dot{\boldsymbol{F}}} R\,]\cdot\delta\dot{\boldsymbol{\varphi}}\,, \\ \partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R : \delta\dot{\boldsymbol{A}}_\mathrm{p} &= -\nabla_{\boldsymbol{X}}\cdot\big[\,[\,\partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\,]^\mathrm{t}\times\delta\dot{\boldsymbol{F}}_\mathrm{p}^\mathrm{t}\,\big] + \nabla^\mathrm{t}_{\boldsymbol{X}}\times[\,\partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\,] : \delta\dot{\boldsymbol{F}}_\mathrm{p}\,, \end{aligned} \tag{12}$$

with $\boldsymbol{U}\times\boldsymbol{V} = [\,\boldsymbol{U}\cdot\boldsymbol{V}^\mathrm{t}\,] : \boldsymbol{E}$ for $\boldsymbol{U}$ and $\boldsymbol{V}$ being second-order tensors. By application of the divergence theorem one obtains

$$\begin{aligned} &\int_{\mathcal{B}_0} [\,\nabla_{\boldsymbol{X}}\cdot\partial_{\dot{\boldsymbol{F}}} R\,]\cdot\delta\dot{\boldsymbol{\varphi}} - \big[\,\partial_{\dot{\boldsymbol{F}}_\mathrm{p}} R + \nabla^\mathrm{t}_{\boldsymbol{X}}\times[\,\partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\,]\big] : \delta\dot{\boldsymbol{F}}_\mathrm{p}\,\mathrm{d}V \\ +&\int_{\partial\mathcal{B}_0} [\,\boldsymbol{t} - \partial_{\dot{\boldsymbol{F}}} R\cdot\boldsymbol{N}\,]\cdot\delta\dot{\boldsymbol{\varphi}} + [\,\boldsymbol{T}_\mathrm{p} - \partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\times\boldsymbol{N}\,] : \delta\dot{\boldsymbol{F}}_\mathrm{p}\,\mathrm{d}A \qquad = \quad 0\,, \end{aligned} \tag{13}$$

wherein the notation $\boldsymbol{U}\times\boldsymbol{v} = [\,\boldsymbol{U}\otimes\boldsymbol{v}\,] : \boldsymbol{E}$, for $\boldsymbol{v}$ being a vector, has been introduced. With these relations in hand, eq. (13) can be further reduced to the local forms

$$\begin{aligned} \nabla_{\boldsymbol{X}}\cdot\partial_{\dot{\boldsymbol{F}}} R = \boldsymbol{0} \quad &\text{in} \quad \mathcal{B}_0 \quad \text{and} \quad \boldsymbol{t} \;= \partial_{\dot{\boldsymbol{F}}} R\cdot\boldsymbol{N} \quad \text{on} \quad \partial\mathcal{B}_0^t\,, \\ \partial_{\dot{\boldsymbol{F}}_\mathrm{p}} R + \nabla^\mathrm{t}_{\boldsymbol{X}}\times[\,\partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\,] = \boldsymbol{0} \quad &\text{in} \quad \mathcal{B}_0 \quad \text{and} \quad \boldsymbol{T}_\mathrm{p} = \partial_{\dot{\boldsymbol{A}}_\mathrm{p}} R\times\boldsymbol{N} \quad \text{on} \quad \partial\mathcal{B}_0^{T_\mathrm{p}}\,. \end{aligned} \tag{14}$$

In summary, these relations represent the primary result of the current approach at the rate level.

Next, emphasis is placed on the incremental form of the derived field equations. In this context, consider the finite time interval $\Delta t = t_{n+1} - t_n \geq 0$ with respect to which the bulk contribution R is now integrated, to be specific

$$w \;=\; \int_{t_n}^{t_{n+1}} R\,\mathrm{d}t \;=\; W_{n+1} - W_n + \int_{t_n}^{t_{n+1}} P\,\mathrm{d}t\,. \tag{15}$$

A straightforward method to numerically integrate P is provided by a simple Euler-forward approach, namely

$$\int_{t_n}^{t_{n+1}} P\,\mathrm{d}t \;\approx\; \Delta t\;P([\boldsymbol{F}_{\mathrm{p}\,n+1} - \boldsymbol{F}_{\mathrm{p}\,n}]/\Delta t;\boldsymbol{X}) = p(\boldsymbol{F}_{\mathrm{p}\,n+1},\Delta t;\boldsymbol{X})\,, \tag{16}$$

so that the incremental form of eq. (14) results in

$$\begin{aligned} \nabla_{\boldsymbol{X}}\cdot\partial_{\boldsymbol{F}_{n+1}} W_{n+1} \;&=\; \boldsymbol{0} \quad \text{in} \quad \mathcal{B}_0 \\ \text{and} \quad \boldsymbol{t} \;&=\; \partial_{\boldsymbol{F}_{n+1}} W_{n+1}\cdot\boldsymbol{N} \quad \text{on} \quad \partial\mathcal{B}_0^t\,, \end{aligned} \tag{17}$$

as well as

$$\partial_{\boldsymbol{F}_{\mathrm{p}\,n+1}} W_{n+1} + \partial_{\boldsymbol{F}_{\mathrm{p}\,n+1}} p + \nabla^{\mathrm{t}}_{\boldsymbol{X}} \times [\, \partial_{\boldsymbol{A}_{\mathrm{p}\,n+1}} W_{n+1} \,] \;=\; \boldsymbol{0} \quad \text{in} \quad \mathcal{B}_0 \qquad \text{and} \quad \boldsymbol{T}_{\mathrm{p}} \;=\; \partial_{\boldsymbol{A}_{\mathrm{p}\,n+1}} W_{n+1} \times \boldsymbol{N} \quad \text{on} \quad \partial\mathcal{B}_0^{T_{\mathrm{p}}} \,. \tag{18}$$

Note that use of the relations $\partial_{\boldsymbol{F}_{n+1}} w = \partial_{\boldsymbol{F}_{n+1}} W_{n+1}$, $\partial_{\boldsymbol{A}_{\mathrm{p}\,n+1}} w = \partial_{\boldsymbol{A}_{\mathrm{p}\,n+1}} W_{n+1}$, and $\partial_{\boldsymbol{F}_{\mathrm{p}\,n+1}} w = \partial_{\boldsymbol{A}_{p\,n+1}} W_{n+1} \times \boldsymbol{N}$ has been made. In addition, it is obvious that $\partial_{\boldsymbol{F}} w$ corresponds to the Piola stresses and, moreover, that (18) represents the algorithmic evolution-field relation for $\boldsymbol{F}_{\mathrm{p}}$.

5. Two configurational field formulations

The subsequent section constitutes the main body of this contribution: two different approaches to formulate configurational field and balance relations are discussed, namely a variational approach and an alternative framework based on a transformation concept applied to standard balance relations.

5.1. Variational approach

In order to derive a configurational field formulation for the variational framework discussed, we first superpose a compatible deformation-type mapping onto the referential arguments of the relevant scalar-valued functions, and second evaluate the respective field relations for this mapping coinciding with the identity mapping; see figure 2 for a graphical illustration. In this context, let $\boldsymbol{x}_\lambda = \boldsymbol{\lambda}(\boldsymbol{X}, t) : \mathcal{B}_0 \times \mathcal{T} \to \mathcal{B}_\lambda$ be a sufficiently smooth mapping, whereas $\boldsymbol{L} = \nabla_{\boldsymbol{X}} \boldsymbol{\lambda}$ denotes the related motion-gradient-type two-point tensor together with $J_\lambda = \det(\boldsymbol{L}) \neq 0$. Accordingly, we next refer the incremental potential energy to the transformation in terms of $\boldsymbol{\lambda}$ so that

$$w \;=\; J_\lambda \, w_\lambda(\boldsymbol{F} \cdot \boldsymbol{L}^{-1}, \boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{L}^{-1}, \boldsymbol{A}_{\mathrm{p}} \cdot \mathrm{cof}(\boldsymbol{L}^{-1}), \boldsymbol{x}_\lambda) \,, \tag{19}$$

compare eq. (4) in view of the Piola transformation of the dislocation density tensor. With these relations in hand, the corresponding variation with respect to $\boldsymbol{\lambda}$ results in

$$\begin{aligned}
\delta \int_{\mathcal{B}_\lambda} w \, \mathrm{d}V \;&=\; \int_{\mathcal{B}_\lambda} w_\lambda \, \partial_{\boldsymbol{L}} J_\lambda : \delta \boldsymbol{L} + J_\lambda \, \partial_{\boldsymbol{\lambda}} w_\lambda \cdot \delta\boldsymbol{\lambda} \, \mathrm{d}V \\
&+ \int_{\mathcal{B}_\lambda} J_\lambda \left[\, \boldsymbol{F}^{\mathrm{t}} \cdot \partial_{\boldsymbol{F}\cdot\boldsymbol{L}^{-1}} w_\lambda + \boldsymbol{F}^{\mathrm{t}}_{\mathrm{p}} \cdot \partial_{\boldsymbol{F}_{\mathrm{p}}\cdot\boldsymbol{L}^{-1}} w_\lambda \,\right] : \delta \boldsymbol{L}^{-1} \, \mathrm{d}V \\
&+ \int_{\mathcal{B}_\lambda} J_\lambda \left[\, \boldsymbol{A}^{\mathrm{t}}_{\mathrm{p}} \cdot \partial_{\boldsymbol{A}_{\mathrm{p}}\cdot\mathrm{cof}(\boldsymbol{L}^{-1})} w_\lambda \,\right] : \delta \, \mathrm{cof}(\boldsymbol{L}^{-1}) \, \mathrm{d}V \\
&=\; \int_{\partial\mathcal{B}_\lambda} \boldsymbol{T} \cdot \delta\boldsymbol{\lambda} \, \mathrm{d}A \,.
\end{aligned} \tag{20}$$

Furthermore, we make use of the relations $\partial_{\boldsymbol{L}} J_\lambda = \mathrm{cof}(\boldsymbol{L})$, $\delta \boldsymbol{L}^{-1} = -\,\boldsymbol{L}^{-1} \cdot \delta\boldsymbol{L} \cdot \boldsymbol{L}^{-1}$, and $\delta \, \mathrm{cof}(\boldsymbol{L}^{-1}) = J_\lambda^{-1} \, \delta \boldsymbol{L}^{\mathrm{t}} - J_\lambda^{-1} [\, \boldsymbol{L}^{-\mathrm{t}} : \delta\boldsymbol{L} \,] \, \boldsymbol{L}^{\mathrm{t}}$, which—together with $\boldsymbol{\lambda}$ coinciding with the identity mapping—enables us to rewrite eq. (20) as

$$\int_{\mathcal{B}_0} \boldsymbol{\Sigma} : \nabla_{\boldsymbol{X}} \, \delta\boldsymbol{\lambda} + \partial_{\boldsymbol{X}} w \cdot \delta\boldsymbol{\lambda} \, \mathrm{d}V \;=\; \int_{\partial\mathcal{B}_0} \boldsymbol{T} \cdot \delta\boldsymbol{\lambda} \, \mathrm{d}A \,, \tag{21}$$

wherein

$$\boldsymbol{\Sigma} \;=\; [\, w - \boldsymbol{A}_{\mathrm{p}} : \partial_{\boldsymbol{A}_{\mathrm{p}}} w \,] \, \boldsymbol{I} - \boldsymbol{F}^{\mathrm{t}} \cdot \partial_{\boldsymbol{F}} w - \boldsymbol{F}^{\mathrm{t}}_{\mathrm{p}} \cdot \partial_{\boldsymbol{F}_{\mathrm{p}}} w + [\, \partial_{\boldsymbol{A}_{\mathrm{p}}} w \,]^{\mathrm{t}} \cdot \boldsymbol{A}_{\mathrm{p}} \tag{22}$$

characterises the Eshelby stresses. In summary, these relations result in the following local form

$$\nabla_{\boldsymbol{X}} \cdot \boldsymbol{\Sigma} - \partial_{\boldsymbol{X}} w \;=\; \boldsymbol{0} \quad \text{in} \quad \mathcal{B}_0 \qquad \text{and} \qquad \boldsymbol{T} \;=\; \boldsymbol{\Sigma} \cdot \boldsymbol{N} \quad \text{on} \quad \partial\mathcal{B}_0^{T} \,. \tag{23}$$

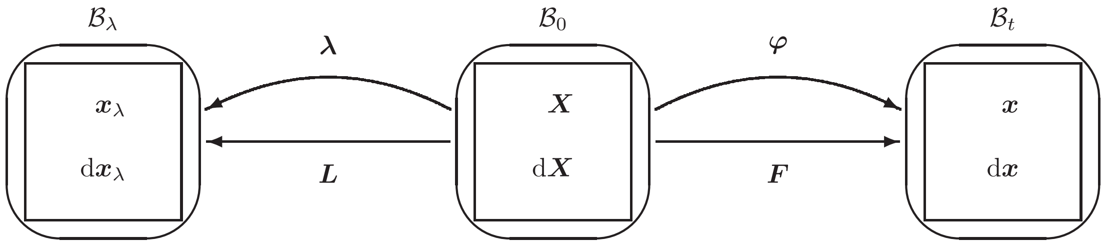

Figure 2: Configurations: illustration of the transformation relations between the referential and spatial configuration as well as the additional configurational setting.

It is also interesting to note that eq. (22) and (23) can be particularised to reduced forms: on the one hand, $\boldsymbol{F}_\mathrm{p}$ may represent a material uniformity so that $\nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p}$ vanishes and $\boldsymbol{\Sigma}$ boils down to a null Lagrangian. On the other hand, the absence of any material heterogeneities eliminates the contribution of $\partial_{\boldsymbol{X}} w$ to the configurational volume forces.

5.2. Transformation-based approach

Next, we place emphasis on what we call the transformation-based approach. To be specific, the standard form of the balance equation (17)—for the quasi static case and in the absence of spatial volume forces—is considered and transformed to the reference configuration via

$$-\boldsymbol{F}^\mathrm{t}\cdot[\,\nabla_{\boldsymbol{X}}\cdot\partial_{\boldsymbol{F}} w\,] = \nabla_{\boldsymbol{X}}\cdot\boldsymbol{\Sigma}+\boldsymbol{B}_0 \quad \text{in } \mathcal{B}_0 \quad \text{and} \quad \boldsymbol{T}=\boldsymbol{\Sigma}\cdot\boldsymbol{N} \quad \text{on } \partial\mathcal{B}_0^T\,, \tag{24}$$

with the index $n+1$ being omitted for notational simplicity. The remaining task consists in identifying $\boldsymbol{\Sigma}$ and $\boldsymbol{B}_0$. Adopting established concepts, we first make use of the compatibility of the overall motion and identify

$$\nabla_{\boldsymbol{X}}\cdot[\,\boldsymbol{F}^\mathrm{t}\cdot\partial_{\boldsymbol{F}} w\,] = \partial_{\boldsymbol{F}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F} + \boldsymbol{F}^\mathrm{t}\cdot[\,\nabla_{\boldsymbol{X}}\cdot\partial_{\boldsymbol{F}} w\,]\,. \tag{25}$$

The first term on the right hand side of eq. (25) can be rewritten by means of the relation

$$\nabla_{\boldsymbol{X}}\cdot[\,w\,\boldsymbol{I}\,] = \partial_{\boldsymbol{F}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F} + \partial_{\boldsymbol{F}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p} + \partial_{\boldsymbol{A}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{A}_\mathrm{p} + \partial_{\boldsymbol{X}} w \tag{26}$$

so that assembling terms yields the well-known formal representation

$$\begin{aligned} -\boldsymbol{F}^\mathrm{t}\cdot[\,\nabla_{\boldsymbol{X}}\cdot\partial_{\boldsymbol{F}} w\,] &= \nabla_{\boldsymbol{X}}\cdot[\,w\,\boldsymbol{I}-\boldsymbol{F}^\mathrm{t}\cdot\partial_{\boldsymbol{F}} w\,] \\ &- \partial_{\boldsymbol{F}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p} - \partial_{\boldsymbol{A}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{A}_\mathrm{p} - \partial_{\boldsymbol{X}} w\,. \end{aligned} \tag{27}$$

In order to obtain a flux term similar to the Eshelby stresses in eq. (22), we further exploit the possibility to introduce the individual contributions to the balance equation of interest either as flux or as source terms. In this regard, it turns out to be useful to consider the relation $\nabla_{\boldsymbol{X}}\boldsymbol{U}^\mathrm{t} : \boldsymbol{V} = \boldsymbol{V} : \nabla_{\boldsymbol{X}}\boldsymbol{U} + 2\,\boldsymbol{V} : [\,\nabla_{\boldsymbol{X}}\boldsymbol{U} : \mathsf{I}^\mathrm{skw}\,]$, whereby $\boldsymbol{U}$ and $\boldsymbol{V}$ are second-order tensors and $\mathsf{I}^\mathrm{skw} = \frac{1}{2}\,\boldsymbol{E}\cdot\boldsymbol{E}$ denotes the skew-symmetric fourth-order identity tensor.

On the one hand, we apply this decomposition to the source term that directly includes the gradient term of $\boldsymbol{F}_\mathrm{p}$, and which can be related to the dislocation density tensor, namely

$$\begin{aligned} \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p}^\mathrm{t} : \partial_{\boldsymbol{F}_\mathrm{p}} w &= \partial_{\boldsymbol{F}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p} + 2\,\partial_{\boldsymbol{F}_\mathrm{p}} w : [\,\nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p} : \mathsf{I}^\mathrm{skw}\,] \\ &= \partial_{\boldsymbol{F}_\mathrm{p}} w : \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p} - [\,\partial_{\boldsymbol{F}_\mathrm{p}} w\,]^\mathrm{t}\times\boldsymbol{A}_\mathrm{p}^\mathrm{t}\,, \end{aligned} \tag{28}$$

compare Menzel and Steinmann (2007) and Menzel (2007). Moreover, the term on the left hand side of eq. (28) allows to be reformulated via

$$\nabla_{\boldsymbol{X}}\cdot[\,\boldsymbol{F}_\mathrm{p}^\mathrm{t}\cdot\partial_{\boldsymbol{F}_\mathrm{p}} w\,] = \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p}^\mathrm{t} : \partial_{\boldsymbol{F}_\mathrm{p}} w + \boldsymbol{F}_\mathrm{p}^\mathrm{t}\cdot[\,\nabla_{\boldsymbol{X}}\cdot\partial_{\boldsymbol{F}_\mathrm{p}} w\,] = \nabla_{\boldsymbol{X}}\boldsymbol{F}_\mathrm{p}^\mathrm{t} : \partial_{\boldsymbol{F}_\mathrm{p}} w\,. \tag{29}$$

Please note that the contribution $\nabla_{\boldsymbol{X}} \cdot \partial_{\boldsymbol{F}_\mathrm{p}} w$ vanishes identically as we conclude from eq. (18) that $\nabla_{\boldsymbol{X}} \cdot \partial_{\boldsymbol{F}_\mathrm{p}} w = -\nabla_{\boldsymbol{X}} \cdot [\nabla^\mathrm{t}_{\boldsymbol{X}} \times [\partial_{\boldsymbol{A}_\mathrm{p}} w]] = \boldsymbol{0}$. As a first intermediate result we note

$$-\partial_{\boldsymbol{F}_\mathrm{p}} w : \nabla_{\boldsymbol{X}} \boldsymbol{F}_\mathrm{p} = -\nabla_{\boldsymbol{X}} \cdot [\boldsymbol{F}^\mathrm{t}_\mathrm{p} \cdot \partial_{\boldsymbol{F}_\mathrm{p}} w] - [\partial_{\boldsymbol{F}_\mathrm{p}} w]^\mathrm{t} \times \boldsymbol{A}^\mathrm{t}_\mathrm{p} . \tag{30}$$

On the other hand, we next consider the last but one term on the right hand side of eq. (27) and conclude—by analogy with eq. (26)—that the following relation holds

$$\nabla_{\boldsymbol{X}} \cdot \big[[\boldsymbol{A}_\mathrm{p} : \partial_{\boldsymbol{A}_\mathrm{p}} w] \boldsymbol{I} \big] = \boldsymbol{A}_\mathrm{p} : \nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w] + \partial_{\boldsymbol{A}_\mathrm{p}} w : \nabla_{\boldsymbol{X}} \boldsymbol{A}_\mathrm{p} . \tag{31}$$

Similar to eq. (28) we, once more, make use of the decomposition of the gradient operation to further specify the first term on the right hand side of eq. (31), namely

$$\nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} : \boldsymbol{A}_\mathrm{p} = \boldsymbol{A}_\mathrm{p} : \nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w] + 2\, \boldsymbol{A}_\mathrm{p} : \big[\nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w] : \mathsf{I}^\mathrm{skw} \big] . \tag{32}$$

Note, to perform a last manipulation, that the left hand side of eq. (32) allows representation in terms of

$$\begin{aligned} \nabla_{\boldsymbol{X}} \cdot \big[[\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} \cdot \boldsymbol{A}_\mathrm{p} \big] &= \nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} : \boldsymbol{A}_\mathrm{p} + [\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} \cdot [\nabla_{\boldsymbol{X}} \cdot \boldsymbol{A}_\mathrm{p}] \\ &= \nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} : \boldsymbol{A}_\mathrm{p} \end{aligned} \tag{33}$$

with $\nabla_{\boldsymbol{X}} \cdot \boldsymbol{A}_\mathrm{p} = \nabla_{\boldsymbol{X}} \cdot [\nabla^\mathrm{t}_{\boldsymbol{X}} \times \boldsymbol{F}_\mathrm{p}] = \boldsymbol{0}$. As a second intermediate result one observes

$$\begin{aligned} -\partial_{\boldsymbol{A}_\mathrm{p}} w : \nabla_{\boldsymbol{X}} \boldsymbol{A}_\mathrm{p} &= \nabla_{\boldsymbol{X}} \cdot \big[[\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} \cdot \boldsymbol{A}_\mathrm{p} - [\boldsymbol{A}_\mathrm{p} : \partial_{\boldsymbol{A}_\mathrm{p}} w] \boldsymbol{I} \big] \\ &- 2\, \boldsymbol{A}_\mathrm{p} : \big[\nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w] : \mathsf{I}^\mathrm{skw} \big] . \end{aligned} \tag{34}$$

Before collecting terms and identifying the Eshelby stresses and related volume forces, we lastly place emphasis on the sum of the last expression of eq. (30) and eq. (34), to be specific

$$\begin{aligned} &- [\partial_{\boldsymbol{F}_\mathrm{p}} w]^\mathrm{t} \times \boldsymbol{A}^\mathrm{t}_\mathrm{p} - 2\, \boldsymbol{A}_\mathrm{p} : \big[\nabla_{\boldsymbol{X}} [\partial_{\boldsymbol{A}_\mathrm{p}} w] : \mathsf{I}^\mathrm{skw} \big] \\ &\qquad = -\big[[\partial_{\boldsymbol{F}_\mathrm{p}} w]^\mathrm{t} \cdot \boldsymbol{A}_\mathrm{p} \big] : \boldsymbol{E} + \boldsymbol{A}_\mathrm{p} : \big[[\nabla^\mathrm{t}_{\boldsymbol{X}} \times [\partial_{\boldsymbol{A}_\mathrm{p}} w]] \cdot \boldsymbol{E} \big] \\ &\qquad = \big[\boldsymbol{A}^\mathrm{t}_\mathrm{p} \cdot [\partial_{\boldsymbol{F}_\mathrm{p}} w - \nabla^\mathrm{t}_{\boldsymbol{X}} \times [\partial_{\boldsymbol{A}_\mathrm{p}} w]] \big] : \boldsymbol{E} \\ &\qquad = 2\, [\boldsymbol{A}^\mathrm{t}_\mathrm{p} \cdot \partial_{\boldsymbol{F}_\mathrm{p}} w] : \boldsymbol{E} \;=\; -2\, [\partial_{\boldsymbol{F}_\mathrm{p}} w]^\mathrm{t} \times \boldsymbol{A}^\mathrm{t}_\mathrm{p} , \end{aligned} \tag{35}$$

wherein use of the field equation (18) has been made.

With these tedious derivations in hand—namely eq. (27), (30), and (34)—we finally are able to identify the Eshelby stresses and volume forces introduced in eq. (24), i.e.

$$\begin{aligned} \boldsymbol{\Sigma} &= [w - \boldsymbol{A}_\mathrm{p} : \partial_{\boldsymbol{A}_\mathrm{p}} w] \boldsymbol{I} - \boldsymbol{F}^\mathrm{t} \cdot \partial_{\boldsymbol{F}} w - \boldsymbol{F}^\mathrm{t}_\mathrm{p} \cdot \partial_{\boldsymbol{F}_\mathrm{p}} w + [\partial_{\boldsymbol{A}_\mathrm{p}} w]^\mathrm{t} \cdot \boldsymbol{A}_\mathrm{p} , \\ \boldsymbol{B}_0 &= -\partial_{\boldsymbol{X}} w - 2\, [\partial_{\boldsymbol{F}_\mathrm{p}} w]^\mathrm{t} \times \boldsymbol{A}^\mathrm{t}_\mathrm{p} . \end{aligned} \tag{36}$$

Note that the manipulations above have been carried out in order to obtain identical representation for the Eshelby stresses based on the variational approach, eq. (22), and the transformation-based approach, eq. (36). The volume forces in the respective formulations, however, do not coincide, which underlines the fundamental difference of the two approaches.

6. Discussion

As a result of the previous derivations, two different versions of the configurational balance of linear momentum representation have been derived. On the one hand, a variational approach has been applied, while, on the other hand, use of what we call a transformation-based approach was made. In general, the overall form of a balance equation allows to shift individual contributions form the flux terms to the source terms and vice versa. In this contribution, such manipulations have been applied to the transformation of the standard spatial balance of linear momentum representation, in order to obtain an identical form for the flux terms—or rather Eshelby stresses—compared to the variational framework. It is interesting to note, that the highlighted version of the Eshelby stresses includes contributions directly determined by the material isomorphism $\boldsymbol{F}_{\mathrm{p}}$ as well as parts defined in terms of the related dislocation density tensor $\boldsymbol{A}_{\mathrm{p}}$. The formally identical representations for the Eshelby stresses derived by means of the variational approach and the transformation-based approach, finally enabled us to compare both formulations. It turned out that different source terms—or rather configurational volume forces—are obtained. In this regard, it is interesting to further discuss the particular contribution that $\boldsymbol{B}_0$ in eq. (36) additionally includes as compared to the source term in eq. (23). In order to specify this contribution and to relate it to the celebrated Peach-Koehler force, consider a single dislocation with $\boldsymbol{A}_{\mathrm{p}} = \Delta\, \boldsymbol{b}_{\mathrm{p}}^{\mathrm{bur}} \otimes \boldsymbol{l}$, wherein Δ denotes the Dirac delta contribution, $\boldsymbol{b}_{\mathrm{p}}^{\mathrm{bur}}$ is the related Burgers vector, and $\boldsymbol{l}$ characterises the tangent vector with respect to the dislocation line. Based on this specification, the additional contribution to $\boldsymbol{B}_0$, i.e. $-[\,\partial_{\boldsymbol{F}_{\mathrm{p}}} w\,]^{\mathrm{t}} \times \boldsymbol{A}_{\mathrm{p}}^{\mathrm{t}}$ with the factor 2 being omitted, can be related to the referential Peach-Koehler force, namely

$$\mathbf{f} = -\int_{\mathcal{V}_0} \Delta\,[\,\partial_{\boldsymbol{F}_{\mathrm{p}}} w\,]^{\mathrm{t}} \times [\,\boldsymbol{l} \otimes \boldsymbol{b}_{\mathrm{p}}^{\mathrm{bur}}\,]\,\mathrm{d}V = \int_{\mathcal{L}_0} \boldsymbol{l} \times \big[\,[\,\partial_{\boldsymbol{F}_{\mathrm{p}}} w\,]^{\mathrm{t}} \cdot \boldsymbol{b}_{\mathrm{p}}^{\mathrm{bur}}\,\big]\,\mathrm{d}L\,. \tag{37}$$

It is interesting to note that eq. (37) recaptures the classical small strain format of the Peach-Koehler force as highlighted in section 1.1, eq. (II.148).

Apart form this, the field relations derived in this contribution—i.e. eq. (17) and (18), as well as eq. (23) and (24)—can be transformed to other configurations. The underlying general transformation relations for the respective divergence and curl operations are provided in eq. (2), which hold for both, (i) compatible transformations, such as $\nabla_{\boldsymbol{X}} \cdot \mathrm{cof}(\boldsymbol{F}) = \boldsymbol{0}$, respectively $\nabla_{\boldsymbol{X}}^{\mathrm{t}} \times \mathrm{cof}(\boldsymbol{F}) = \boldsymbol{0}$, as well as for (ii) incompatible transformations, such as $\nabla_{\boldsymbol{X}} \cdot \mathrm{cof}(\boldsymbol{F}_{\mathrm{p}}) \neq \boldsymbol{0}$, respectively $\nabla_{\boldsymbol{X}}^{\mathrm{t}} \times \mathrm{cof}(\boldsymbol{F}_{\mathrm{p}}) \neq \boldsymbol{0}$. From a computational point of view, it is of particular interest to further investigate algorithmic aspects and simulation results of the different configurational balance of linear momentum representations based on the three different forms of the flux and source terms determined by eq. (22), (27), and (36).

References

Bertram, A. (1999). An alternative approach to finite plasticity based on material isomorphisms, *International Journal of Plasticity* **15(3)**, pp. 353–374.

Capriz, G. (1989). Continua with microstructure, *Springer Tracts in Natural Philosophy* **35**.

Carstensen, C., Hackl, K. and Mielke., A. (2002). Non–convex potentials and microstructures in finite–strain plasticity, *Proceedings of the Royal Society A* **458**, pp. 299–317.

Ciarlet, P. (1988). Mathematical elasticity – volume 1: Three dimensional elasticity, *Volume 20 of Studies in Mathematics and its Applications, North–Holland* .

Dassiso, G. and Lindell, I. (2001). On the Helmholtz decomposition for polyadics, *Quarterly of Applied Mathematics* **59**, pp. 787–796.

Epstein, M. (2002). The Eshelby tensor and the theory of continuous distributions of dislocations, *Mechanics Research Communications* **29**, pp. 501–506.

Epstein, M. and Elżanowski, M. (2007). The Eshelby tensor and the theory of continuous distributions of dislocations, *Interaction of Mechanics and Mathematics, Springer* .

Epstein, M. and Maugin, G. (1990). The energy–momentum tensor and material uniformity in finite elasticity, *Acta Mechanica* **83**, pp. 127–133.

Ericksen, J. (1998). Introduction to the thermodynamics of solids, *Volume 131 of Applied Mathematical Science, Springer, revised edition* .

G. de Saxcé (2001). Divergence and curl of a product of linear mapping fileds and applications to the large deformations, *International Journal of Engineering Science* **39**, pp. 555–561.

Gurtin, M. (2000a). Configurational forces as basic concept in continuum physics, *Volume 137 of Applied Mathematical Sciences, Springer* .

Gurtin, M. (2000b). On the plasticity of single crystals: free energy, microforces, plastic–strain gradients, *Journal of the Mechanics and Physics of Solids* **48**, pp. 989–1036.

Gurtin, M. (2002). A gradient theory of single–crystal viscoplasticity that accounts for geometrically necessary dislocations, *Journal of the Mechanics and Physics of Solids* **50**, pp. 5–32.

Hackl, K. (1997). Generalized media and variational principles in classical and finite strain elastoplasticity, *Journal of the Mechanics and Physics of Solids* **45**, pp. 667–688.

Hanyga, A. (1985). Mathematical theory of non–linear elasticity, *Polish Scientific Publishers – Ellis Horwood* .

Hirschberger, C., Kuhl, E. and Steinmann, P. (2007). On deformational and configurational mechanics of micromorphic hyperelasticity – Theory and computations, *Computer Methods in Applied Mechanics and Engineering* **196**, pp. 4027–4044.

Kirchner, N. and Steinmann, P. (2007). On the material setting of gradient hyperelasticity, *Mathematics and Mechanics of Solids* **12**, pp. 559–580.

Kröner, E. (1958). Kontinuumstheorie der Versetzungen und Eigenspannungen, *Erg. Angew. Math., Springer* **5**.

Levkovitch, V. and Svendsen, B. (2006). On the large deformation and continuum based formulation of models for extended crystal plasticity, *International Journal of Solids and Structures* **43**, pp. 7246–7267.

Markenscoff, X. and Gupta, A. (2006). Collected works of J.D. Eshelby – the mechanics of defects and inhomogeneities, *Volume 133 of Solid Mechanics and its Applications, Springer* .

Maugin, G. (1993). Material inhomogeneities in elasticity, *Volume 3 of Applied Mathematics and Mathematical Computation, Chapman* & *Hall* .

Maugin, G. (2003). Pseudo–plasticity and pseudo–inhomogeneity effects in materials mechanics, *Journal of Elasticity* **71**, pp. 81–103.

Menzel, A. (2007). Frontiers in inelastic continuum mechanics, *Habilitation thesis, Chair of Applied Mechanics, Technical University of Kaiserslautern, http://kluedo.ub.uni-kl.de/volltexte/2007/2127/* **UKL/LTM T07-03**.

Menzel, A., Denzer, R. and Steinmann, P. (2004). On the comparison of two approaches to compute material forces for inelastic materials. Application to single–slip crystal–plasticity, *Computer Methods in Applied Mechanics and Engineering* **193(48-51)**, pp. 5411–5428.

Menzel, A., Denzer, R. and Steinmann, P. (2005). Material forces in computational single–slip crystal–plasticity, *Computational Materials Science* **32(3–4)**, pp. 446–454.

Menzel, A. and Steinmann, P. (2000). On the continuum formulation of higher gradient plasticity for single and polycrystals, *Journal of the Mechanics and Physics of Solids* **48(8)**, pp. 1777–1796.

Menzel, A. and Steinmann, P. (2005). A note on material forces in finite inelasticity, *Archive of Applied Mechanics* **74**, pp. 800–807.

Menzel, A. and Steinmann, P. (2007). On configurational forces in multiplicative elastoplasticity, *International Journal of Solids and Structures* **44(13)**, pp. 4442–4471.

Miehe, C. (2002). Strain–driven homogenization of inelastic microstructures and composites based on an incremental variational formulation, *International Journal for Numerical Methods in Engineering* **55**, pp. 1285–1322.

Negahban, M. and Wineman, A. (1992). The evolution of anisotropies in the elastic response of an elastic-plastic material, *International Journal of Plasticity* **8(5)**, pp. 519–542.

Noll, W. (1967). Materially uniform simple bodies with inhomogeneities, *Archive for Rational Mechanics and Analysis* **27**, pp. 1–32.

Ogden, R. (1997). Non–linear elastic deformations, *Dover* .

Ortiz, M. and Repetto, E. (1999). Nonconvex energy minimization and dislocation structures in ductile single crystals, *Journal of the Mechanics and Physics of Solids* **47**, pp. 397–462.

Peach, M. and Koehler, J. (1950). The forces exerted on dislocations and the stress field produced by them, *Physical Review Letters* **80**, pp. 436–439.

Podio-Guidugli, P. (2001). Configurational balances via variational arguments, *Interfaces and Free Boundaries* **3**, pp. 223–232.

Šilhavý, M. (1997). The mechanics and thermomechanics of continuous media, *Texts and Monographs in Physics. Springer* .

Steinmann, P. (2002a). On spatial and material settings of hyperelastostatic crystal defects, *Journal of the Mechanics and Physics of Solids* **50(8)**, pp. 1743–1766.

Steinmann, P. (2002b). On spatial and material settings of thermo–hyperelastodynamics, *Journal of Elasticity* **66**, pp. 109–157.

Svendsen, B. (1998). Continuum thermodynamic and variational models for continua with microstructure and material inhomogeneity, *International Journal of Plasticity* **6**, pp. 473–488.

Svendsen, B. (2002). Continuum thermodynamic models for crystal plasticity including the effects of geometrically–necessary dislocations, *Journal of the Mechanics and Physics of Solids* **50**, pp. 1297–1330.

Svendsen, B. (2005). Continuum thermodynamic and variational models for continua with microstructure and material inhomogeneity, *Volume 11 of Advances in Mechanics and Mathematics, Springer* , pp. 173–180.

Svendsen, B., Neff, P. and Menzel, A. (2009). On some constitutive and configurational aspects of gradient continua with microstructure, *Z. Angew. Math. Mech.* **89(8)**, pp. 687–697.