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On the Sensitivity of the Rate of Global Energy Dissipation due to Configurational Changes

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Abstract

The thermodynamic framework for combined configurational and deformational changes was recently discussed by Runesson et al. (2008). One key ingredient in this setting is the (fixed) absolute configuration, relative to which both physical and virtual (variational) changes of the material and spatial configurations can be described. In the present paper we consider dissipative material response and emphasize the fact that it is possible to identify *explicit* energetic changes due to configurational changes for "frozen" spatial configuration (a classical view) and the *configuration-induced* material dissipation. The classical assumption (previously adopted in the literature) is to ignore this dissipation, i.e. the internal variables are considered as fixed fields in the material configuration. In this paper, however, we define configurational forces by considering the *total variation* of the total dissipation with respect to configurational changes. The key task is then to compute the *sensitivity* of the internal variable rates to such configurational changes, which results in a global tangent problem based on the balance equations (momentum and energy) for a given body. In this paper we restrict to quasistatic loading under isothermal conditions and for elastic-plastic response, and we apply the modeling to the case of a moving interface of dissimilar materials.

1. Introduction

The notion of configurational changes refers basically to the motion of "property surfaces", that are either internal to a given finite body or identical to (some part of) the external boundary. An important class is defined by the motion/evolution of "singular surfaces" representing discontinuities (or defects) in the material properties and, consequently, in the state variables when the body is loaded. Typical examples of internal processes are the evolution of defects, phase transformation (microstructural changes that are mostly accompanied by change of volume and mechanical properties), and internal cracks. Typical boundary processes are the evolution of surface (biological) growth and surface cracks. Crack propagation may in this context be seen as a degenerated boundary motion.

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Since the literature on configurational mechanics is very rich, we do not intend to give a comprehensive account. We only mention the pioneering work by Eshelby (1951) and the contributions by Abeyaratne and Knowles (1990), Maugin (1993, 1995, 1997, 1998a,b, 1999), Maugin and Trimarco (1992, 1995), Gurtin (1995, 2000), and Kienzler and Herrmann (2000). Some of these works also contain comprehensive overviews with a discussion of various aspects of configurational mechanics ("material" mechanics in Maugin's terminology). As to the physical motivation, a major application is the "driving force" on singular surfaces. In the seminal contributions by Gurtin (1995, 2000), balance equations for interfaces are derived from a non-standard (material) observer invariance argument with strong relations to the celebrated NOETHER'S theorem, Noether (1918). The effects of configurational changes of surfaces in terms of physical properties intrinsically attached to the surfaces (e.g. energy) have been addressed by, among others, Gurtin and Murdoch (1975); Gurtin and Struthers (1990), Simha and Bhattacharya (1998). A recent comprehensive treatment of "surface energies" is given by Steinmann (2008). Indeed, it appears that there is a strong link to the analysis in this paper on "sensitivity".

The concept of "configurational forces" has been exploited extensively in recent years in computational fracture mechanics, cf. Steinmann (2000); Steinmann et al. (2001); Steinmann (2002b,a); Menzel et al. (2004); Steinmann (2008), Fagerström and Larsson (2008). The suggestion in Steinmann et al. (2001) to compute the crack-driving force based on the concept of "nodal material forces" generalized, in fact, the domain integral format suggested previously by Li et al. (1985). A posteriori error control and adaptivity of the J-integral in its different equivalent formats were investigated by Heintz et al. (2004). A recent paper by Guerses and Miehe (2008), which is closely related to the present paper concerning the thermodynamic setting, addresses r -adaptive remeshing for a propagating crack.

Most studies so far are explicitly confined to elastic material response. While the state of affairs seems to be quite clear in this case, it is not so in the case (local) material dissipation occurs as a result of the configurational change in addition to the energy release from a propagating crack. The formulation of the crack-driving force in such a case and the computational aspects have been discussed by Maugin and Trimarco (1992), Simha et al. (2003), Simha et al. (2008), Liebe et al. (2003), Menzel et al. (1995), Nguyen et al. (2005). However, there seems to be a lack of consensus as to the appropriate basic formulation.

In this contribution we aim at shedding some further light on the energetic consequences of configurational changes for rate-independent dissipative material response. We focus on the dissipation of mechanical energy of a given finite body that is undergoing configurational changes in conjunction with (or as a result of) mechanical loading. More specifically, we put forward the idea that it is the *total variation* of the appropriately defined dissipation functional for the whole body that represents the "driving force" for the physical process that is described by configurational changes¹. However, which definition

¹This choice has distinct advantages; one being that it is possible to check analytical results by comparison with numerical perturbations of the functional.

of the driving force to use is basically a matter of modeling, although the choice is strongly guided by thermodynamics considerations.

In order to increase clarity in the variational framework, we adopt a description that allows for the combined configurational (material) and deformational (spatial) motions. To this end we first introduce an auxiliary (fictitious) reference configuration that is *fixed* in space; in particular, its *boundary is fixed* and thus defines a time-invariant domain under (possible) configurational and deformational changes. It is important to note that the introduction of such an absolute reference configuration *does not* simply mean a change of computational domain (associated with a change of coordinates). As a special case, we may choose this referential domain to be the current configuration (the Eulerian view), which corresponds to the study of the "inverse motion", and this approach is common in the literature on configurational forces (crack-driving force) within the context of singular cracks, e.g. Steinmann (2000). With such a choice, however, the combined action of configurational and material changes is never revealed.

The paper is organized as follows: Section 2 introduces definitions and preliminaries related to the unified representation of configurational (material) and deformational (spatial) motions in terms of an absolute reference configuration. A generic balance law is established in Section 3, whereby "configurational flux" across the boundary is allowed, and it is applied to the mechanical dissipation inequality. In Section 4, we establish the pertinent dissipation functional due to imposed configurational changes while assuming rather general constitutive response based on the presence of internal variables in the free energy. In Section 5, we define generalized configurational forces from the "total variation of the global dissipation", which is the main novel result of the paper. This result is applied, and further specified, in Section 6 to a material singular surface. Explicit computational results are given in Section 7 for a non-homogeneous plate with dissimilar elastic-plastic material properties. Finally, conclusions and an outlook to future developments are given in Section 8.

2. Representation of configurational and deformational motions

2.1. Preliminaries

We first note that the spatial (deformational or direct) motion problem (SMP) is expressed in terms of a spatial motion map $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X}, t)$, $\mathcal{B}_X \mapsto \mathcal{B}_x(t)$, such that the reference position of the material particles, \boldsymbol{X} , in the fixed (time-invariant) *material* configuration \mathcal{B}_X , are mapped onto the *deformed* position, \boldsymbol{x} , in the *spatial* configuration $\mathcal{B}_x(t)$. It is emphasized that $\mathcal{B}_X = \mathcal{B}_x(0)$ is the actual configuration of the body at $t = 0$ in the classical setting.

In this paper, we generalize the classical view of motion slightly, cf. Figure 1, since the material configuration is allowed to change with time in the sense that the boundary $\partial\mathcal{B}_X$ of the body \mathcal{B}_X may change with time. It is important to note that this case also embodies the case of an evolving internal singular surface, since it is possible to view the two parts separated by the singular surface as changing configurations. It is then convenient to take the view that both the "undeformed" (material) and "deformed" (spatial) configurations

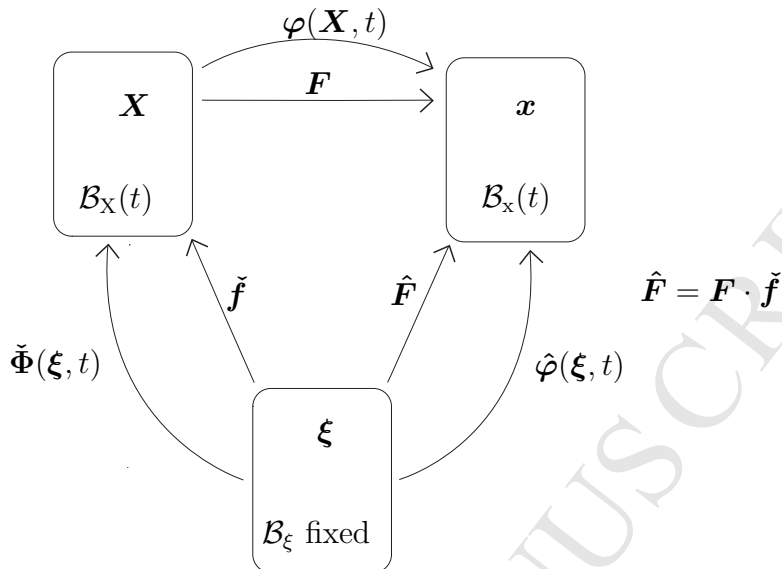


Figure 1: *Spatial (current) configuration, $\mathcal{B}_x(t)$, material configuration, $\mathcal{B}_X(t)$, and absolute (fixed) configuration, \mathcal{B}_ξ .*

will undergo time-dependent changes with respect to an *absolute* (fixed, time-invariant) configuration \mathcal{B}_ξ . We may then introduce the map $\mathbf{X} = \check{\Phi}(\boldsymbol{\xi}, t)$ for the time-dependent "motion" of $\mathcal{B}_X(t)$ w.r.t. \mathcal{B}_ξ , and we introduce the *absolute* spatial motion map $\mathbf{x} = \hat{\varphi}(\boldsymbol{\xi}, t)$ for the time-dependent motion (including deformation) of $\mathcal{B}_x(t)$ w.r.t. \mathcal{B}_ξ . It is clear that $\hat{\varphi}(\boldsymbol{\xi}, t), \mathcal{B}_\xi \mapsto \mathcal{B}_x(t)$, represents the composite map $\hat{\varphi}(\boldsymbol{\xi}, t) \stackrel{\text{def}}{=} (\varphi \circ \check{\Phi})(\boldsymbol{\xi}, t)$. We may introduce the convenient *assumption* that $\mathcal{B}_\xi = \mathcal{B}_X(0) = \mathcal{B}_x(0)$.

The gradients corresponding to the introduced mappings (see also Figure 1) are the spatial motion gradient $\mathbf{F} \stackrel{\text{def}}{=} \varphi \otimes \nabla_X$, the *absolute* spatial motion gradient $\hat{\mathbf{F}} \stackrel{\text{def}}{=} \hat{\varphi} \otimes \nabla_\xi$, and the absolute material motion gradient $\check{\mathbf{f}} \stackrel{\text{def}}{=} \check{\Phi} \otimes \nabla_\xi$ ². Upon using the chain rule, we obtain the relation $\hat{\mathbf{F}} = \mathbf{F} \cdot \check{\mathbf{f}}$. We shall also frequently use the determinant $\check{j} = \det \check{\mathbf{f}}$, which is relevant both for the volume mapping³ $dV_X = \check{j} dV_\xi$ and for the area mapping $dS_X = \check{j} \sqrt{\mathbf{N}_\xi \cdot \check{\mathbf{f}}^{-1} \cdot \check{\mathbf{f}}^{-T} \cdot \mathbf{N}_\xi} dS_\xi$ when the computational domain is changed from \mathcal{B}_X to \mathcal{B}_ξ .

2.2. Absolute and material time differentiation

We shall introduce absolute and material time derivatives of a field f , parametrized in \mathcal{B}_X or \mathcal{B}_ξ , as follows:

$$\Delta_t f \stackrel{\text{def}}{=} \partial_t f|_\xi, \quad D_t f \stackrel{\text{def}}{=} \partial_t f|_X \quad (1)$$

²The gradient vectors ∇_ξ and ∇_X refer to coordinates in \mathcal{B}_ξ and \mathcal{B}_X , respectively.

³ \mathbf{N}_ξ is the unit normal vector on $\partial\mathcal{B}_\xi$ resulting from a pullback of the unit normal $\mathbf{N}(= \mathbf{N}_X)$ from $\partial\mathcal{B}_X$.

where $\partial_t[\bullet] \stackrel{\text{def}}{=} \partial[\bullet]/\partial t$ denotes the ordinary partial time derivative. In particular, the material velocity, \mathbf{v} , the *absolute* velocity, $\dot{\mathbf{x}}$, and the (absolute) configurational rate, $\dot{\mathbf{X}}$, are defined as

$$\mathbf{v} \stackrel{\text{def}}{=} D_t \mathbf{x} = \partial_t \boldsymbol{\varphi}(\mathbf{X}, t), \quad \dot{\mathbf{x}} \stackrel{\text{def}}{=} \Delta_t \mathbf{x} = \partial_t \hat{\boldsymbol{\varphi}}(\boldsymbol{\xi}, t), \quad \dot{\mathbf{X}} \stackrel{\text{def}}{=} \Delta_t \mathbf{X} = \partial_t \check{\boldsymbol{\Phi}}(\boldsymbol{\xi}, t) \quad (2)$$

However, using the chain rule to differentiate the composite function $\hat{\boldsymbol{\varphi}}(\boldsymbol{\xi}, t) \stackrel{\text{def}}{=} (\boldsymbol{\varphi} \circ \check{\boldsymbol{\Phi}})(\boldsymbol{\xi}, t)$, we obtain the relation

$$\mathbf{v} = \dot{\mathbf{x}} - \mathbf{F} \cdot \dot{\mathbf{X}} \quad (3)$$

where the definitions in (1) were used.

We shall later make use of the absolute and material time derivatives of a (tensor-valued) *operator* field $y(\mathbf{X}(\boldsymbol{\xi}, t), \mathbf{x}(\boldsymbol{\xi}, t), \alpha_1(\boldsymbol{\xi}, t), \alpha_2(\boldsymbol{\xi}, t), \dots, t)$ or, for the sake of brevity, $y(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$ ⁴⁵. Let us first consider a volume-specific field, $y(\bullet, t)$ for $\mathbf{X} \in \mathcal{B}_X(t)$, for which the relation between the absolute and material time derivatives can be computed as

$$D_t y(\bullet, t) = \Delta_t y(\bullet, t) - [y(\bullet, t) \otimes \nabla_X] \cdot \dot{\mathbf{X}} \quad (4)$$

The total and material time derivatives of a few selected fields, $\check{\mathbf{f}}(\mathbf{X})$ and $\check{\mathbf{j}}(\mathbf{X})$, are given as follows:

$$\Delta_t \check{\mathbf{f}} = [\dot{\mathbf{X}} \otimes \nabla_X] \cdot \check{\mathbf{f}}, \quad \Delta_t \check{\mathbf{j}} = \check{\mathbf{j}} \dot{\mathbf{X}} \cdot \nabla_X \quad (5)$$

In particular, we obtain

$$\Delta_t (dV_X) = \check{\mathbf{j}} \dot{\mathbf{X}} \cdot \nabla_X dV_\xi = \dot{\mathbf{X}} \cdot \nabla_X dV_X \quad (6)$$

We may also compute the absolute and material time derivatives of $\mathbf{F}(\mathbf{X}, \mathbf{x})$ as

$$\Delta_t \mathbf{F} = -\mathbf{F} \cdot [\dot{\mathbf{X}} \otimes \nabla_X] + \dot{\mathbf{x}} \otimes \nabla_X \quad (7)$$

$$D_t \mathbf{F} = \mathbf{v} \otimes \nabla_X = -[\mathbf{F} \cdot \dot{\mathbf{X}}] \otimes \nabla_X + \dot{\mathbf{x}} \otimes \nabla_X. \quad (8)$$

Next, we consider a surface-specific field, $\hat{y}(\bullet, t)$ for $\mathbf{X} \in \partial \mathcal{B}_X(t)$, for which the absolute time-derivative is given as for the volume-specific field. The reason is that $\partial \mathcal{B}_\xi$ is fixed (stationary). However, the relation between the absolute and *surface-specific material* time-derivatives is given as

$$\hat{D}_t \hat{y}(\bullet, t) \stackrel{\text{def}}{=} \Delta_t \hat{y}(\bullet, t) - [\hat{y}(\bullet, t) \otimes \hat{\nabla}_X] \cdot \dot{\mathbf{X}} \quad (9)$$

where we introduced the surface gradient operator $\hat{\nabla}_X \stackrel{\text{def}}{=} \nabla_X \cdot \hat{\mathbf{I}}$ with the surface-specific identity tensor $\hat{\mathbf{I}} \stackrel{\text{def}}{=} \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$. We may combine the relations (4) and (9) to obtain the useful result

$$\hat{D}_t \hat{y}(\bullet, t) = D_t \hat{y}(\bullet, t) + [\hat{y}(\bullet, t) \otimes \nabla_X] \cdot \mathbf{N} \otimes \dot{\mathbf{X}} \cdot \mathbf{N} \quad (10)$$

⁴An example is the deformation gradient $\mathbf{F}(\mathbf{X}, \mathbf{x}) = \mathbf{x} \otimes \nabla_X$.

⁵The column vector $\underline{\alpha}$ contains the set of fields α_i , which may have different tensorial character.

for $\dot{\mathbf{X}} \in \partial\mathcal{B}_X$. This relation is used in the Appendix to establish the so-called "tangent problem".

Corresponding to (6), we obtain

$$\Delta_t(dS_X) = \check{j} \sqrt{\mathbf{N}_\xi \cdot \check{\mathbf{f}}^{-1} \cdot \check{\mathbf{f}}^{-T} \cdot \mathbf{N}_\xi} \dot{\mathbf{X}} \cdot \hat{\nabla}_X dS_\xi = \dot{\mathbf{X}} \cdot \hat{\nabla}_X dS_X \quad (11)$$

2.3. Conservation laws

2.3.1. Time-derivative of volume integral

Subsequently we shall establish the time derivative of suitably defined conservation quantities. To this end, suppose that $f_X(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$, for $\mathbf{X} \in \mathcal{B}_X(t)$, is a volume-specific quantity. Now, consider a typical conservation quantity F

$$F \stackrel{\text{def}}{=} \int_{\mathcal{B}_X} f_X dV_X \quad (12)$$

The time-derivative of F , for time-dependent \mathcal{B}_X , is then given as

$$\begin{aligned} \frac{d}{dt} F &= \int_{\mathcal{B}_X} \left[\Delta_t f_X + f_X \dot{\mathbf{X}} \cdot \nabla_X \right] dV_X \\ &= \int_{\mathcal{B}_X} \left[D_t f_X + \left[f_X \dot{\mathbf{X}} \right] \cdot \nabla_X \right] dV_X = \int_{\mathcal{B}_X} D_t f_X dV_X + \int_{\partial\mathcal{B}_X} f_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (13)$$

In order to derive (13), we first performed a pull-back of the integration domain from the time-dependent $\mathcal{B}_X(t)$ ⁶ to \mathcal{B}_ξ , while using the relation $dV_X = \check{j} dV_\xi$ with the Jacobian (volume ratio) $\check{j} = \det(\check{\mathbf{f}})$, then used the expression for $\Delta_t(dV_X)$ from (6) and, finally, pushed forward to \mathcal{B}_X . The expression in (13) is clearly analogous to the classical Reynolds' transport theorem, that is commonly established to express the material time derivative of an integral on the spatial domain \mathcal{B}_X .

2.3.2. Time-derivative of surface integral

It is of interest to consider a surface-specific quantity $\hat{f}_X(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$, for $\mathbf{X} \in \partial\mathcal{B}_X(t)$, and the corresponding extensive quantity

$$\hat{F} \stackrel{\text{def}}{=} \int_{\partial\mathcal{B}_X} \hat{f}_X dS_X \quad (14)$$

The time-derivative of \hat{F} , for time-dependent $\partial\mathcal{B}_X$, is given as

$$\begin{aligned} \frac{d}{dt} \hat{F} &= \int_{\partial\mathcal{B}_X} \left[\Delta_t \hat{f}_X + \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\nabla}_X \right] dS_X \\ &= \int_{\partial\mathcal{B}_X} \left[\hat{D}_t \hat{f}_X + \left[\hat{f}_X \dot{\mathbf{X}} \right] \cdot \hat{\nabla}_X \right] dS_X \end{aligned} \quad (15)$$

⁶Henceforth, the explicit dependence on time of \mathcal{B}_X is dropped for brevity of notation.

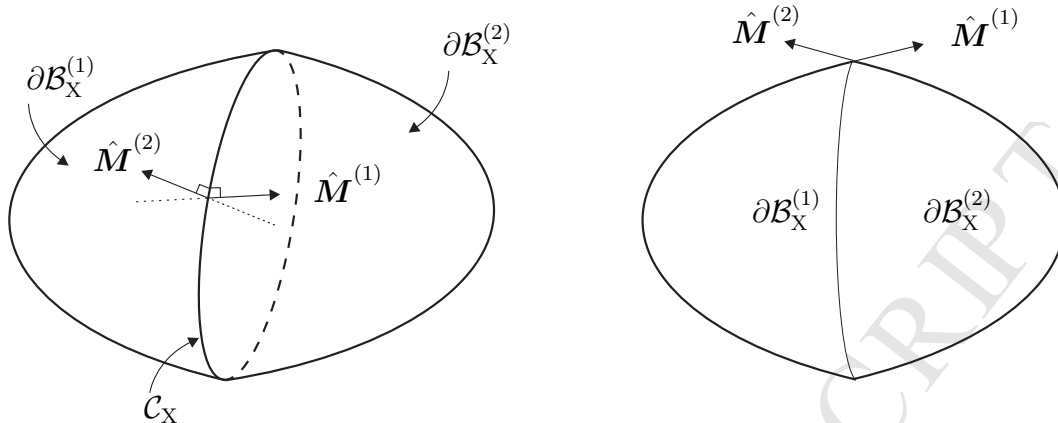


Figure 2: Finite body whose material (reference) configuration occupies the volume, $\mathcal{B}_X = \mathcal{B}_X^{(1)} \cup \mathcal{B}_X^{(2)}$ with boundary surface $\partial\mathcal{B}_X = \partial\mathcal{B}_X^{(1)} \cup \partial\mathcal{B}_X^{(2)}$. The (open) surface parts $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$ are joined along the curve \mathcal{C}_X .

where we used the definition of $\hat{\mathbf{D}}_t$ in (9), and where we, once again, used the surface-specific gradient operator $\hat{\nabla}_X$ (as defined above in terms of the surface-specific identity tensor $\hat{\mathbf{I}} \stackrel{\text{def}}{=} \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$). In order to derive (15), we first performed a pull-back of $\partial\mathcal{B}_X$ to $\partial\mathcal{B}_\xi$, while using the relation in (11).

The divergence theorem for surfaces may be used in order to transform the last term of the integrand in (15): We then consider the situation that $\partial\mathcal{B}_X = \partial\mathcal{B}_X^{(1)} \cup \partial\mathcal{B}_X^{(2)}$ is non-smooth and can be decomposed into the two smooth parts $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$, joined along the common curve \mathcal{C}_X , as shown in Figure 2. For each open surface $\partial\mathcal{B}_X^{(i)}$, $i = 1, 2$, we may apply the divergence theorem for surfaces to obtain

$$\int_{\partial\mathcal{B}_X^{(i)}} \left[\hat{f}_X \dot{\mathbf{X}} \right] \cdot \hat{\nabla}_X dS_X = \int_{\mathcal{C}_X} \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\mathbf{M}}^{(i)} dL_X - \int_{\partial\mathcal{B}_X^{(i)}} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X, \quad i = 1, 2 \quad (16)$$

where the unit vector $\hat{\mathbf{M}}^{(i)}$ is normal to \mathbf{N} on $\partial\mathcal{B}_X^{(i)}$ and the tangent of \mathcal{C}_X . Moreover, $k = -\mathbf{N} \cdot \hat{\nabla}_X$ is the total curvature of $\partial\mathcal{B}_X$ at any regular point. Several useful results pertaining to configurational changes on surfaces, including (16), can be found in Steinmann (2008).

We shall now assume that $\dot{\mathbf{X}}$ is continuous across \mathcal{C}_X , whereas \hat{f}_X may be discontinuous across \mathcal{C}_X . Upon adding the two results in (16) pertinent to $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$, we obtain

$$\int_{\partial\mathcal{B}_X} \left[\hat{f}_X \dot{\mathbf{X}} \right] \cdot \hat{\nabla}_X dS_X = \int_{\mathcal{C}_X} \left[\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)} \right] \cdot \dot{\mathbf{X}} dL_X - \int_{\partial\mathcal{B}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \quad (17)$$

Remark: If the closed surface $\partial\mathcal{B}_X$ is smooth across \mathcal{C}_X , i.e. if $\hat{\mathbf{M}}^{(1)} + \hat{\mathbf{M}}^{(2)} = \mathbf{0}$, and \hat{f}_X is continuous, i.e. $\hat{f}_X^{(1)} = \hat{f}_X^{(2)}$, we obtain the identity

$$\int_{\partial\mathcal{B}_X} \left[\hat{f}_X \dot{\mathbf{X}} \right] \cdot \hat{\nabla}_X dS_X = - \int_{\partial\mathcal{B}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \quad (18)$$

□

As a generalization, we may compose the closed surface into several multiple smooth parts to obtain

$$\int_{\partial\mathcal{B}_X} [\hat{f}_X \dot{\mathbf{X}}] \cdot \hat{\nabla}_X \, dS_X = \int_{\partial^2\mathcal{B}_X} [\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} \, dL_X - \int_{\partial\hat{\mathcal{B}}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (19)$$

where $\partial^2\mathcal{B}_X$ is the union of all curves defining "edges" on $\partial\mathcal{B}_X$. Finally, using the relation in (19) we may reformulate (15) as

$$\begin{aligned} \frac{d}{dt} \hat{F} &= \int_{\partial\mathcal{B}_X} [\Delta_t \hat{f}_X + \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\nabla}_X] \, dS_X \\ &= \int_{\partial\mathcal{B}_X} [\hat{D}_t \hat{f}_X - k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N}] \, dS_X + \int_{\partial^2\mathcal{B}_X} [\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} \, dL_X \end{aligned} \quad (20)$$

3. Thermodynamic relations in the material format

3.1. The generic balance law

It is convenient to establish a generic balance law for a given body occupying the *current* material domain \mathcal{B}_X with boundary $\partial\mathcal{B}_X$ (and unit normal \mathbf{N}), as shown schematically in Figure 2.

$$\frac{d}{dt} F = \mathcal{G}^{\text{GEN}} + \mathcal{G}^{\text{TRAN}} + \mathcal{F}^{\text{CONF}} \quad (21)$$

where \mathcal{G}^{GEN} is the (prescribed) internally generated source, $\mathcal{G}^{\text{TRAN}}$ is the standard (prescribed) "material flux", or transfer, through the boundary if the domain \mathcal{B}_X is held fixed, whereas $\mathcal{F}^{\text{CONF}}$ is the non-conventional "configurational flux" across the boundary due to the configurational motion of \mathcal{B}_X ⁷. These source terms are defined in terms of volume- and surface-specific quantities as follows:

$$\mathcal{G}^{\text{GEN}} = \int_{\mathcal{B}_X} g_X^{\text{GEN}} \, dV_X, \quad \mathcal{G}^{\text{TRAN}} = \int_{\partial\mathcal{B}_X} g_X^{\text{TRAN}} \, dS_X, \quad \mathcal{F}^{\text{CONF}} = \int_{\partial\mathcal{B}_X} f_X^{\text{CONF}} \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (22)$$

Within a smooth part of \mathcal{B}_X , the "configurational flux" f_X^{CONF} coincides with the convection of f_X due to the configurational motion, thus providing the basis for recovering the classical balance law for f_X . At a free boundary of a *finite body* Ω_X , it is necessary that f_X^{CONF} is assigned a constitutively prescribed quantity \bar{f}_X^{CONF} (that may be related to surface growth).

Subsequently, we apply (21) to the simplest situation of (in)balance of mechanical dissipation, whereby we restrict to *quasistatic motion* (i.e. dynamic forces are ignored) and isothermal conditions. Moreover, we make the classical assumption that mass is conserved. For a more comprehensive discussion of the different balance laws pertinent to mass, momentum, energy and entropy, for the general situation of dynamic motion and non-isothermal conditions, the reader is referred to Runesson et al. (2008).

⁷This represents an alternative (but in principle equivalent) formulation of the "observer-objective" paradigm by Gurtin (2000).

3.2. Global and localized dissipation inequality

The global free energy is given as

$$\Psi \stackrel{\text{def}}{=} \int_{\mathcal{B}_X} \psi_X \, dV_X \quad (23)$$

where ψ_X is the volume-specific free energy. The configurational flux of free energy is thus given as

$$\Psi^{\text{CONF}} = \int_{\partial\mathcal{B}_X} \psi_X^{\text{CONF}} \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (24)$$

Moreover, the total mechanical power supply, \mathcal{W} , is given as

$$\mathcal{W} = \int_{\mathcal{B}_X} \mathbf{b}_X \cdot \mathbf{v} \, dV_X + \int_{\partial\mathcal{B}_X} \mathbf{t}_X \cdot \mathbf{v} \, dS_X = \int_{\mathcal{B}_X} \mathbf{P} : D_t \mathbf{F} \, dV_X \quad (25)$$

In order to obtain the last expression in (25), the momentum balance $\mathbf{P} \cdot \nabla_X + \mathbf{b}_X = \mathbf{0}$, was used, where \mathbf{P} is the 1st Piola-Kirchhoff stress, and \mathbf{b}_X is the volume-specific load.

It is *proposed* that the total mechanical dissipation is expressed as

$$\mathcal{D} = \mathcal{W} - \frac{d}{dt} \Psi + \Psi^{\text{CONF}} \geq 0 \quad (26)$$

In the special case of isothermal *elastic* material response (volume-specific free energy $\psi_X(\mathbf{F}, \mathbf{X})$), and no configurational flux ($\psi_X^{\text{CONF}} = 0$), the expression in (26) was proposed by Guerses and Miehe (2008) in the context of crack propagation.

In order to obtain the localized form of (26), we consider an arbitrary domain \mathcal{B}_X that is embedded totally within a finite body. In such a case $\psi_X^{\text{CONF}} = \psi_X$ and we obtain the standard expression

$$d_X = \mathbf{P} : D_t \mathbf{F} - D_t \psi_X \geq 0 \quad (27)$$

where d_X is the volume-specific mechanical dissipation.

Next, we introduce the parametrization of the free energy density, $\psi_X(\mathbf{F}, \theta, \underline{k}; \mathbf{X})$, pertinent to a *dissipative* material response, where \underline{k} represents a set of internal variables. It is noted that a possible explicit dependence of \mathbf{X} is included as argument in ψ (representing inhomogeneous variation of material parameters in \mathcal{B}_X). Upon evaluating the material time derivative $D_t \psi_X$, and using standard arguments of the COLEMANN-NOLL type, we obtain the constitutive state equation

$$\mathbf{P} = \frac{\partial \psi_X}{\partial \mathbf{F}} \quad (28)$$

such that (24) reduces to

$$d_X = \underline{K} \star D_t \underline{k} \geq 0 \quad \text{with } \underline{K} \stackrel{\text{def}}{=} -\frac{\partial \psi_X}{\partial \underline{k}} \quad (29)$$

where we introduced dissipative stresses \underline{K} that are energy-conjugated to the internal variables \underline{k} ⁸.

4. Dissipation functional for changing material configuration

4.1. Preliminaries

We shall consider the global (mechanical) dissipation inequality for a given *finite* body occupying the current material domain Ω_X with external boundary $\partial\Omega_X$. It is assumed that the body undergoes configurational changes, expressed as $\dot{\mathbf{X}} \neq \mathbf{0}$, while it is subjected to prescribed loading. For simplicity, we restrict to *isothermal conditions* henceforth. The resulting thermodynamic process is then characterized by time-changes of all the independent thermodynamic fields, \mathbf{F} and \underline{k} , since they are solutions of the pertinent balance and state equations (equilibrium and constitutive equations) and thus depend on the configurational motion $\mathbf{X} = \Phi(\boldsymbol{\xi}, t)$ in an *implicit* manner. As a result, the global dissipation functional \mathcal{D} depends, apart from $\dot{\mathbf{X}}$, *potentially* on the fields $\dot{\mathbf{x}}$ and $\dot{\underline{k}}$ in the most general case of combined configurational and deformational motion for general loading; hence we denote $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{x}}, \dot{\underline{k}})$ the *global dissipation functional*.

Remark: For the SMP, involving the momentum equation, the boundary is subdivided into parts with essential and natural boundary conditions for the spatial field \mathbf{x} . The generic notion of these (Dirichlet and Neumann) boundary parts are $\partial\Omega_{X,D}$ (with prescribed placements) and $\partial\Omega_{X,N}$ (with prescribed tractions). It is important to note that the boundary in the expressions for \mathcal{W} in (25) is the total one, i.e. $\partial\Omega_X = \partial\Omega_{X,D} \cup \partial\Omega_{X,N}$. For example, both a prescribed and a "support" traction will contribute to \mathcal{W} in the general situation when the support is defined by prescribed non-zero configurational rate. \square

Below, we present explicit forms of $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{x}}, \dot{\underline{k}})$. As a preliminary for these developments, we recall the equilibrium equation rephrased as

$$-\mathbf{P} \cdot \nabla_X = \mathbf{b}_X \quad \text{in } \Omega_X, \quad \mathbf{P} \cdot \mathbf{N} \stackrel{\text{def}}{=} \mathbf{t}_X \quad \text{on } \partial\Omega_X \quad (30)$$

We shall also use the standard weak format⁹ of the equilibrium equation (30)

$$\int_{\Omega_X} [\mathbf{P} : [\delta\mathbf{x} \otimes \nabla_X] - \mathbf{b}_X \cdot \delta\mathbf{x}] dV_X - \int_{\partial\Omega_X} \mathbf{t}_X \cdot \delta\mathbf{x} dS_X = 0, \quad \forall \delta\mathbf{x} \in \mathbb{V} \quad (31)$$

where the virtual (placements) $\delta\mathbf{x} \in \mathbb{V}$ must be sufficiently smooth to allow for the gradient $\delta\mathbf{x} \otimes \nabla_X$ to be meaningful. We remark that no specific assumption has been made as to the value of $\delta\mathbf{x}$ on the Dirichlet boundary $\partial\Omega_{X,D}$.

⁸The "scalar star product" has the appropriate interpretation depending on the tensorial order of variables in the column vector \underline{k} .

⁹To simplify matters, it is assumed in this Section that sufficient regularity for using the divergence theorem is present in the whole Ω_X . In the subsequent application to material interfaces, this requirement does not necessarily hold; however, it can be circumvented as shown.

4.2. Basic formats of the dissipation functional – Split in configurational and material parts

It was shown in Runesson et al. (2008) that (i) the dissipation functional \mathcal{D} does not depend explicitly on $\dot{\mathbf{x}}$, i.e. the parametrization $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ suffices, (ii) it is natural to split $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ as

$$\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \mathcal{D}^{\text{CONF}}(\dot{\mathbf{X}}) + \mathcal{D}^{\text{MAT}}(\dot{\mathbf{k}}) \quad (32)$$

where $\mathcal{D}^{\text{CONF}}$ and \mathcal{D}^{MAT} are the *configurational* and *material* dissipation function, respectively.

More specifically, it was shown in Runesson et al. (2008) that two possible formats of $\mathcal{D}^{\text{CONF}}$, labelled (I) and (II), are those defined as

$$\begin{aligned} \mathcal{D}^{\text{CONF}}(\dot{\mathbf{X}}) &= \mathcal{D}_I^{\text{CONF}}(\dot{\mathbf{X}}) \stackrel{\text{def}}{=} \\ &\int_{\Omega_X} \left[-\boldsymbol{\Sigma} : \left[\dot{\mathbf{X}} \otimes \boldsymbol{\nabla}_X \right] + \mathbf{B}_I \cdot \dot{\mathbf{X}} \right] dV_X + \int_{\partial\Omega_X} \mathbf{T}_I \cdot \dot{\mathbf{X}} dS_X \end{aligned} \quad (33)$$

$$\begin{aligned} &= \mathcal{D}_{II}^{\text{CONF}}(\dot{\mathbf{X}}) \stackrel{\text{def}}{=} \\ &\int_{\Omega_X} \left[-\mathbf{B}_{II} \cdot \dot{\mathbf{X}} \right] dV_X + \int_{\partial\Omega_X} \left[-\mathbf{T}_{II} \cdot \dot{\mathbf{X}} \right] dS_X \end{aligned} \quad (34)$$

where we introduced the following notation: $\boldsymbol{\Sigma}$ is the "quasi-static" ESHELBY (energy-momentum) tensor, associated with ψ_X , which is defined as

$$\boldsymbol{\Sigma} \stackrel{\text{def}}{=} \psi_X \mathbf{I} - \mathbf{F}^T \cdot \frac{\partial \psi_X}{\partial \mathbf{F}} = \psi_X \mathbf{I} - \mathbf{F}^T \cdot \mathbf{P}, \quad (35)$$

$\mathbf{B}_I, \mathbf{B}_{II}$ are configurational volume forces, whereas $\mathbf{T}_I, \mathbf{T}_{II}$ are configurational boundary tractions, that are defined as

$$\mathbf{B}_I = -\frac{\partial \psi_X}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} - \mathbf{F}^T \cdot \mathbf{b}_X, \quad \mathbf{T}_I = -\mathbf{F}^T \cdot \mathbf{t}_X + \psi_X^{\text{CONF}} \mathbf{N} \quad (36)$$

$$\mathbf{B}_{II} = \underline{\mathbf{K}} \star [\underline{\mathbf{k}} \otimes \boldsymbol{\nabla}_X], \quad \mathbf{T}_{II} = [\psi_X - \psi_X^{\text{CONF}}] \mathbf{N} \quad (37)$$

Moreover, \mathcal{D}^{MAT} is given as

$$\mathcal{D}^{\text{MAT}}(\dot{\mathbf{k}}) \stackrel{\text{def}}{=} \int_{\Omega_X} \underline{\mathbf{K}} \star \dot{\mathbf{k}} dV_X \quad (38)$$

Once again, it must be noted that the expressions $\mathcal{D}_I^{\text{CONF}}$ and $\mathcal{D}_{II}^{\text{CONF}}$ in (33) and (34) are but two possible expressions for the purely configurational part of the dissipation. Moreover, they are completely equivalent provided certain regularity requirements are satisfied, e.g. $\dot{\mathbf{X}}$ is sufficiently regular.

Remark: It turns out that it is often more useful to introduce the alternative split of $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ as compared to (32):

$$\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) + \bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) \quad (39)$$

where we introduced

$$\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = \int_{\partial\Omega_X} [-\mathbf{T}_{\text{II}} \cdot \dot{\mathbf{X}}] \, dS_X = - \int_{\partial\Omega_X} [\psi_X - \psi_X^{\text{CONF}}] \mathbf{N} \cdot \dot{\mathbf{X}} \, dS_X \quad (40)$$

and

$$\bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \int_{\Omega_X} \underline{\mathbf{K}} \star D_t \underline{\mathbf{k}} \, dV_X = \int_{\Omega_X} \underline{\mathbf{K}} \star [\dot{\mathbf{k}} - [\underline{\mathbf{k}} \otimes \nabla_X] \cdot \dot{\mathbf{X}}] \, dV_X \quad (41)$$

It appears readily that $\bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ represents precisely the ordinary material dissipation. Moreover, if we introduce the condition of vanishing net dissipation across the external boundary, i.e. $\mathbf{N} \cdot \dot{\mathbf{X}} = 0$ on $\partial\Omega_X$, then it follows that $\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = 0$ independent of the nature of loading, boundary conditions and possible material inhomogeneity in Ω_X . In such a case the mapping $\mathbf{X}(\boldsymbol{\xi}, t)$ represents merely a coordinate transformation under which the result $\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = 0$ is invariant, cf. NOETHER'S theorem, Noether (1918). \square

4.3. Material equilibrium - Other formats of dissipation

It is useful to establish "configurational volume loads", \mathbf{B} , and "configurational surface tractions", \mathbf{T} , that equilibrate the pertinent Eshelby stress via the "configurational equilibrium equations"

$$-\boldsymbol{\Sigma} \cdot \nabla_X = \mathbf{B} \quad \text{in } \Omega_X, \quad \boldsymbol{\Sigma} \cdot \mathbf{N} = \mathbf{T} \quad \text{on } \partial\Omega_X \quad (42)$$

Upon direct differentiation of $\boldsymbol{\Sigma}$, as defined in (35), we obtain

$$\mathbf{B} = - \frac{\partial \psi_X}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} - \mathbf{F}^T \cdot \mathbf{b}_X + \underline{\mathbf{K}} \star [\underline{\mathbf{k}} \otimes \nabla_X] \quad (43)$$

where we used the strong format of (spatial) equilibrium for \mathbf{P} in (30). We also obtain the material traction as

$$\mathbf{T} = \boldsymbol{\Sigma} \cdot \mathbf{N} = \psi_X \mathbf{N} - \mathbf{F}^T \cdot \mathbf{t}_X \quad (44)$$

Remark: $\mathbf{B} = \mathbf{B}_{\text{I}} + \mathbf{B}_{\text{II}}$ and $\mathbf{T} = \mathbf{T}_{\text{I}} + \mathbf{T}_{\text{II}}$.

Remark: Since the "equilibrium equation" $(42)_1$ is a derived *identity*, it does not add any new physical information.

It is useful to establish the weak format of the configurational equilibrium equations in $(42)_1$. To this end we consider "virtual velocities" $\delta \dot{\mathbf{X}} \in \mathbb{X}$ and recast $(42)_1$ in the variational format

$$\int_{\Omega'_X} [\boldsymbol{\Sigma} : [\delta \dot{\mathbf{X}} \otimes \nabla_X] - \mathbf{B} \cdot \delta \dot{\mathbf{X}}] \, dV_X - \int_{\partial\Omega'_X} \mathbf{T} \cdot \delta \dot{\mathbf{X}} \, dS_X = 0, \quad \forall \delta \dot{\mathbf{X}} \in \mathbb{X} \quad (45)$$

where the virtual velocities $\delta \dot{\mathbf{X}} \in \mathbb{X}$ must be sufficiently smooth to allow for the gradient $\delta \dot{\mathbf{X}} \otimes \nabla_X$ to be meaningful. We remark that no specific assumption has been made as to the value of $\delta \dot{\mathbf{X}}$ on the Dirichlet boundary $\partial\Omega_{X,D}$.

5. Configurational-induced global dissipation – Generalized configurational forces

5.1. Total variation of the rate of global dissipation due to configurational changes

Henceforth, we shall restrict our attention to the situation that a physical process is manifested by fields $D_t \mathbf{x}$ and $D_t \underline{k}$ that are *brought about solely by configurational changes*. In other words, for a given field $\dot{\mathbf{X}}(\boldsymbol{\xi}, t)$, it is possible to solve for all other fields, $\dot{\mathbf{x}}\{\dot{\mathbf{X}}\}$ and $\underline{k}\{\dot{\mathbf{X}}\}$, as (implicit) functions of $\dot{\mathbf{X}}$ from the momentum equation and the pertinent constitutive relations. It is noted that the *actual physical problem* involves $\dot{\mathbf{X}}(\boldsymbol{\xi}, t)$ as part of the total solution, which requires a constitutive relation for $\dot{\mathbf{X}}$ in terms of a suitably defined field of "driving forces". However, these driving forces will be of such nature that they can only be determined when the solutions $\dot{\mathbf{x}}\{\dot{\mathbf{X}}\}$ and $\underline{k}\{\dot{\mathbf{X}}\}$ are known; hence, the problem of computing the driving forces is indeed nonlinear and must be solved by some sort of iterative procedure in practice.

Next, we shall be concerned with the issue of defining the field of thermodynamically consistent *generalized configurational forces* that are energy-conjugated to a given differential change (variation) of the field $\dot{\mathbf{X}}$, henceforth denoted $d\dot{\mathbf{X}}$, in the sense that they represent the total variation of \mathcal{D} with respect to $\dot{\mathbf{X}}$. The total differential of $\mathcal{D} \stackrel{\text{def}}{=} \mathcal{D}(\dot{\mathbf{X}}, \underline{k}\{\dot{\mathbf{X}}\})$ can be expressed as

$$\begin{aligned} d_{\dot{\mathbf{X}}} \mathcal{D} &= \mathcal{D}'(\dot{\mathbf{X}}, \underline{k}\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \\ &= (\bar{\mathcal{D}}^{\text{CONF}})'_{\dot{\mathbf{X}}}(\dot{\mathbf{X}}; d\dot{\mathbf{X}}) + (\bar{\mathcal{D}}^{\text{MAT}})'_{\dot{\mathbf{X}}}(\dot{\mathbf{X}}, \underline{k}; d\dot{\mathbf{X}}) + (\bar{\mathcal{D}}^{\text{MAT}})'_{\underline{k}}(\dot{\mathbf{X}}, \underline{k}; \underline{k}'\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \\ &= \bar{\mathcal{D}}^{\text{CONF}}(d\dot{\mathbf{X}}) + \bar{\mathcal{D}}^{\text{MAT}}(d\dot{\mathbf{X}}, \underline{k}'\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \end{aligned} \quad (46)$$

where it was used that both $\bar{\mathcal{D}}^{\text{CONF}}$ and $\bar{\mathcal{D}}^{\text{MAT}}$ are linear in their arguments ($\dot{\mathbf{X}}$ and $\dot{\mathbf{X}}, \underline{k}$, respectively). In order to carry out the total variation, it is necessary to compute the *sensitivity* fields:

$$d\dot{\mathbf{x}} = \dot{\mathbf{x}}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}, \quad d\underline{k} = \underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\} \quad (47)$$

which are directional (or Gateaux) derivatives in the classical sense¹⁰. The sensitivity fields $\dot{\mathbf{x}}'$ and \underline{k}' must satisfy *global tangent (or sensitivity) relations*, which are derivable from linearization of the equilibrium equation together with the constitutive rate equations for \underline{k} . It is emphasized that the sensitivity fields, say $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$, are *linear* in $d\dot{\mathbf{X}}$; however, they represent "spatially global" relations in Ω_X . This means, in particular, that the configurational dissipation is not necessarily confined to the (possibly small) part of Ω_X where $d\dot{\mathbf{X}} \neq \mathbf{0}$ has been assumed.

Remark: Although it is only $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ that appears in \mathcal{D}' , it is still necessary in the general case to solve for both $\dot{\mathbf{x}}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ and $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ in a truly coupled fashion via the sensitivity problem for a given field $d\dot{\mathbf{X}}$. \square

¹⁰A more explicit definition of sensitivities is possible if we define the "unit sensitivity" fields $\dot{\mathbf{x}}'^{(i)}$, $i = 1, 2, \dots, \text{NDIM}$, via the identity $d\dot{\mathbf{x}} = \sum_{i=1}^{\text{NDIM}} \dot{\mathbf{x}}'^{(i)} d(\dot{X}_i)$.

Remark: In practice, it is sometimes more convenient to compute the sensitivities in the material time derivatives. In order to link the relevant quantities, we consider a generic field z and obtain

$$\dot{z} = D_t z + [z \otimes \nabla_{\mathbf{X}}] \cdot \dot{\mathbf{X}} \quad \Rightarrow \quad \dot{z}'\{\bullet; d\dot{\mathbf{X}}\} = (D_t z)'\{\bullet; d\dot{\mathbf{X}}\} + [z \otimes \nabla_{\mathbf{X}}] \cdot d\dot{\mathbf{X}} \quad (48)$$

For example, we note that $\dot{\mathbf{x}}'\{\bullet; d\dot{\mathbf{X}}\} = \mathbf{v}'\{\bullet; d\dot{\mathbf{X}}\} + \mathbf{F} \cdot d\dot{\mathbf{X}}$. \square

Next, we shall assume that $d\dot{\mathbf{X}}$ can be parametrized as follows:

$$d\dot{\mathbf{X}} = \sum_{i=1}^{N_W} \mathbf{W}_i d\dot{a}_i \quad (49)$$

where $\mathbf{W}_i(\mathbf{X})$, $i = 1, 2, \dots, N_W$, are "weight functions" (or shape functions), the choice of which represents a model assumption in general. Upon inserting (49) into (46), we obtain the representation

$$d_{\dot{\mathbf{X}}} \mathcal{D} = \underline{\mathcal{G}}^T d\dot{\mathbf{a}} \quad (50)$$

where $\underline{\mathcal{G}}$ is the generalized configurational force that is energy-conjugated to $\dot{\mathbf{a}}$. Using (46), we may split $\underline{\mathcal{G}}$ as

$$\underline{\mathcal{G}} = \underline{\mathcal{G}}^{\text{CONF}} + \underline{\mathcal{G}}^{\text{MAT}} \quad (51)$$

where the components of $\underline{\mathcal{G}}^{\text{CONF}}$ and $\underline{\mathcal{G}}^{\text{MAT}}$ are given as

$$\mathcal{G}_i^{\text{CONF}} = \bar{\mathcal{D}}^{\text{CONF}}(\mathbf{W}_i), \quad \mathcal{G}_i^{\text{MAT}} = \bar{\mathcal{D}}^{\text{MAT}}(\mathbf{W}_i, \underline{k}'\{\dot{\mathbf{X}}; \mathbf{W}_i\}) \quad (52)$$

5.2. Constitutive relation for rate-independent plasticity

We shall consider rate-independent material response, typical for classical plasticity. In such a case \underline{k} represents the plastic strain, "hardening strain", etc. The standard material format of the rate equations for such material response then reads ¹¹

$$D_t \underline{k} = \lambda \underline{g}, \quad \lambda = \frac{1}{h} \langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle, \quad \underline{k}(\mathbf{X}, 0) = \underline{0} \quad (53)$$

where $\langle [\bullet] \rangle \stackrel{\text{def}}{=} \frac{1}{2} (|[\bullet]| + [\bullet])$ is the McCauley bracket; hence, it is noted that λ is a *first order homogeneous (but nonlinear)* function ¹² in $D_t \mathbf{F}$. This specific structure reflects the loading/unloading conditions expressed in terms of the sign of the "loading indicator" function $\boldsymbol{\mu} : D_t \mathbf{F}$ in a "strain-controlled" format" such that plastic loading, (L), is signalled by $\boldsymbol{\mu} : D_t \mathbf{F} > 0$, whereas elastic unloading, (U), is signalled by $\boldsymbol{\mu} : D_t \mathbf{F} \leq 0$. These cases are thus defined by

$$\lambda = \frac{1}{h} \boldsymbol{\mu} : D_t \mathbf{F} \quad (\text{L}), \quad \lambda = 0 \quad (\text{U}) \quad (54)$$

¹¹To simplify notation, it is assumed that the "flow rule" is regular (corresponding to a smooth flow potential).

¹²A function $f(x)$ is first order homogeneous if, for $\alpha > 0$, $f(\alpha x) = \alpha f(x)$.

As to the explicit definition of the state functions ¹³ g , h and $\boldsymbol{\mu}$, they are model dependent. (A prototype model of plasticity based on linearized elastic relations will be employed in conjunction with the motion of a singular material surface, see below.)

The appropriate continuum tangent relation for \mathbf{P} in terms of \mathbf{F} and \underline{k} can now be written as

$$\mathbf{D}_t \mathbf{P} = \mathbf{L}^e : \mathbf{D}_t \mathbf{F} + \underline{\mathbf{M}} \star \mathbf{D}_t \underline{k} \quad (55)$$

where we introduced the tangent operators

$$\mathbf{L}^e \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{k}, \mathbf{X}}, \quad \underline{\mathbf{M}} \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \underline{k}} \Big|_{\mathbf{F}, \mathbf{X}} \quad (56)$$

In particular, \mathbf{L}^e is the elastic continuum tangent stiffness (CTS) tensor. Upon inserting (53)₁ into (55), we obtain

$$\mathbf{D}_t \mathbf{P} = \mathbf{L}^{\text{ep}} : \mathbf{D}_t \mathbf{F} \quad (\text{L}), \quad \mathbf{D}_t \mathbf{P} = \mathbf{L}^e : \mathbf{D}_t \mathbf{F} \quad (\text{U}) \quad (57)$$

where \mathbf{L}^{ep} is the elastic-plastic continuum tangent stiffness (CTS) tensor, defined as

$$\mathbf{L}^{\text{ep}} \stackrel{\text{def}}{=} \mathbf{L}^e + \frac{1}{h} \underline{\mathbf{M}} \star \underline{g} \boldsymbol{\mu} \quad (58)$$

We note that the CTS-tensor takes two distinct expressions depending on whether plastic loading (L) or elastic unloading (U) is at hand at a given position $\mathbf{X} \in \Omega_X$. Hence, $\mathbf{D}_t \underline{k}$ and $\mathbf{D}_t \mathbf{P}$ are nonlinear functions in $\mathbf{D}_t \mathbf{F}$.

Now, we shall take the total variation of $\mathbf{D}_t \mathbf{P}$ with respect to variation of $\dot{\mathbf{X}}$ to obtain the sensitivity relation

$$(\mathbf{D}_t \mathbf{P})' = \mathbf{L}^e : (\mathbf{D}_t \mathbf{F})' + \underline{\mathbf{M}} \star (\mathbf{D}_t \underline{k})' \quad (59)$$

From (53)₁ we obtain

$$(\mathbf{D}_t \underline{k})' = \underline{\mathbf{R}}_T : (\mathbf{D}_t \mathbf{F})' \quad \text{with} \quad \underline{\mathbf{R}}_T \stackrel{\text{def}}{=} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F}|} \underline{g} \otimes \boldsymbol{\mu} \quad (60)$$

which (i) depends on the current value of \mathbf{v} (or $\dot{\mathbf{x}}$ and $\dot{\mathbf{X}}$) via the relation in (9), (ii) is linear in the sensitivity $(\mathbf{D}_t \mathbf{F})'$. The expression in (60) is well-defined for all solutions except at neutral loading defined by $\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} = 0$. In particular, it can be evaluated for the situation $\dot{\mathbf{X}} = \mathbf{0}$, corresponding to vanishing configurational motion.

Upon combining (59,60), we obtain the desired relation

$$(\mathbf{D}_t \mathbf{P})' = \mathbf{L}_T : (\mathbf{D}_t \mathbf{F})' \quad \text{with} \quad \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}^e + \frac{1}{h} \frac{\langle \boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F}|} \underline{\mathbf{M}} \star \underline{g} \otimes \boldsymbol{\mu} \quad (61)$$

where \mathbf{L}_T is the tangent stiffness tensor that depends on $\mathbf{D}_t \mathbf{F}$ and which holds for both (L) and (U).

¹³E.g. $\underline{g}(\mathbf{F}[\mathbf{X}, \mathbf{x}], \underline{k})$

Remark: For a more general rate-independent relation than (53) of the generic form

$$D_t \underline{k} = \underline{f}(D_t \mathbf{F}) \quad (62)$$

where \underline{f} is 1st order homogeneous in its argument, we may generalize (60) to

$$(D_t \underline{k})' = \underline{f}'(D_t \mathbf{F}; (D_t \mathbf{F})') \quad (63)$$

where $\underline{f}'(\bullet; (\bullet)')$ represents the directional derivative. \square

5.3. Basic format of the tangent problem for quasistatic equilibrium

5.3.1. Preliminaries

Consider the basic problem of a finite body with Dirichlet and Neumann boundary conditions $\mathbf{x} = \bar{\mathbf{x}}$ on $\partial\Omega_{X,D}$ and $\mathbf{t}_X \stackrel{\text{def}}{=} \mathbf{P} \cdot \mathbf{N} = \bar{\mathbf{t}}_X$ on $\partial\Omega_{X,N} = \partial\Omega_X \setminus \partial\Omega_{X,D}$. Moreover, we assume the constitutive state relation $\mathbf{P}(\mathbf{F}, \underline{k}; \mathbf{X})$. The weak format of the equilibrium equation can then be written in standard fashion:

$$a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) = l(\delta \mathbf{x}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (64)$$

where

$$a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) \stackrel{\text{def}}{=} \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P}(\mathbf{F}, \underline{k}; \mathbf{X}) \, dV_X \quad (65)$$

$$l(\delta \mathbf{x}) \stackrel{\text{def}}{=} \int_{\Omega_X} \delta \mathbf{x} \cdot \mathbf{b}_X \, dV_X + \int_{\partial\Omega_{X,N}} \delta \mathbf{x} \cdot \mathbf{t}_X \, dS_X \quad (66)$$

The SMP is then to find $\mathbf{x} \in \mathbb{V}$ and $\underline{k} \in \mathbb{K}$ that solve (64) together with the pertinent evolution equation for \underline{k} , as defined in (53).

Since Ω_X is not time-invariant at configurational changes, the test functions $\delta \mathbf{x} \in \mathbb{V}^0$ are time-dependent in the parametrization $\delta \mathbf{x}(\mathbf{X}, t)$; however, this relation is constrained by the condition that $\delta \mathbf{x}(\mathbf{X}, t)$ is stationary in the absolute configuration, i.e.

$$\delta \mathbf{x}(\mathbf{X}(\boldsymbol{\xi}, t), t) \stackrel{\text{def}}{=} \delta \mathbf{x}(\boldsymbol{\xi}, t) = \delta \mathbf{x}(\boldsymbol{\xi}) \quad (67)$$

In particular, this means that

$$\Delta_t \delta \mathbf{x} = \mathbf{0}, \quad D_t \delta \mathbf{x} = -[\delta \mathbf{x} \otimes \nabla_X] \cdot \dot{\mathbf{X}} \quad (68)$$

$$\Delta_t [\delta \mathbf{x} \otimes \nabla_X] = -[\delta \mathbf{x} \otimes \nabla_X] \cdot [\dot{\mathbf{X}} \otimes \nabla_X], \quad D_t [\delta \mathbf{x} \otimes \nabla_X] = [D_t \delta \mathbf{x}] \otimes \nabla_X \quad (69)$$

Our purpose is to first solve for the sensitivity field $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$ from the tangent problem

$$d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} a(\bullet; \delta \mathbf{x}) - \frac{d}{dt} l(\delta \mathbf{x}) \right] = 0, \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (70)$$

for given variations¹⁴ $d\dot{\mathbf{X}} \in \mathbb{X}^0$, and then to compute $\underline{k}'\{\bullet, d\dot{\mathbf{X}}\}$.

Remark: The format for the tangent problem based on $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\}$ as the primary unknown field is considered henceforth as the "operational" format, since each field $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$ is continuous across any singular surface where the state variables (such as \mathbf{F}) may be discontinuous. In such a case, $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} = \dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} - \mathbf{F} \cdot d\dot{\mathbf{X}}$ is discontinuous across the singular surface, and it follows that $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} \notin \mathbb{V}^0$, as shown in Figure 3. Nevertheless, the special situation that the solution is smooth, i.e. $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$, is of particular relevance. Hence, both situations will be discussed subsequently. \square

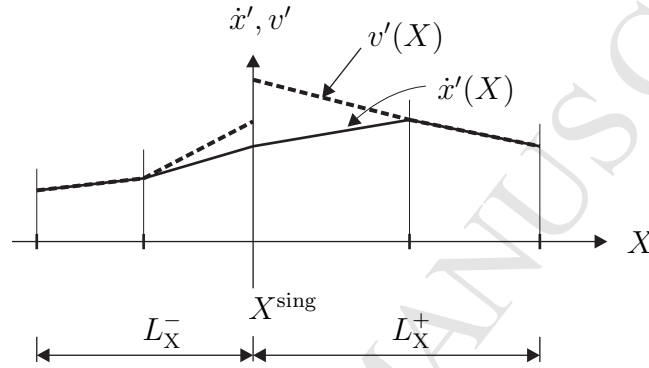


Figure 3: Illustration of the general situation that $\dot{\mathbf{x}}'$ is continuous while \mathbf{v}' is discontinuous across Γ_X^{sing} .

5.3.2. Operational format (based on $\dot{\mathbf{x}}$)

We shall first consider the general case that \mathbf{v}' is only p.w. smooth in Ω_X . In such a case $\dot{\mathbf{x}}' \in \mathbb{V}^0$ is solved from the tangent relation

$$a_T(\bullet; \delta \mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (71)$$

where the pertinent tangent forms are defined as¹⁵

$$a_T(\bullet; \delta \mathbf{x}, \dot{\mathbf{x}}') \stackrel{\text{def}}{=} \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X] dV_X \quad (72)$$

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \\ & + \int_{\partial\Omega_X} \left[- \left[\delta \mathbf{x} \otimes \hat{\nabla}_X \right] : \left[\mathbf{t}_X \otimes d\dot{\mathbf{X}} \right] + \left[\delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X \right] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dS_X \\ & + \int_{\hat{c}_X} \delta \mathbf{x} \cdot \left[\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)} \right] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (73)$$

¹⁴The required regularity of \mathbb{X}^0 depends on the chosen format; here, we assume that $d\dot{\mathbf{X}}$ is continuous and that $d\dot{\mathbf{X}} = \mathbf{0}$ on $\partial\Omega_{X,D}$ for any $d\dot{\mathbf{X}} \in \mathbb{X}^0$.

¹⁵Henceforth, in order to retain maximal generality we do not distinguish explicitly between the Dirichlet and Neumann boundary parts in the various surface integrals.

The continuum tangent stiffness tensor \mathbf{L}_T , defined by the relation $(D_t \mathbf{P})' = \mathbf{L}_T : (D_t \mathbf{F})'$, was defined in (61). In order to define the "loading" $l_T^{(x)}$ of the tangent problem, we introduced the 4th order tensor \mathbf{P} (which has generally minor non-symmetry), and the 3rd order tensor \mathbf{r}_X , defined as follows:

$$\mathbf{P} \stackrel{\text{def}}{=} \underline{\mathbf{P}} \otimes \mathbf{I} - \mathbf{P} \otimes \mathbf{I} \quad (74)$$

$$\mathbf{r}_X = \Delta \mathbf{L}_T : [\mathbf{F} \otimes \nabla_X] - \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_X] - \frac{\partial \mathbf{P}}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} \quad (75)$$

where $\Delta \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}_T - \mathbf{L}^e$. Details of the derivation are given in the Appendix.

5.3.3. Non-operational format (based on \mathbf{v})

Next, we consider the special case that \mathbf{v}' is smooth in Ω_X . In such a case $\mathbf{v}' \in \mathbb{V}^0$ can be solved from the tangent relation

$$a_T(\bullet; \delta \mathbf{x}, \mathbf{v}') = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (76)$$

where the tangent form a_T was defined in (72), whereas $l_T^{(v)}$ is given as

$$\begin{aligned} l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\partial \Omega_X} [-[\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} + \delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}]] d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ & + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (77)$$

Details of the derivation are given in the Appendix.

6. Application to moving material (singular) interface

6.1. Problem definition

Consider the situation when an embedded (open) singular surface Γ_X^{sing} , across which the material properties may be discontinuous. The surface Γ_X^{sing} , with boundary curve \mathcal{C}_X , can move through the material domain Ω_X with (closed) *external* boundary $\partial \Omega_X$, which is assumed to be sufficiently smooth. In fact, it suffices that $\partial \Omega_X$ is smooth where $d\dot{\mathbf{X}} \neq \mathbf{0}$. The domain Ω_X is split into two parts, Ω_X^- and Ω_X^+ ($\Omega_X = \Omega_X^- \cup \Omega_X^+$ and $\partial \Omega_X = \partial \Omega_X^- \cup \partial \Omega_X^+$), as shown in Figure 4, whereby the boundary of the two parts are given as $\partial(\Omega_X^-) = \partial \Omega_X^- \cup \Gamma_X^{\text{sing}}$ and $\partial(\Omega_X^+) = \partial \Omega_X^+ \cup \Gamma_X^{\text{sing}}$, respectively. Since the state variables, such as \mathbf{F} and \underline{k} , are generally discontinuous across Γ_X^{sing} , the volume-specific free energy ψ_X is also discontinuous across Γ_X^{sing} .

The normal on Γ_X^{sing} pointing into Ω_X^+ is denoted $\mathbf{N}^- (= \mathbf{N})$, as shown in Figure 4; hence, we use the notation $\mathbf{N}^+ (= -\mathbf{N})$ for the normal in the opposite direction. The cotangents $\hat{\mathbf{M}}^-$ and $\hat{\mathbf{M}}^+$, located on the curve \mathcal{C}_X , are normal to \mathcal{C}_X and lie in the tangent plane of $\partial \Omega_X^-$ and $\partial \Omega_X^+$, respectively. Hence, $\hat{\mathbf{M}}^+ + \hat{\mathbf{M}}^- \neq \mathbf{0}$ in general. The cotangent $\hat{\mathbf{M}}^{\text{tang}}$, which is also located on and directed normal to \mathcal{C}_X , lies in the tangent plane of Γ_X^{sing} . It is thus unique on both sides of the interface.

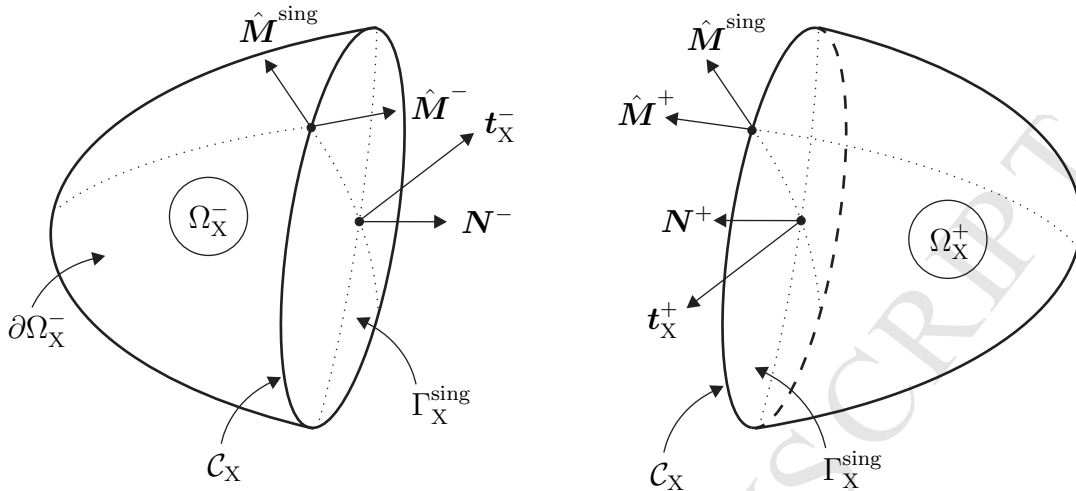


Figure 4: Moving material (singular) interface Γ_X^{sing} splitting the domain Ω_X in the parts Ω_X^- and Ω_X^+ . Other notation is explained in the main text.

6.2. Explicit (classical) configurational forces along material interface

The explicit expression for $\mathcal{D}^{\text{CONF}}$ was discussed in some detail in Runesson et al. (2008). Upon introducing the assumption of vanishing net dissipation across the exterior boundary, i.e. $\mathbf{N} \cdot \dot{\mathbf{X}} = 0$ on $\partial\Omega_X$, we obtain the classical representation

$$\bar{\mathcal{D}}^{\text{CONF}}(d\dot{\mathbf{X}}) = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{CONF}} \cdot d\dot{\mathbf{X}} dS_X, \quad \mathcal{G}^{\text{CONF}} \stackrel{\text{def}}{=} \|\Sigma\| \cdot \mathbf{N} \quad (78)$$

where $\mathcal{G}^{\text{CONF}}$ is the explicitly localized (distributed) configurational "traction" that "lives" on Γ_X^{sing} and, moreover, that represents the dissipation along Γ_X^{sing} .

Remark: Since the deformation gradient \mathbf{F} can be discontinuous only in the normal direction, \mathbf{N} , across Γ_X^{sing} , it is possible to express $\mathcal{G}^{\text{CONF}}$ as

$$\mathcal{G}^{\text{CONF}} = \|\Sigma\| \cdot \mathbf{N} = \alpha \mathbf{N} \quad (79)$$

where $\alpha = \|\Psi_X\| - \mathbf{N} \cdot \|\mathbf{F}^T\| \cdot \langle \mathbf{P} \rangle \cdot \mathbf{N}$ ¹⁶. Hence, the configurational dissipation along Γ_X^{sing} is invariant (vanishes) for any choice of $\dot{\mathbf{X}}$ s.t. $\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ on $\partial\Omega_X \cup \Gamma_X^{\text{sing}}$. \square

6.3. Implicit (configurational-induced) configurational forces along interface – Tangent problem

6.3.1. Operational format of tangent problem

We shall use the fact that all fields are sufficiently smooth in the parts Ω_X^- and Ω_X^+ , whereby the tangent problem introduced in (71) applies to Ω_X^- and Ω_X^+ separately. However, although \mathbf{v}' is expected to be discontinuous across the singular surface Γ_X^{sing} (since \mathbf{F} is discontinuous in general), $\dot{\mathbf{x}}'$ is still continuous across this surface. This means that the

¹⁶ $\langle \mathbf{P} \rangle$ denotes mean value, i.e. $\langle \mathbf{P} \rangle = \frac{1}{2}[\mathbf{P}^- + \mathbf{P}^+]$.

operational format of the tangent problem for a discontinuity surface is conveniently based on $\dot{\mathbf{x}}' \in \mathbb{V}^0$ as the primary unknown field.

At the outset we shall choose $d\dot{\mathbf{X}}$ continuous across Γ_X^{sing} . In order to simplify the resulting expression as far as possible without loss of essential features, we shall also assume that the external boundary $\partial\Omega_X$ is smooth along \mathcal{C}_X . Referring to the notation introduced in Figure 4, we then note the following identities relating to the singular surface Γ_X^{sing} :

$$\hat{\mathbf{M}}^+ + \hat{\mathbf{M}}^- = \mathbf{0}, \quad \mathbf{t}_X^+ + \mathbf{t}_X^- = \mathbf{0}, \quad k^+ + k^- = 0 \quad (80)$$

Clearly, (80)₁ represents the smoothness condition on $\partial\Omega_X$, (80)₂ expresses the condition that the physical tractions on each side of the interface Γ_X^{sing} equilibrate each other, whereas the relation (80)₃ follows from the identities $\hat{\nabla}_X^- = \hat{\nabla}_X^+ \stackrel{\text{def}}{=} \hat{\nabla}_X$ and $-\mathbf{N}^+ = \mathbf{N}^- \stackrel{\text{def}}{=} \mathbf{N}$.

In addition, we shall introduce the assumption that the applied volume load \mathbf{b}_X and surface load (traction) $\bar{\mathbf{t}}_X$ are continuous across \mathcal{C}_X , i.e. $\mathbf{b}_X^- = \mathbf{b}_X^+$ and $\bar{\mathbf{t}}_X^- = \bar{\mathbf{t}}_X^+$ on \mathcal{C}_X .

It is now possible to "tie together" the tangent problems for Ω_X^- and Ω_X^+ , as defined in (71), upon simply adding the pertinent relations and using the "continuity" conditions in (80). We then obtain the tangent problem for the body with interface: Solve for $\dot{\mathbf{x}}' \in \mathbb{V}^0$ from

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (81)$$

where $a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}')$ is still given by (72), whereas $l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}})$ in (73) is now condensed to

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \\ & + \int_{\partial\Omega_X} \left[- \left[\delta\mathbf{x} \otimes \hat{\nabla}_X \right] : \left[\mathbf{t}_X \otimes d\dot{\mathbf{X}} \right] + [\delta\mathbf{x} \cdot \mathbf{b}_X - k \delta\mathbf{x} \cdot \mathbf{t}_X] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dA_X \end{aligned} \quad (82)$$

An important special case is defined by the choice $d\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ and $\bar{\mathbf{t}}_X = \mathbf{0}$ on the exterior Neumann boundary part $\partial\Omega_{X,N}$. In such a case the boundary integral in (82) vanishes, and we are left with the simpler expression

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}) = & \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \end{aligned} \quad (83)$$

In practice, the operational format is based on the parametrization in (49), whereby we obtain

$$\dot{\mathbf{x}}' \{ \dot{\mathbf{X}}; d\dot{\mathbf{X}} \} = \sum_{i=1}^{N_w} \dot{\mathbf{x}}' \{ \dot{\mathbf{X}}; \mathbf{W}_i \} d\dot{a}_i = \sum_{i=1}^{N_w} \dot{\mathbf{x}}'_i d\dot{a}_i \quad (84)$$

Consequently, (81) is replaced by the set of problems: Solve for $\dot{\mathbf{x}}'_i \in \mathbb{V}^0, i = 1, 2, \dots, N_w$:

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}'_i) = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, \mathbf{W}_i), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (85)$$

For known fields $\dot{\mathbf{x}}'_i$, it is possible to compute the generalized configurational force components $(\underline{\mathcal{G}}^{\text{MAT}})_i$ in a post-processing step: $\dot{\mathbf{x}}'_i \rightarrow \mathbf{v}'_i \rightarrow (\mathbf{D}_t \mathbf{F})'_i \rightarrow (\mathbf{D}_t \underline{k})'_i \rightarrow \mathcal{G}_i^{\text{MAT}} \stackrel{\text{def}}{=} (\underline{\mathcal{G}}^{\text{MAT}})_i$ with

$$\mathcal{G}_i^{\text{MAT}} \stackrel{\text{def}}{=} \int_{\Omega_X} \underline{K} \star (\mathbf{D}_t \underline{k})'_i \, dV_X. \quad (86)$$

Finally, we may define the "localizable" (distributed) configurational force vector \mathcal{G}^{MAT} via the identity (least squares projection)

$$\mathcal{G}_i^{\text{MAT}} = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{MAT}} \cdot \mathbf{W}_i \, dS_X \quad (87)$$

This equation is solved approximately in practice using FE-discretization, whereby \mathbf{W}_i are taken as the nodal basis functions along Γ_X^{sing} , and \mathcal{G}^{MAT} is expanded in this basis (as discussed below).

6.3.2. Issue of unique sensitivity field (tangent solution)

It is of considerable interest to note that the sensitivity field $\dot{\mathbf{x}}'$ (or \mathbf{v}') are unique with respect to the choice of the field $d\dot{\mathbf{X}}$ in Ω_X as long as the following conditions are satisfied: (i) The normal component of $d\dot{\mathbf{X}}$ is uniquely chosen on the external boundary $\partial\Omega_X$ as well as on the interface Γ_X^{sing} , (ii) $d\dot{\mathbf{X}}$ is unique along \mathcal{C}_X .

In order to show this result, we consider two given fields $d\dot{\mathbf{X}}^{(1)}$ and $d\dot{\mathbf{X}}^{(2)}$ defined on Ω_X^- . Their difference is denoted $d\dot{\mathbf{X}}^{(1,2)} \stackrel{\text{def}}{=} d\dot{\mathbf{X}}^{(1)} - d\dot{\mathbf{X}}^{(2)}$, corresponding to the sensitivity $(\mathbf{v}^{(1,2)})'$. Now, in view of (76), we conclude that $(\mathbf{v}^{(1,2)})'$ is the solution of the tangent problem

$$a_T(\bullet; \delta \mathbf{x}, (\mathbf{v}^{(1,2)})') = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (88)$$

where

$$\begin{aligned} l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}) \stackrel{\text{def}}{=} & \int_{\partial(\Omega_X^-)} [-[\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} + \delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X \\ & + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}]] \, d\dot{\mathbf{X}}^{(1,2)} \cdot \mathbf{N} \, dS_X \\ & + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X \otimes \hat{\mathbf{M}} + \mathbf{t}_X^- \otimes \hat{\mathbf{M}}^-] \cdot d\dot{\mathbf{X}}^{(1,2)} \, dL_X \end{aligned} \quad (89)$$

However, if we impose the conditions (i) $d\dot{\mathbf{X}}^{(1,2)} \cdot \mathbf{N} = 0$ on $\partial(\Omega_X^-)$ and (ii) $d\dot{\mathbf{X}}^{(1,2)} = \mathbf{0}$ along \mathcal{C}_X , which situation is illustrated in Figure 5, then it is obvious that $l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}) = 0$. Hence, it is concluded that $(\mathbf{v}^{(1,2)})' = \mathbf{0}$ in Ω_X^- . Similarly, we may consider the part Ω_X^+ and conclude that $(\mathbf{v}^{(1,2)})' = \mathbf{0}$ in Ω_X^+ under the same assumptions. We have thus shown that $(\mathbf{v}^{(1)})' = (\mathbf{v}^{(2)})' = \mathbf{v}'$ is unique in the entire domain Ω_X , from which it is concluded that $(\mathbf{D}_t \mathbf{F})'$ is unique and, finally, $(\mathbf{D}_t \underline{k})'$ is unique (which will also be verified numerically below).

In summary, we have shown that \mathcal{G}^{MAT} will not be affected by the particular choice of the variation $d\dot{\mathbf{X}}$ in the entire domain Ω_X as long as the conditions (i) and (ii) are satisfied. That $\mathcal{G}^{\text{CONF}}$ is not affected by the choice of $d\dot{\mathbf{X}}$ whatsoever is clear from (78).

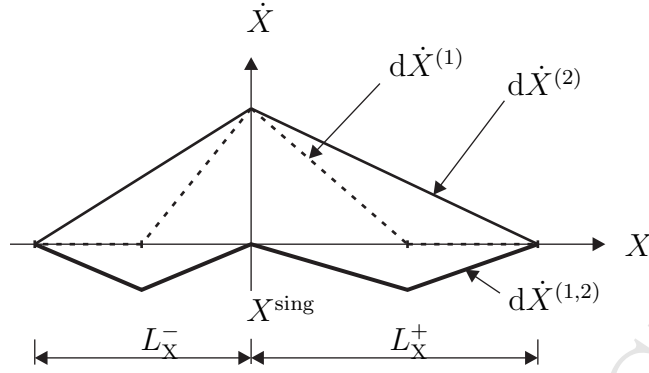


Figure 5: Two choices of $d\dot{\mathbf{X}}$ which give the same field $(D_t \underline{\mathbf{k}})'$ and, hence, identical values of \mathcal{G}^{MAT} .

7. Numerical example: Plate with interface separating parts with dissimilar material properties

7.1. Elastic-plastic model – Linearized format

We adopt a simple elastic-plastic model based on the von Mises yield criterion with isotropic hardening. A linearization of the spatially objective large deformation formulation is obtained by introducing the volume-specific free energy as

$$\psi_{\mathbf{X}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}, k) = \psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}) + \psi_{\mathbf{X}}^{\text{p}}(k) \quad (90)$$

where the part $\psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}})$ represents linear elasticity and is given as

$$\psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}) = \frac{1}{2} [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] : \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] \quad (91)$$

with $\mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}}) \stackrel{\text{def}}{=} \mathbf{I} + \boldsymbol{\epsilon}^{\text{P}}$, and where $\psi_{\mathbf{X}}^{\text{p}}(k)$ is the "plastic" (or rather hardening) free energy corresponding to isotropic hardening and given as

$$\psi_{\mathbf{X}}^{\text{p}}(k) = \frac{1}{2} H k^2 \quad (92)$$

In (91), we introduced the constant "small strain" stiffness tensor in standard fashion representing isotropic linear elastic properties

$$\mathbf{E}^{\text{e}} = 2G \mathbf{I}_{\text{dev}}^{\text{sym}} + K \mathbf{I} \otimes \mathbf{I}, \quad \mathbf{I}_{\text{dev}}^{\text{sym}} = \mathbf{I}^{\text{sym}} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \quad (93)$$

where G and K are the shear and bulk moduli, respectively. In (92), H is the constant isotropic hardening modulus. Obviously, this model gives the thermodynamically consistent stresses

$$\mathbf{P} = \frac{\partial \psi_{\mathbf{X}}}{\partial \mathbf{F}} = \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] \quad (94)$$

$$\boldsymbol{\sigma}^{\text{P}} = -\frac{\partial \psi_{\mathbf{X}}}{\partial \boldsymbol{\epsilon}^{\text{P}}} = \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] = \mathbf{P} \quad (95)$$

$$K = -\frac{\partial \psi_{\mathbf{X}}}{\partial k} = -Hk \quad (96)$$

We may thus express the (local) volume-specific material rate of dissipation $d_X = \underline{K} \star D_t \underline{k}$ according to (29) with the matrices \underline{k} and \underline{K} defined as

$$\underline{k} \stackrel{\text{def}}{=} \begin{bmatrix} \boldsymbol{\epsilon}^P \\ k \end{bmatrix}, \quad \underline{K} \stackrel{\text{def}}{=} \begin{bmatrix} \mathbf{P} \\ K \end{bmatrix} \quad (97)$$

The von Mises yield criterion with isotropic hardening is expressed as

$$\Phi(\mathbf{P}, K) = P_e - [Y + K] = 0, \quad P_e \stackrel{\text{def}}{=} \sqrt{\frac{3}{2}} |\mathbf{P}_{\text{dev}}| \quad (98)$$

where Y is the uniaxial yield stress and P_e is the effective (1st Piola-Kirchhoff) stress.

To complete the model, we adopt the evolution rules of the associated type, i.e.

$$D_t \boldsymbol{\epsilon}^P = \lambda \frac{\partial \Phi}{\partial \mathbf{P}} = \lambda \frac{3 \mathbf{P}_{\text{dev}}}{2 P_e} \quad (99)$$

$$D_t k = \lambda \frac{\partial \Phi}{\partial K} = -\lambda \quad (100)$$

where λ is the plastic multiplier. Due to the linearized structure and since \mathbf{E}^e has both major and minor symmetry, \mathbf{P} becomes symmetrical; hence, the conventional small strain model is retrieved in the case that deformations are indeed small such that $|\boldsymbol{\epsilon}^P| \ll 1$.

Next, we obtain from (56) the basic tangent operators

$$\mathbf{L}^e \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{k}, X} = \mathbf{E}^e, \quad \underline{\mathbf{M}} \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \underline{\mathbf{k}}} \Big|_{\mathbf{F}, X} = \begin{bmatrix} \frac{\partial \mathbf{P}}{\partial \boldsymbol{\epsilon}^P} \\ \frac{\partial \mathbf{P}}{\partial k} \end{bmatrix} = \begin{bmatrix} -\mathbf{E}^e \\ \mathbf{0} \end{bmatrix} \quad (101)$$

In order to obtain explicit expressions of the tangent operators $\underline{\mathbf{R}}_T$ and \mathbf{L}_T , defined in (60) and (61), respectively, we may evaluate the condition $D_t \Phi = 0$ at plastic loading for "deformation control" to compute the state functions

$$h = 3G + H, \quad \boldsymbol{\mu} = \frac{3G}{P_e} \mathbf{P}_{\text{dev}}, \quad \underline{\mathbf{g}} = \begin{bmatrix} \frac{3}{2P_e} \mathbf{P}_{\text{dev}} \\ -1 \end{bmatrix} \quad (102)$$

and we obtain

$$\mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{E}^e - \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \boldsymbol{\mu} \otimes \boldsymbol{\mu}, \quad \Delta \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}_T - \mathbf{L}^e = -\frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \boldsymbol{\mu} \otimes \boldsymbol{\mu} \quad (103)$$

where it was used that $\underline{\mathbf{M}} \star \underline{\mathbf{g}} = -\boldsymbol{\mu}$. Finally, we may use (101) and (102) to obtain

$$\begin{aligned} \mathcal{G}_i^{\text{MAT}} &= \int_{\Omega_X^p} \underline{K} \star \underline{\mathbf{R}}_T : (D_t \mathbf{F})' dV_X = \int_{\Omega_X^p} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \underline{K} \star \underline{\mathbf{g}} \boldsymbol{\mu} : (D_t \mathbf{F})' dV_X \\ &= \int_{\Omega_X^p} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} Y \boldsymbol{\mu} : (D_t \mathbf{F})' dV_X \end{aligned} \quad (104)$$

In order to obtain the last expression in (104), we used that $\underline{K} \star \underline{g} = P_e - K = Y$ in the plastic domain Ω_X^p , defined by the current state satisfying the yield criterion, $\Phi = 0$.

When the quantities $\mathcal{G}_i^{\text{MAT}}$, which correspond to nodal values da_i , are known, it is possible to "localize" the "configurational traction" \mathcal{G}^{MAT} via the *ansatz*, cf. Figure 6,

$$\mathcal{G}^{\text{MAT}} = \sum_{j=1}^{N_W} \mathbf{W}_j \bar{\mathcal{G}}_j^{\text{MAT}} \quad (105)$$

where $\bar{\mathcal{G}}_i^{\text{MAT}}$ and \mathbf{W}_i , $i = 1, 2, \dots, N_W$, are the nodal values (intensities) and the basis functions, respectively. A least squares projection on the set of basis functions in the sense that

$$\mathcal{G}_i^{\text{MAT}} = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{MAT}} \cdot \mathbf{W}_i \, dS_X \quad (106)$$

then gives the intensities $\bar{\mathcal{G}}_i^{\text{MAT}}$, collected in the column matrix $\underline{\bar{\mathcal{G}}}^{\text{MAT}} = [\bar{\mathcal{G}}_1^{\text{MAT}}, \bar{\mathcal{G}}_2^{\text{MAT}}, \dots, \bar{\mathcal{G}}_{N_W}^{\text{MAT}}]^T$, from the matrix equation

$$\underline{W} \underline{\bar{\mathcal{G}}}^{\text{MAT}} = \underline{\mathcal{G}}^{\text{MAT}}, \quad W_{ij} \stackrel{\text{def}}{=} \int_{\Gamma_X^{\text{sing}}} \mathbf{W}_i \cdot \mathbf{W}_j \, dS_X \quad (107)$$

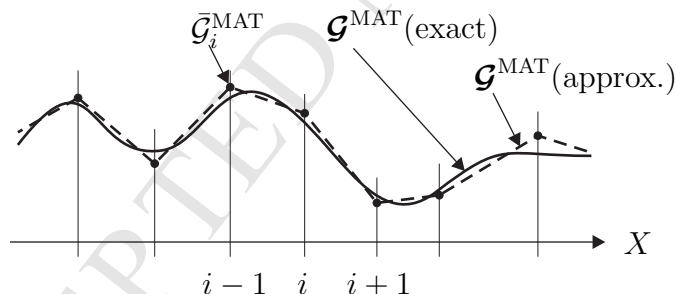


Figure 6: Representation of \mathcal{G}^{MAT} in terms of the nodal values on Γ_X^{sing} for a given FE-mesh.

7.2. Problem formulation

Consider a plate in plane strain, with length L and width $H = 0.5L$, which is subjected to prescribed end displacements at the right end, as shown in Figure 7(a). The maximal displacement is $\bar{u}_{\text{max}}/L = 0.5 \cdot 10^{-3}$. This is the sole loading, i. e. $\mathbf{b}_X = \mathbf{0}$ in Ω_X and $\bar{\mathbf{t}}_X = \mathbf{0}$ on $\partial\Omega_{X,N}$. Since we shall also assume that $d\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ on the external boundary $\partial\Omega_X$, we obtain the following simplified version of (83) as the data for the tangent problem:

$$\begin{aligned} l_T^{(\dot{x})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) = & \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : [d\dot{\mathbf{X}} \otimes \nabla_X] \right. \\ & \left. + \mathbf{L}_T : \left[\mathbf{F} \cdot [d\dot{\mathbf{X}} \otimes \nabla_X] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} \right] dV_X \end{aligned} \quad (108)$$

Using the fact that the material properties are homogeneous in each of the two subdomains separated by the singular surface, i.e. $\frac{\partial \mathbf{P}}{\partial \mathbf{X}}|_{\mathbf{F},k} = \mathbf{0}$, it is possible to reformulate \mathbf{r}_X , the general expression of which was given in (75), more explicitly as

$$\mathbf{r}_X = \Delta \mathbf{L}_T : [\mathbf{F} \otimes \nabla_X] + \mathbf{E}^e : [\epsilon^p \otimes \nabla_X] \quad (109)$$

where $\Delta \mathbf{L}_T$ was given in (103).

The material parameters for the elastic-plastic model are: $E, \nu = 0.3, Y, H$ with $E_{\text{ref}}, Y_{\text{ref}} = 0.001 E_{\text{ref}}, H_{\text{ref}} = 0.2 E_{\text{ref}}$. They assume different values on each side of the interface, as shown schematically in Figure 7(b).

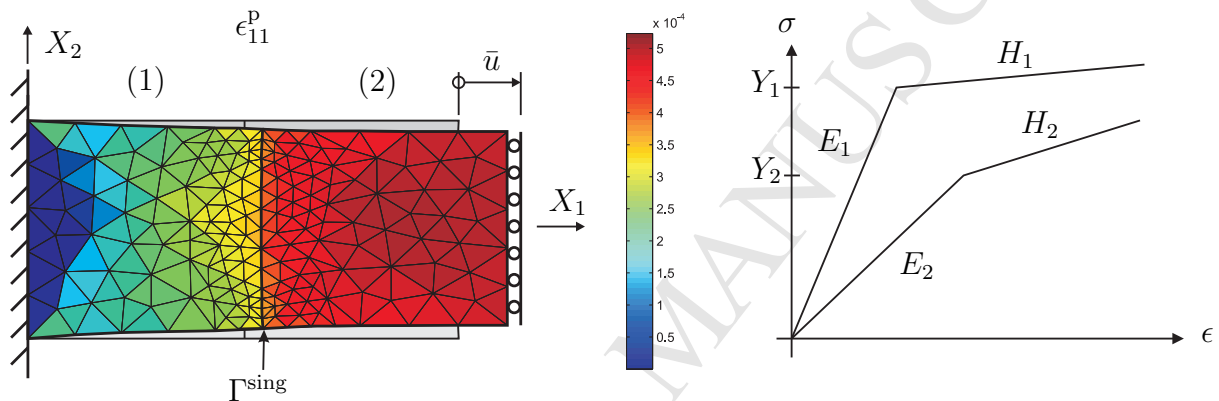


Figure 7: Plate in plane strain with discontinuity in material properties along central interface. (a) Deformed configuration and plastic deformations for $\bar{u}/\bar{u}_{\text{max}} = 1$, (b) Linear elastic-hardening stress-strain response curves.

7.3. Numerical results

The first set of computations were carried out to verify the theoretical result in Subsubsection 6.3.2 that the values of both $\mathcal{G}^{\text{CONF}}$ and \mathcal{G}^{MAT} are independent of the choice of the variation of $\dot{\mathbf{X}}$ under certain conditions. To this end, we considered three different fields $d\dot{\mathbf{X}}_i$, $i = I, II, III$, which all satisfied the condition that $d\dot{\mathbf{X}}_i \cdot \mathbf{N} = 1$ on Γ^{sing} , and that $d\dot{\mathbf{X}}_i \cdot \mathbf{N} = c(\mathbf{X})$ for $\mathbf{X} \in \partial\Omega_X$, where $c(\mathbf{X})$ is a given function. Otherwise, the fields differed from each other only in the interior of Ω_X , as shown in Figure 8. As a consequence, all the requirements discussed in Subsubsection 6.3.2 for satisfying the condition $l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_I - d\dot{\mathbf{X}}_{II}) = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_{II} - d\dot{\mathbf{X}}_{III}) = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_{III} - d\dot{\mathbf{X}}_I) = 0$ in both the left and right part of the singular surface in Figure 7 were satisfied. Indeed, the numerical results verified that the values of $\mathcal{G}^{\text{CONF}}$ and \mathcal{G}^{MAT} were the same for all three fields $d\dot{\mathbf{X}}_i$ in Figure 8.

Next, the mesh (in)sensitivity and convergence properties for mesh refinement were studied for two types of element approximations: linear (CTS) and quadratic (LST) displacement approximation. The results are depicted in Figure 9, and they show that the quadratic element approximation gives superior convergence properties (as expected).

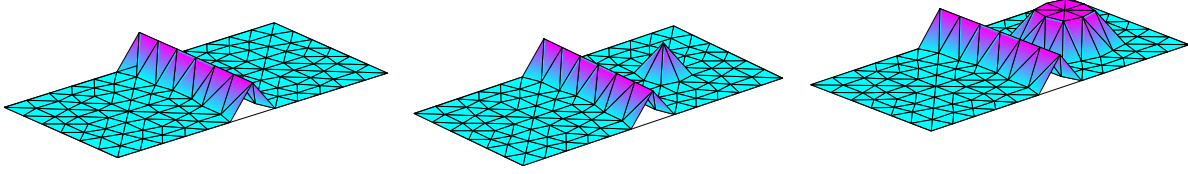


Figure 8: Choice of variations of the field $d\mathbf{X}_i$, $i = I, II, III$. All choices give identical results of the sensitivity \mathbf{v}' .

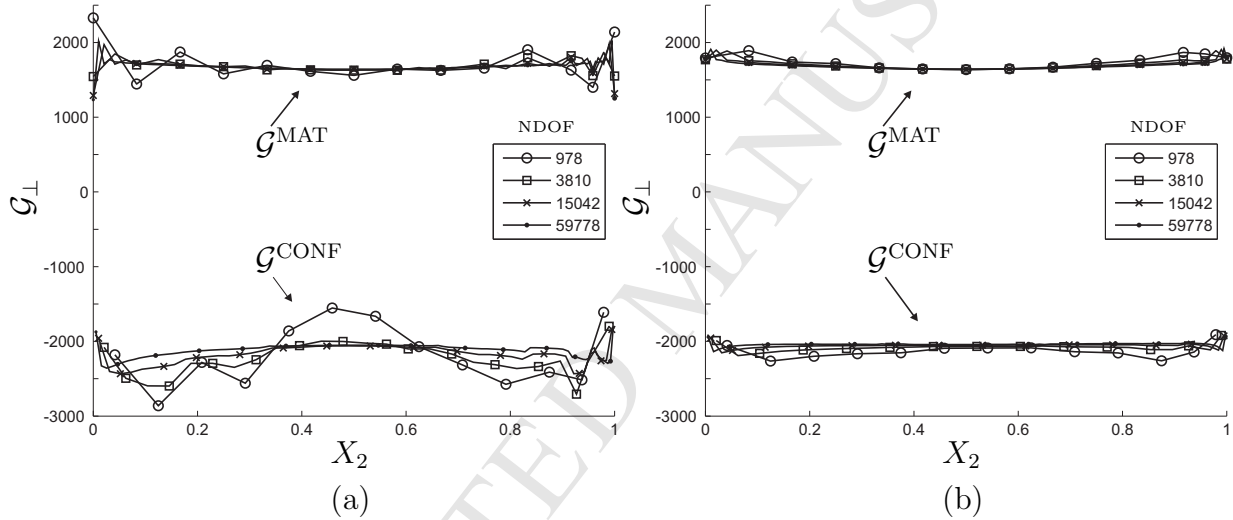


Figure 9: Mesh-sensitivity/convergence of components (fields) $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of the material data: $E_2 = 0.5E_{\text{ref}}$. All results obtained for $\bar{u}/\bar{u}_{\text{max}} = 1$.

The next series of computations concerned the development of $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ with increasing (prescribed) displacement, while it was assumed that there is a mismatch across the interface of the elastic and the plastic (hardening) properties. These results are shown in Figure 10.

In order to further provoke the triaxiality in the stress and strain states, we next considered the case when a circular hole is introduced in the right part of the plate, as shown in Figure 11(a). The base set of material parameter values are still the same as those given in Figure 7(b).

The distribution of components $\mathcal{G}_{\perp}^{\text{CONF}}$, $\mathcal{G}_{\perp}^{\text{MAT}}$ and $\mathcal{G}_{\perp} = \mathcal{G}_{\perp}^{\text{CONF}} + \mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of elasticity, $E_2 = 0.5E_{\text{ref}}$, are shown in Figure 12 for the LST approximation and a mesh that represents a converged state.

The final series of computations concerned the development of $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ with increasing (prescribed) displacement, while it was assumed that there is a mismatch across

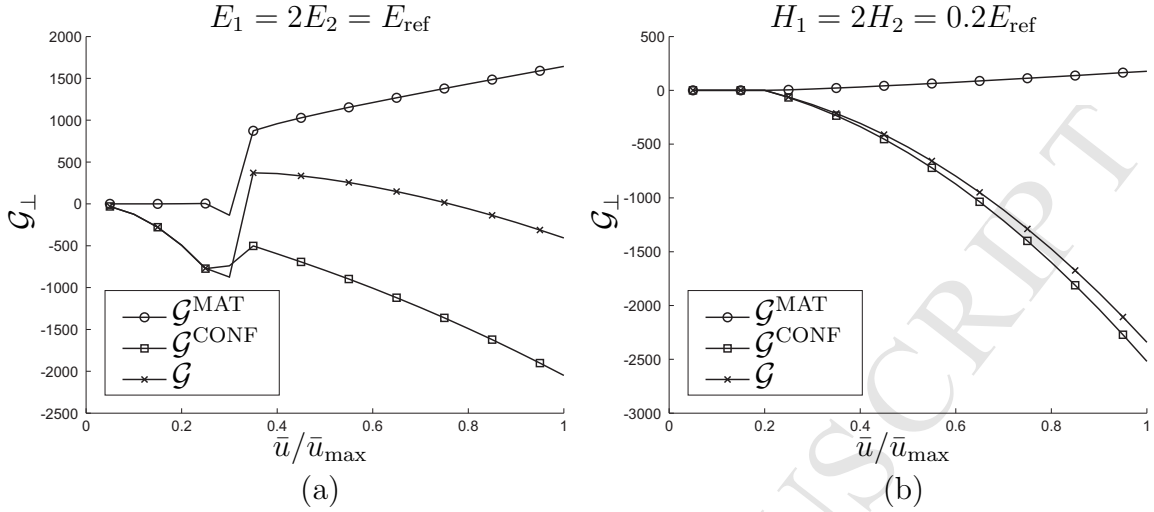


Figure 10: Development of components $\mathcal{G}_\perp^{\text{CONF}}$, $\mathcal{G}_\perp^{\text{MAT}}$ and $\mathcal{G}_\perp = \mathcal{G}_\perp^{\text{CONF}} + \mathcal{G}_\perp^{\text{MAT}}$ with increasing loading (prescribed displacement) for (a) mismatch of elasticity: $E_2 = 0.5E_{\text{ref}}$, and (b) mismatch of hardening: $H_2 = 0.5H_{\text{ref}}$.

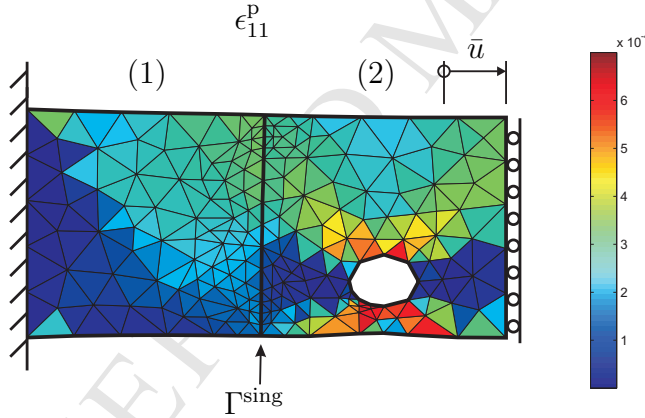


Figure 11: Plate in plane strain with discontinuity in material properties along central interface and with eccentric hole. Deformed configuration and plastic deformations for $\bar{u}/\bar{u}_{\text{max}} = 1$.

the interface of the elastic and the plastic (hardening) properties. These results are shown in Figure 13.

8. Discussion, conclusions and outlook

In this paper we have presented a novel investigation in the context of configurational changes for a rate-independent dissipative material; namely, we considered the *total variation* of the rate of global dissipation with respect to the rate of configurational motion. Such a variation may, alternatively, be considered as the evaluation of the *total sensitivity* due to configurational changes, which may be brought about (in their turn) by physical

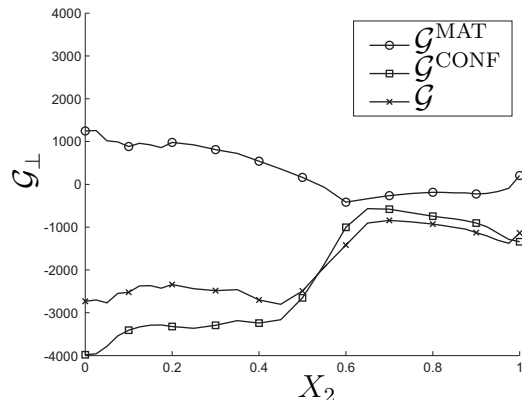


Figure 12: Distribution of components $\mathcal{G}_{\perp}^{\text{CONF}}$, $\mathcal{G}_{\perp}^{\text{MAT}}$ and $\mathcal{G}_{\perp} = \mathcal{G}_{\perp}^{\text{CONF}} + \mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of elasticity: $E_2 = 0.5E_{\text{ref}}$. All results obtained for $\bar{u}/\bar{u}_{\text{max}} = 1$.

changes. It is then clear that the *material part of the dissipation* is indeed coupled (and sensitive) to configurational changes. However, it is not at all clear how to use this information. The classical approach in defining the "driving force" for configurational changes, advocated in the current literature, is to account only for the explicit part of the total configurational force, denoted $\mathcal{G}^{\text{CONF}}$ in this paper. An alternative, perhaps more natural, approach is to assume that the "driving force" for configurational changes is identified precisely by the total sensitivity, which means that the total configurational force \mathcal{G} is the proper choice in constitutive models for configurational changes. Whatever the choice made, it is clearly a model assumption.

The paper discussed essentially two aspects: (1) How to formulate (or construct) the total dissipation in the presence of configurational changes, and (2) how to compute the total sensitivity of the global dissipation via the appropriate formulation of a tangent problem. In the present paper only isothermal (thermomechanically uncoupled) quasistatic problems are considered, which means that the only balance equation for establishing the pertinent tangent problem is the standard equilibrium equation. We remark that we chose to linearize the weak form of equilibrium by observing that the virtual (test) functions are time-invariant in the absolute configuration \mathcal{B}_{ξ} ; however, it would have been possible to linearize the strong format of equilibrium in \mathcal{B}_{ξ} , establish the weak format and, finally, push forward to obtain the tangent problem in \mathcal{B}_X .

A few issues deserve further comments: The tangent stiffness \mathbf{L}_T appearing in the "sensitivity version" of the constitutive continuum tangent relation (61) in the case of plastic loading (L) is not necessarily identical to the actual \mathbf{L}^{ep} for two reasons: (1) the relation (57) represents essentially a nonlinear (bilinear) relation in $D_t \mathbf{F}$, (2) \mathbf{L}_T can be linearized at the *actual* value of $\dot{\mathbf{X}}$ or at $\dot{\mathbf{X}} = \mathbf{0}$ corresponding to a stationary singular surface. If we choose the actual value of $\dot{\mathbf{X}}$ it is obvious that \mathcal{G}^{MAT} depends on the solution to the physical motion problem at each point in time. Hence, if indeed \mathcal{G}^{MAT} is part of the "driving force", then the computation of the sensitivity problem is nonlinear and can only be carried out for a given field $\dot{\mathbf{X}}$ as part of an iteration process to compute the actual

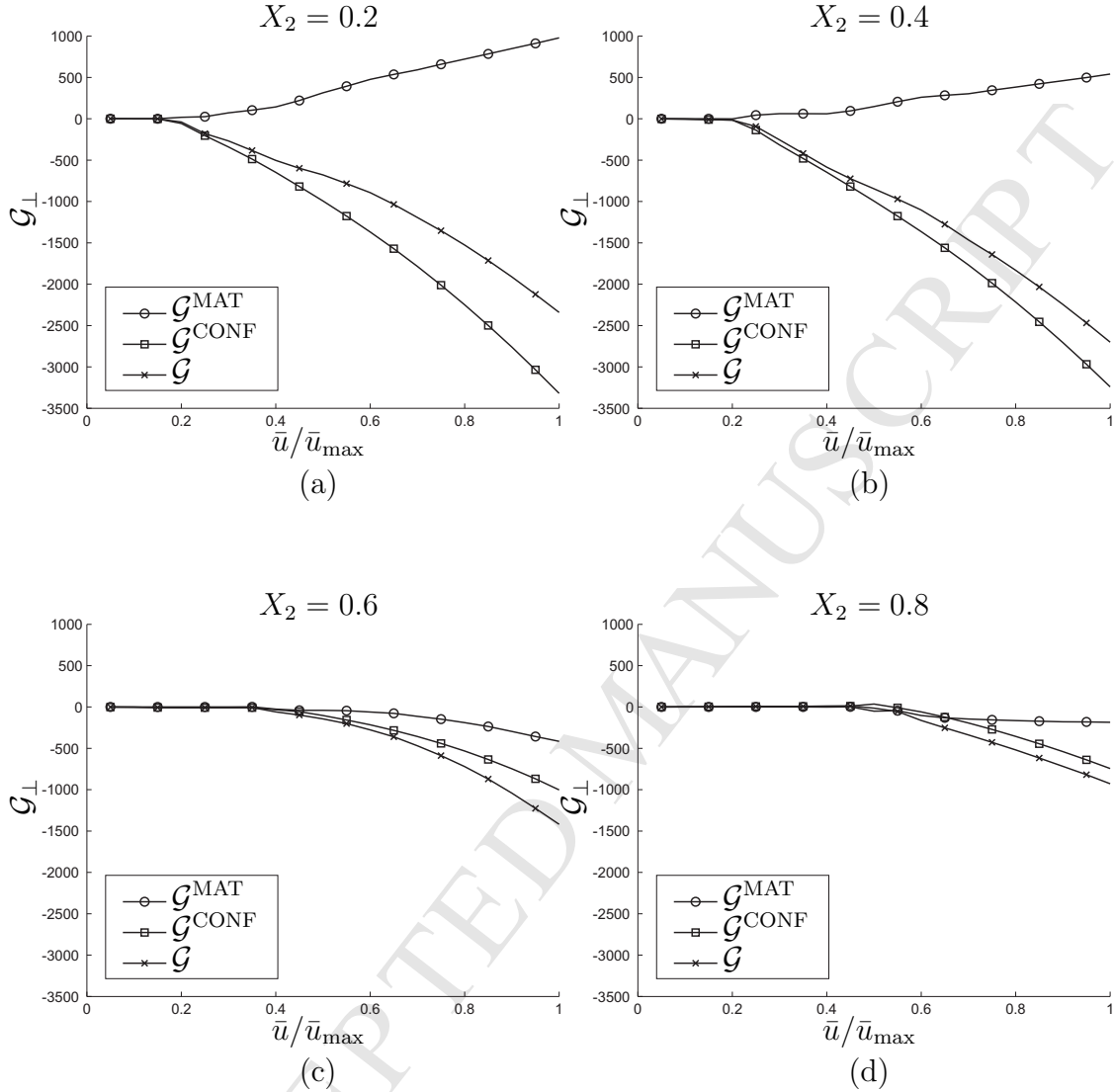


Figure 13: Development of components $\mathcal{G}_\perp^{\text{CONF}}$, $\mathcal{G}_\perp^{\text{MAT}}$ and $\mathcal{G}_\perp = \mathcal{G}_\perp^{\text{CONF}} + \mathcal{G}_\perp^{\text{MAT}}$ with increasing loading (prescribed displacement) for mismatch of hardening: $H_2 = 0.5H_{\text{ref}}$. Results are given for different positions across the interface: (a) $X_2 = 0.2$, (a) $X_2 = 0.4$, (a) $X_2 = 0.6$, (a) $X_2 = 0.8$.

field $\dot{\mathbf{X}}$.

It was shown theoretically that the variation $d\dot{\mathbf{X}}$ can be chosen arbitrarily in the interior of the material domain $\Omega_{\mathbf{X}}$ without affecting the value of \mathcal{G}^{MAT} , as long as certain conditions on the external boundary and the singular interface are satisfied. This was confirmed by numerical results for selected choices of $d\dot{\mathbf{X}}$. For uniform cross-section of the investigated plate, a separate parameter study (not discussed explicitly in the paper) showed, in the case $\nu \rightarrow 0$, that $\mathcal{G}_\perp^{\text{MAT}}$ converges to the value that is obtained for uniaxial stress (which confirms the soundness of the numerical evaluation). The numerical results obtained for dissimilar material properties across the singular surface showed that a misfit

in the elasticity modulus resulted in larger value of $\mathcal{G}_\perp^{\text{MAT}}$ than did a misfit in the hardening modulus.

Although it follows from the local (strong) version of dissipation inequality that $\bar{\mathcal{D}}(\dot{\underline{k}}) \geq 0$ must always hold, it is possible that the corresponding sensitivity to configurational changes becomes non-positive, i.e. $\bar{\mathcal{D}}^{\text{MAT}}(\text{d}\dot{\underline{X}}, \dot{\underline{k}}\{\dot{\underline{X}}; \text{d}\dot{\underline{X}}\}) \leq 0$ is certainly possible. An example of this situation is given in Figure 13 for the two last cross-sections (for the plate with a hole), where it appears that $\mathcal{G}_\perp^{\text{MAT}} \leq 0$.

Whenever in doubt, we checked the results by numerical differentiation. This is doable since we are interested in the total variation of the global dissipation (and not only a partial variation corresponding to $\mathcal{G}^{\text{CONF}}$). As to the practical calculation of the configurational force, it appears that the classical configurational rate, $\mathcal{G}^{\text{CONF}}$, is *spatially localized a priori* to a singular surface by the analytical expression. On the other hand, the material rate of dissipation, \mathcal{G}^{MAT} , is *spatially localizable a posteriori* via a suitable parametrization and least squares projection (in practice) on the FE-shape functions.

Finally, we mention some possible future developments. The total configurational force \mathcal{G} will be exploited as the "driving force" in a crack-propagation model for fatigue cracks in railway steel under complex loading. As to the efficient computation of global dissipation for the mesh-parametrized material motion, it is possible to use a so-called "dual" method, whereby only one single dual solution is needed even if there are a multitude of nodal values \mathcal{G}_i to compute, cf. the sensitivity problem in the context of parameter identification discussed by Johansson et al. (2007).

9. Acknowledgements

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A. Appendix

A.1. Tangent problem – Format based on $\dot{\mathbf{x}}$

The derivations leading to (70) with (71) and (72) are outlined as follows: From the definition of $a(\mathbf{x}, \underline{k}; \delta \mathbf{x})$ in (64), together with the identity in (13), we derive

$$\begin{aligned} \frac{\text{d}}{\text{d}t} a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) &= \int_{\Omega_{\mathbf{x}}} [\Delta_t[\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \mathbf{P} + [\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \Delta_t \mathbf{P} + \\ &\quad [\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \mathbf{P} \otimes \dot{\underline{X}} \cdot \nabla_{\mathbf{x}}] \text{d}V_{\mathbf{x}} \end{aligned} \quad (1)$$

Upon using the relations

$$\begin{aligned} \Delta_t \mathbf{P} &= \text{D}_t \mathbf{P} + [\mathbf{P} \otimes \nabla_{\mathbf{x}}] \cdot \dot{\underline{X}} \\ &= \text{D}_t \mathbf{P} + [\mathbf{L}^e : [\mathbf{F} \otimes \nabla_{\mathbf{x}}] + \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_{\mathbf{x}}] + \frac{\partial \mathbf{P}}{\partial \underline{\mathbf{X}}} \Big|_{\mathbf{F}, \underline{k}} \cdot \dot{\underline{X}} \end{aligned} \quad (2)$$

together with (68), we may reformulate this expression in (1) as

$$\begin{aligned} \frac{d}{dt}a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) &= \int_{\Omega_X} \left[[\delta \mathbf{x} \otimes \nabla_X] : D_t \mathbf{P} - [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} : [\dot{\mathbf{X}} \otimes \nabla_X] \right. \\ &\quad \left. + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{L}^e : [\mathbf{F} \otimes \nabla_X] + \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_X] + \frac{\partial \mathbf{P}}{\partial \mathbf{X}}|_{F, \underline{k}} \cdot \dot{\mathbf{X}}] \right] dV_X \end{aligned} \quad (3)$$

Now, taking the total variation of (3) w.r.t. $\dot{\mathbf{X}}$, while using the tangent relation (60) expressed explicitly as

$$(D_t \mathbf{P})' = \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X - [\mathbf{F} \cdot d\dot{\mathbf{X}}] \otimes \nabla_X] \quad (4)$$

we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt}a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) \right] &= \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X] dV_X \\ &\quad - \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : [d\dot{\mathbf{X}} \otimes \nabla_X] + \mathbf{L}_T : [\mathbf{F} \cdot [d\dot{\mathbf{X}} \otimes \nabla_X]] \right. \\ &\quad \left. + \mathbf{r}_X \cdot d\dot{\mathbf{X}} \right] dV_X \end{aligned} \quad (5)$$

Next, from the definition of $l(\delta \mathbf{x})$ in (65) together with (13) and (15), we derive

$$\begin{aligned} \frac{d}{dt}l(\delta \mathbf{x}) &= \int_{\Omega_X} D_t[\delta \mathbf{x} \cdot \mathbf{b}_X] dV_X + \int_{\partial \Omega_X} [\delta \mathbf{x} \cdot \mathbf{b}_X] \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{\partial \Omega_{X,N}} [\hat{D}_t[\delta \mathbf{x} \cdot \mathbf{t}_X] - k[\delta \mathbf{x} \cdot \mathbf{t}_X] \dot{\mathbf{X}} \cdot \mathbf{N}] dS_X \\ &\quad + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_X \end{aligned} \quad (6)$$

where we used that $\delta \mathbf{x}$ and $\dot{\mathbf{X}}$ are continuous on $\partial \Omega_X$, in particular across \mathcal{C}_X .

In order to obtain operational expressions, we note the relations

$$D_t[\delta \mathbf{x} \cdot \mathbf{b}_X] = D_t[\delta \mathbf{x}] \cdot \mathbf{b}_X + \delta \mathbf{x} \cdot D_t \mathbf{b}_X = -[\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes \dot{\mathbf{X}}] + \delta \mathbf{x} \cdot D_t \mathbf{b}_X \quad \text{in } \Omega_X \quad (7)$$

$$\hat{D}_t[\delta \mathbf{x} \cdot \mathbf{t}_X] = \hat{D}_t[\delta \mathbf{x}] \cdot \mathbf{t}_X + \delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X = -[\delta \mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes \dot{\mathbf{X}}] + \delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X \quad \text{on } \partial \Omega_X \quad (8)$$

where we used the relations (4), (9) and (68), which may be inserted into (6) to give

$$\begin{aligned} \frac{d}{dt}l(\delta \mathbf{x}) &= \int_{\Omega_X} \left[\delta \mathbf{x} \cdot D_t \mathbf{b}_X - [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes \dot{\mathbf{X}}] \right] dV_X \\ &\quad + \int_{\partial \Omega_X} \left[\delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X - [\delta \mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes \dot{\mathbf{X}}] \right] dS_X \\ &\quad + \int_{\partial \Omega_X} [[\delta \mathbf{x} \cdot \mathbf{b}_X] - k[\delta \mathbf{x} \cdot \mathbf{t}_X]] \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_X \end{aligned} \quad (9)$$

Upon taking the total variation of (9) w.r.t. $\dot{\mathbf{X}}$, while assuming that \mathbf{b}_X , \mathbf{t}_X , $D_t\mathbf{b}_X$ and $\hat{D}_t\mathbf{t}_X$ are independent on $\dot{\mathbf{X}}$, i.e.

$$\mathbf{b}'_X = \mathbf{t}'_X = (D_t\mathbf{b}_X)' = (\hat{D}_t\mathbf{t}_X)' = \mathbf{0} \quad (10)$$

we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} l(\delta\mathbf{x}) \right] &= - \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes d\dot{\mathbf{X}}] dV_X \\ &\quad - \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes d\dot{\mathbf{X}}] dS_X \\ &\quad + \int_{\partial\Omega_X} [[\delta\mathbf{x} \cdot \mathbf{b}_X] - k[\delta\mathbf{x} \cdot \mathbf{t}_X]] d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{c_X} \delta\mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (11)$$

Remark: Assuming that $\hat{D}_t\mathbf{t}_X$ does not depend on $\dot{\mathbf{X}}$ pertains to the assumption that \mathbf{t}_X is defined only on $\partial\Omega_X$. \square

Finally, upon using (5) and (11), we may rephrase (70) as

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (12)$$

where the tangent forms a_T and $l_T^{(\dot{\mathbf{x}})}$ are given in (72) and (73), respectively.

A.2. Tangent problem – Format based on \mathbf{v}

The derivations leading to (76) with (77) are outlined as follows: From the definition of $a(\mathbf{x}, \underline{k}; \delta\mathbf{x})$ in (64), together with the identity in (13), we derive

$$\begin{aligned} \frac{d}{dt} a(\mathbf{x}, \underline{k}; \delta\mathbf{x}) &= \int_{\Omega_X} [[D_t[\delta\mathbf{x}] \otimes \nabla_X] : \mathbf{P} + [\delta\mathbf{x} \otimes \nabla_X] : D_t\mathbf{P}] dV_X \\ &\quad + \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{P} \otimes \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (13)$$

where we used the relation $D_t[\delta\mathbf{x} \otimes \nabla_X] = D_t[\delta\mathbf{x}] \otimes \nabla_X$.

Taking the total variation of (13) w.r.t. $\dot{\mathbf{X}}$, while using the tangent relation (60), we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} a(\mathbf{x}, \underline{k}; \delta\mathbf{x}) \right] &= \int_{\Omega_X} [[(D_t[\delta\mathbf{x}])' \otimes \nabla_X] : \mathbf{P} + [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\mathbf{v}' \otimes \nabla_X]] dV_X \\ &\quad + \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{P} \otimes d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (14)$$

As to the time-derivative of $l(\delta\mathbf{x})$, the expression (6) is taken as the point of departure. While the decomposition of $D_t[\delta\mathbf{x} \cdot \mathbf{b}_X]$ in (7) is retained, we shall use the following decomposition of $\hat{D}_t[\delta\mathbf{x} \cdot \mathbf{t}_X]$, instead of (8):

$$\hat{D}_t[\delta\mathbf{x} \cdot \mathbf{t}_X] = D_t[\delta\mathbf{x}] \cdot \mathbf{t}_X + [\delta\mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}] \dot{\mathbf{X}} \cdot \mathbf{N} + \delta\mathbf{x} \cdot \hat{D}_t\mathbf{t}_X \quad (15)$$

where we used the relation (10) to replace $\hat{D}_t[\delta\mathbf{x}]$ by $D_t[\delta\mathbf{x}] + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] \cdot \mathbf{N}[\dot{\mathbf{X}} \cdot \mathbf{N}]$. Upon introducing the relations (13) and (15) in (6), we obtain

$$\begin{aligned} \frac{d}{dt}l(\delta\mathbf{x}) &= \int_{\Omega_{\mathbf{X}}} [\delta\mathbf{x} \cdot D_t\mathbf{b}_{\mathbf{X}} + D_t[\delta\mathbf{x}] \cdot \mathbf{b}_{\mathbf{X}}] dV_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} \left[\delta\mathbf{x} \cdot \hat{D}_t\mathbf{t}_{\mathbf{X}} + D_t[\delta\mathbf{x}] \cdot \mathbf{t}_{\mathbf{X}} + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] : [\mathbf{t}_{\mathbf{X}} \otimes \mathbf{N}]\dot{\mathbf{X}} \cdot \mathbf{N} \right] dS_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} [\delta\mathbf{x} \cdot \mathbf{b}_{\mathbf{X}} - k[\delta\mathbf{x} \cdot \mathbf{t}_{\mathbf{X}}]] \dot{\mathbf{X}} \cdot \mathbf{N} dS_{\mathbf{X}} \\ &+ \int_{\mathcal{C}_{\mathbf{X}}} \delta\mathbf{x} \cdot [\mathbf{t}_{\mathbf{X}}^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_{\mathbf{X}}^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_{\mathbf{X}} \end{aligned} \quad (16)$$

Again, upon taking the total variation of (16) w.r.t. $\dot{\mathbf{X}}$, while assuming that $\mathbf{b}_{\mathbf{X}}$, $\mathbf{t}_{\mathbf{X}}$, $D_t\mathbf{b}_{\mathbf{X}}$ and $\hat{D}_t\mathbf{t}_{\mathbf{X}}$ are independent on $\dot{\mathbf{X}}$, i.e. (10) holds, then we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt}l(\delta\mathbf{x}) \right] &= \int_{\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{b}_{\mathbf{X}} dV_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} \left[(D_t[\delta\mathbf{x}])' \cdot \mathbf{t}_{\mathbf{X}} + [\delta\mathbf{x} \cdot \mathbf{b}_{\mathbf{X}} - k[\delta\mathbf{x} \cdot \mathbf{t}_{\mathbf{X}}] + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] : [\mathbf{t}_{\mathbf{X}} \otimes \mathbf{N}]] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dV_{\mathbf{X}} \\ &+ \int_{\mathcal{C}_{\mathbf{X}}} \delta\mathbf{x} \cdot [\mathbf{t}_{\mathbf{X}}^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_{\mathbf{X}}^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_{\mathbf{X}} \end{aligned} \quad (17)$$

Finally, upon using the divergence theorem to note that

$$\int_{\Omega_{\mathbf{X}}} [(D_t[\delta\mathbf{x}])' \otimes \nabla_{\mathbf{X}}] : \mathbf{P} dV_{\mathbf{X}} = \int_{\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{b}_{\mathbf{X}} dV_{\mathbf{X}} + \int_{\partial\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{t}_{\mathbf{X}} dS_{\mathbf{X}}, \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (18)$$

we may use (14) and (17) together with (69) to arrive at

$$a_{\mathbf{T}}(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_{\mathbf{T}}^{(v)}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (19)$$

where the tangent forms $a_{\mathbf{T}}$ and $l_{\mathbf{T}}^{(v)}$ are given in (71) and (76).

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On the Sensitivity of the Rate of Global Energy Dissipation due to Configurational Changes

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Abstract

The thermodynamic framework for combined configurational and deformational changes was recently discussed by Runesson et al. (2008). One key ingredient in this setting is the (fixed) absolute configuration, relative to which both physical and virtual (variational) changes of the material and spatial configurations can be described. In the present paper we consider dissipative material response and emphasize the fact that it is possible to identify *explicit* energetic changes due to configurational changes for "frozen" spatial configuration (a classical view) and the *configuration-induced* material dissipation. The classical assumption (previously adopted in the literature) is to ignore this dissipation, i.e. the internal variables are considered as fixed fields in the material configuration. In this paper, however, we define configurational forces by considering the *total variation* of the total dissipation with respect to configurational changes. The key task is then to compute the *sensitivity* of the internal variable rates to such configurational changes, which results in a global tangent problem based on the balance equations (momentum and energy) for a given body. In this paper we restrict to quasistatic loading under isothermal conditions and for elastic-plastic response, and we apply the modeling to the case of a moving interface of dissimilar materials.

1. Introduction

The notion of configurational changes refers basically to the motion of "property surfaces", that are either internal to a given finite body or identical to (some part of) the external boundary. An important class is defined by the motion/evolution of "singular surfaces" representing discontinuities (or defects) in the material properties and, consequently, in the state variables when the body is loaded. Typical examples of internal processes are the evolution of defects, phase transformation (microstructural changes that are mostly accompanied by change of volume and mechanical properties), and internal cracks. Typical boundary processes are the evolution of surface (biological) growth and surface cracks. Crack propagation may in this context be seen as a degenerated boundary motion.

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Since the literature on configurational mechanics is very rich, we do not intend to give a comprehensive account. We only mention the pioneering work by Eshelby (1951) and the contributions by Abeyaratne and Knowles (1990), Maugin (1993, 1995, 1997, 1998a,b, 1999), Maugin and Trimarco (1992, 1995), Gurtin (1995, 2000), and Kienzler and Herrmann (2000). Some of these works also contain comprehensive overviews with a discussion of various aspects of configurational mechanics ("material" mechanics in Maugin's terminology). As to the physical motivation, a major application is the "driving force" on singular surfaces. In the seminal contributions by Gurtin (1995, 2000), balance equations for interfaces are derived from a non-standard (material) observer invariance argument with strong relations to the celebrated NOETHER'S theorem, Noether (1918). The effects of configurational changes of surfaces in terms of physical properties intrinsically attached to the surfaces (e.g. energy) have been addressed by, among others, Gurtin and Murdoch (1975); Gurtin and Struthers (1990), Simha and Bhattacharya (1998). A recent comprehensive treatment of "surface energies" is given by Steinmann (2008). Indeed, it appears that there is a strong link to the analysis in this paper on "sensitivity".

The concept of "configurational forces" has been exploited extensively in recent years in computational fracture mechanics, cf. Steinmann (2000); Steinmann et al. (2001); Steinmann (2002b,a); Menzel et al. (2004); Steinmann (2008), Fagerström and Larsson (2008). The suggestion in Steinmann et al. (2001) to compute the crack-driving force based on the concept of "nodal material forces" generalized, in fact, the domain integral format suggested previously by Li et al. (1985). A posteriori error control and adaptivity of the J-integral in its different equivalent formats were investigated by Heintz et al. (2004). A recent paper by Guerses and Miehe (2008), which is closely related to the present paper concerning the thermodynamic setting, addresses r -adaptive remeshing for a propagating crack.

Most studies so far are explicitly confined to elastic material response. While the state of affairs seems to be quite clear in this case, it is not so in the case (local) material dissipation occurs as a result of the configurational change in addition to the energy release from a propagating crack. The formulation of the crack-driving force in such a case and the computational aspects have been discussed by Maugin and Trimarco (1992), Simha et al. (2003), Simha et al. (2008), Liebe et al. (2003), Menzel et al. (1995), Nguyen et al. (2005). However, there seems to be a lack of consensus as to the appropriate basic formulation.

In this contribution we aim at shedding some further light on the energetic consequences of configurational changes for rate-independent dissipative material response. We focus on the dissipation of mechanical energy of a given finite body that is undergoing configurational changes in conjunction with (or as a result of) mechanical loading. More specifically, we put forward the idea that it is the *total variation* of the appropriately defined dissipation functional for the whole body that represents the "driving force" for the physical process that is described by configurational changes¹. However, which definition

¹This choice has distinct advantages; one being that it is possible to check analytical results by comparison with numerical perturbations of the functional.

of the driving force to use is basically a matter of modeling, although the choice is strongly guided by thermodynamics considerations.

In order to increase clarity in the variational framework, we adopt a description that allows for the combined configurational (material) and deformational (spatial) motions. To this end we first introduce an auxiliary (fictitious) reference configuration that is *fixed* in space; in particular, its *boundary is fixed* and thus defines a time-invariant domain under (possible) configurational and deformational changes. It is important to note that the introduction of such an absolute reference configuration *does not* simply mean a change of computational domain (associated with a change of coordinates). As a special case, we may choose this referential domain to be the current configuration (the Eulerian view), which corresponds to the study of the "inverse motion", and this approach is common in the literature on configurational forces (crack-driving force) within the context of singular cracks, e.g. Steinmann (2000). With such a choice, however, the combined action of configurational and material changes is never revealed.

The paper is organized as follows: Section 2 introduces definitions and preliminaries related to the unified representation of configurational (material) and deformational (spatial) motions in terms of an absolute reference configuration. A generic balance law is established in Section 3, whereby "configurational flux" across the boundary is allowed, and it is applied to the mechanical dissipation inequality. In Section 4, we establish the pertinent dissipation functional due to imposed configurational changes while assuming rather general constitutive response based on the presence of internal variables in the free energy. In Section 5, we define generalized configurational forces from the "total variation of the global dissipation", which is the main novel result of the paper. This result is applied, and further specified, in Section 6 to a material singular surface. Explicit computational results are given in Section 7 for a non-homogeneous plate with dissimilar elastic-plastic material properties. Finally, conclusions and an outlook to future developments are given in Section 8.

2. Representation of configurational and deformational motions

2.1. Preliminaries

We first note that the spatial (deformational or direct) motion problem (SMP) is expressed in terms of a spatial motion map $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X}, t)$, $\mathcal{B}_X \mapsto \mathcal{B}_x(t)$, such that the reference position of the material particles, \boldsymbol{X} , in the fixed (time-invariant) *material* configuration \mathcal{B}_X , are mapped onto the *deformed* position, \boldsymbol{x} , in the *spatial* configuration $\mathcal{B}_x(t)$. It is emphasized that $\mathcal{B}_X = \mathcal{B}_x(0)$ is the actual configuration of the body at $t = 0$ in the classical setting.

In this paper, we generalize the classical view of motion slightly, cf. Figure 1, since the material configuration is allowed to change with time in the sense that the boundary $\partial\mathcal{B}_X$ of the body \mathcal{B}_X may change with time. It is important to note that this case also embodies the case of an evolving internal singular surface, since it is possible to view the two parts separated by the singular surface as changing configurations. It is then convenient to take the view that both the "undeformed" (material) and "deformed" (spatial) configurations

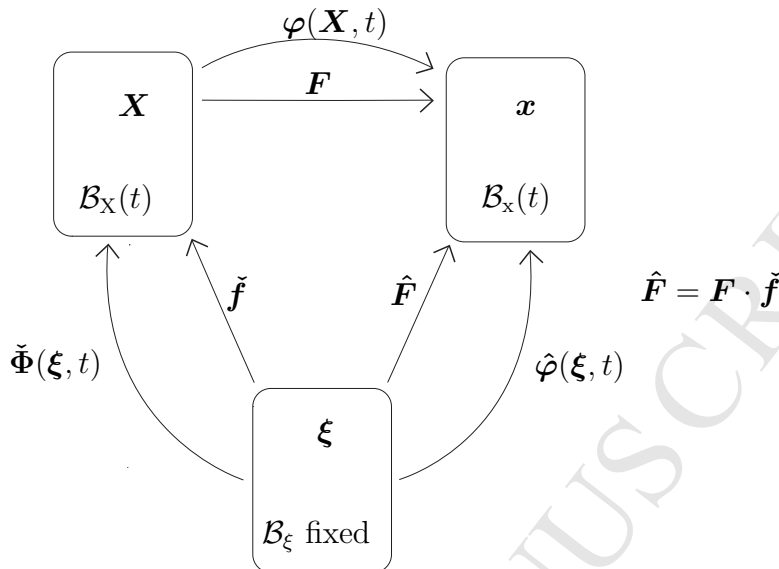


Figure 1: *Spatial (current) configuration, $\mathcal{B}_x(t)$, material configuration, $\mathcal{B}_X(t)$, and absolute (fixed) configuration, \mathcal{B}_ξ .*

will undergo time-dependent changes with respect to an *absolute* (fixed, time-invariant) configuration \mathcal{B}_ξ . We may then introduce the map $\mathbf{X} = \check{\Phi}(\boldsymbol{\xi}, t)$ for the time-dependent "motion" of $\mathcal{B}_X(t)$ w.r.t. \mathcal{B}_ξ , and we introduce the *absolute* spatial motion map $\mathbf{x} = \hat{\varphi}(\boldsymbol{\xi}, t)$ for the time-dependent motion (including deformation) of $\mathcal{B}_x(t)$ w.r.t. \mathcal{B}_ξ . It is clear that $\hat{\varphi}(\boldsymbol{\xi}, t), \mathcal{B}_\xi \mapsto \mathcal{B}_x(t)$, represents the composite map $\hat{\varphi}(\boldsymbol{\xi}, t) \stackrel{\text{def}}{=} (\varphi \circ \check{\Phi})(\boldsymbol{\xi}, t)$. We may introduce the convenient *assumption* that $\mathcal{B}_\xi = \mathcal{B}_X(0) = \mathcal{B}_x(0)$.

The gradients corresponding to the introduced mappings (see also Figure 1) are the spatial motion gradient $\mathbf{F} \stackrel{\text{def}}{=} \varphi \otimes \nabla_X$, the *absolute* spatial motion gradient $\hat{\mathbf{F}} \stackrel{\text{def}}{=} \hat{\varphi} \otimes \nabla_\xi$, and the absolute material motion gradient $\check{\mathbf{f}} \stackrel{\text{def}}{=} \check{\Phi} \otimes \nabla_\xi$ ². Upon using the chain rule, we obtain the relation $\hat{\mathbf{F}} = \mathbf{F} \cdot \check{\mathbf{f}}$. We shall also frequently use the determinant $\check{j} = \det \check{\mathbf{f}}$, which is relevant both for the volume mapping³ $dV_X = \check{j} dV_\xi$ and for the area mapping $dS_X = \check{j} \sqrt{\mathbf{N}_\xi \cdot \check{\mathbf{f}}^{-1} \cdot \check{\mathbf{f}}^{-T} \cdot \mathbf{N}_\xi} dS_\xi$ when the computational domain is changed from \mathcal{B}_X to \mathcal{B}_ξ .

2.2. Absolute and material time differentiation

We shall introduce absolute and material time derivatives of a field f , parametrized in \mathcal{B}_X or \mathcal{B}_ξ , as follows:

$$\Delta_t f \stackrel{\text{def}}{=} \partial_t f|_\xi, \quad D_t f \stackrel{\text{def}}{=} \partial_t f|_X \quad (1)$$

²The gradient vectors ∇_ξ and ∇_X refer to coordinates in \mathcal{B}_ξ and \mathcal{B}_X , respectively.

³ \mathbf{N}_ξ is the unit normal vector on $\partial\mathcal{B}_\xi$ resulting from a pullback of the unit normal $\mathbf{N}(= \mathbf{N}_X)$ from $\partial\mathcal{B}_X$.

where $\partial_t[\bullet] \stackrel{\text{def}}{=} \partial[\bullet]/\partial t$ denotes the ordinary partial time derivative. In particular, the material velocity, \mathbf{v} , the *absolute* velocity, $\dot{\mathbf{x}}$, and the (absolute) configurational rate, $\dot{\mathbf{X}}$, are defined as

$$\mathbf{v} \stackrel{\text{def}}{=} D_t \mathbf{x} = \partial_t \boldsymbol{\varphi}(\mathbf{X}, t), \quad \dot{\mathbf{x}} \stackrel{\text{def}}{=} \Delta_t \mathbf{x} = \partial_t \hat{\boldsymbol{\varphi}}(\boldsymbol{\xi}, t), \quad \dot{\mathbf{X}} \stackrel{\text{def}}{=} \Delta_t \mathbf{X} = \partial_t \check{\boldsymbol{\Phi}}(\boldsymbol{\xi}, t) \quad (2)$$

However, using the chain rule to differentiate the composite function $\hat{\boldsymbol{\varphi}}(\boldsymbol{\xi}, t) \stackrel{\text{def}}{=} (\boldsymbol{\varphi} \circ \check{\boldsymbol{\Phi}})(\boldsymbol{\xi}, t)$, we obtain the relation

$$\mathbf{v} = \dot{\mathbf{x}} - \mathbf{F} \cdot \dot{\mathbf{X}} \quad (3)$$

where the definitions in (1) were used.

We shall later make use of the absolute and material time derivatives of a (tensor-valued) *operator* field $y(\mathbf{X}(\boldsymbol{\xi}, t), \mathbf{x}(\boldsymbol{\xi}, t), \alpha_1(\boldsymbol{\xi}, t), \alpha_2(\boldsymbol{\xi}, t), \dots, t)$ or, for the sake of brevity, $y(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$ ⁴⁵. Let us first consider a volume-specific field, $y(\bullet, t)$ for $\mathbf{X} \in \mathcal{B}_X(t)$, for which the relation between the absolute and material time derivatives can be computed as

$$D_t y(\bullet, t) = \Delta_t y(\bullet, t) - [y(\bullet, t) \otimes \nabla_X] \cdot \dot{\mathbf{X}} \quad (4)$$

The total and material time derivatives of a few selected fields, $\check{\mathbf{f}}(\mathbf{X})$ and $\check{\mathbf{j}}(\mathbf{X})$, are given as follows:

$$\Delta_t \check{\mathbf{f}} = [\dot{\mathbf{X}} \otimes \nabla_X] \cdot \check{\mathbf{f}}, \quad \Delta_t \check{\mathbf{j}} = \check{\mathbf{j}} \dot{\mathbf{X}} \cdot \nabla_X \quad (5)$$

In particular, we obtain

$$\Delta_t (dV_X) = \check{\mathbf{j}} \dot{\mathbf{X}} \cdot \nabla_X dV_\xi = \dot{\mathbf{X}} \cdot \nabla_X dV_X \quad (6)$$

We may also compute the absolute and material time derivatives of $\mathbf{F}(\mathbf{X}, \mathbf{x})$ as

$$\Delta_t \mathbf{F} = -\mathbf{F} \cdot [\dot{\mathbf{X}} \otimes \nabla_X] + \dot{\mathbf{x}} \otimes \nabla_X \quad (7)$$

$$D_t \mathbf{F} = \mathbf{v} \otimes \nabla_X = -[\mathbf{F} \cdot \dot{\mathbf{X}}] \otimes \nabla_X + \dot{\mathbf{x}} \otimes \nabla_X. \quad (8)$$

Next, we consider a surface-specific field, $\hat{y}(\bullet, t)$ for $\mathbf{X} \in \partial \mathcal{B}_X(t)$, for which the absolute time-derivative is given as for the volume-specific field. The reason is that $\partial \mathcal{B}_\xi$ is fixed (stationary). However, the relation between the absolute and *surface-specific material* time-derivatives is given as

$$\hat{D}_t \hat{y}(\bullet, t) \stackrel{\text{def}}{=} \Delta_t \hat{y}(\bullet, t) - [\hat{y}(\bullet, t) \otimes \hat{\nabla}_X] \cdot \dot{\mathbf{X}} \quad (9)$$

where we introduced the surface gradient operator $\hat{\nabla}_X \stackrel{\text{def}}{=} \nabla_X \cdot \hat{\mathbf{I}}$ with the surface-specific identity tensor $\hat{\mathbf{I}} \stackrel{\text{def}}{=} \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$. We may combine the relations (4) and (9) to obtain the useful result

$$\hat{D}_t \hat{y}(\bullet, t) = D_t \hat{y}(\bullet, t) + [\hat{y}(\bullet, t) \otimes \nabla_X] \cdot \mathbf{N} \otimes \dot{\mathbf{X}} \cdot \mathbf{N} \quad (10)$$

⁴An example is the deformation gradient $\mathbf{F}(\mathbf{X}, \mathbf{x}) = \mathbf{x} \otimes \nabla_X$.

⁵The column vector $\underline{\alpha}$ contains the set of fields α_i , which may have different tensorial character.

for $\dot{\mathbf{X}} \in \partial\mathcal{B}_X$. This relation is used in the Appendix to establish the so-called "tangent problem".

Corresponding to (6), we obtain

$$\Delta_t(dS_X) = \check{j} \sqrt{\mathbf{N}_\xi \cdot \check{\mathbf{f}}^{-1} \cdot \check{\mathbf{f}}^{-T} \cdot \mathbf{N}_\xi} \dot{\mathbf{X}} \cdot \hat{\nabla}_X dS_\xi = \dot{\mathbf{X}} \cdot \hat{\nabla}_X dS_X \quad (11)$$

2.3. Conservation laws

2.3.1. Time-derivative of volume integral

Subsequently we shall establish the time derivative of suitably defined conservation quantities. To this end, suppose that $f_X(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$, for $\mathbf{X} \in \mathcal{B}_X(t)$, is a volume-specific quantity. Now, consider a typical conservation quantity F

$$F \stackrel{\text{def}}{=} \int_{\mathcal{B}_X} f_X dV_X \quad (12)$$

The time-derivative of F , for time-dependent \mathcal{B}_X , is then given as

$$\begin{aligned} \frac{d}{dt} F &= \int_{\mathcal{B}_X} \left[\Delta_t f_X + f_X \dot{\mathbf{X}} \cdot \nabla_X \right] dV_X \\ &= \int_{\mathcal{B}_X} \left[D_t f_X + \left[f_X \dot{\mathbf{X}} \right] \cdot \nabla_X \right] dV_X = \int_{\mathcal{B}_X} D_t f_X dV_X + \int_{\partial\mathcal{B}_X} f_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (13)$$

In order to derive (13), we first performed a pull-back of the integration domain from the time-dependent $\mathcal{B}_X(t)$ ⁶ to \mathcal{B}_ξ , while using the relation $dV_X = \check{j} dV_\xi$ with the Jacobian (volume ratio) $\check{j} = \det(\check{\mathbf{f}})$, then used the expression for $\Delta_t(dV_X)$ from (6) and, finally, pushed forward to \mathcal{B}_X . The expression in (13) is clearly analogous to the classical Reynolds' transport theorem, that is commonly established to express the material time derivative of an integral on the spatial domain \mathcal{B}_X .

2.3.2. Time-derivative of surface integral

It is of interest to consider a surface-specific quantity $\hat{f}_X(\mathbf{X}, \mathbf{x}, \underline{\alpha}, t)$, for $\mathbf{X} \in \partial\mathcal{B}_X(t)$, and the corresponding extensive quantity

$$\hat{F} \stackrel{\text{def}}{=} \int_{\partial\mathcal{B}_X} \hat{f}_X dS_X \quad (14)$$

The time-derivative of \hat{F} , for time-dependent $\partial\mathcal{B}_X$, is given as

$$\begin{aligned} \frac{d}{dt} \hat{F} &= \int_{\partial\mathcal{B}_X} \left[\Delta_t \hat{f}_X + \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\nabla}_X \right] dS_X \\ &= \int_{\partial\mathcal{B}_X} \left[\hat{D}_t \hat{f}_X + \left[\hat{f}_X \dot{\mathbf{X}} \right] \cdot \hat{\nabla}_X \right] dS_X \end{aligned} \quad (15)$$

⁶Henceforth, the explicit dependence on time of \mathcal{B}_X is dropped for brevity of notation.

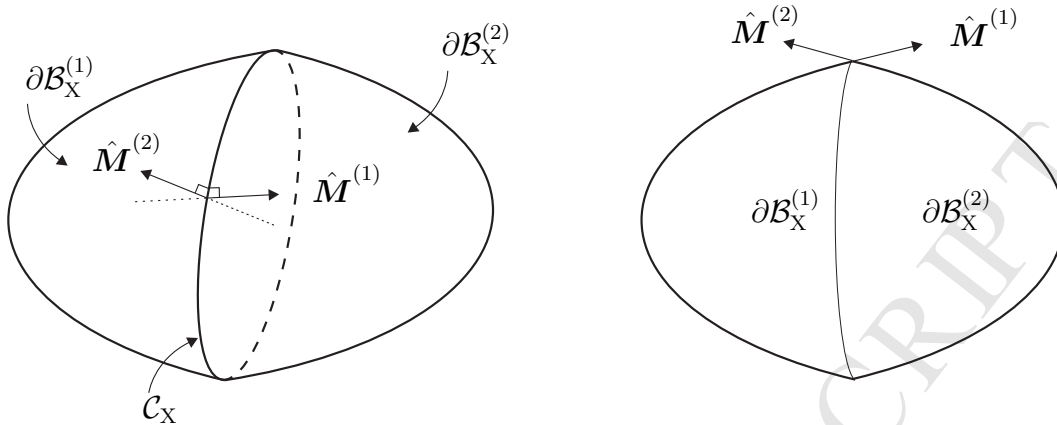


Figure 2: Finite body whose material (reference) configuration occupies the volume, $\mathcal{B}_X = \mathcal{B}_X^{(1)} \cup \mathcal{B}_X^{(2)}$ with boundary surface $\partial\mathcal{B}_X = \partial\mathcal{B}_X^{(1)} \cup \partial\mathcal{B}_X^{(2)}$. The (open) surface parts $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$ are joined along the curve \mathcal{C}_X .

where we used the definition of $\hat{\mathbf{D}}_t$ in (9), and where we, once again, used the surface-specific gradient operator $\hat{\nabla}_X$ (as defined above in terms of the surface-specific identity tensor $\hat{\mathbf{I}} \stackrel{\text{def}}{=} \mathbf{I} - \mathbf{N} \otimes \mathbf{N}$). In order to derive (15), we first performed a pull-back of $\partial\mathcal{B}_X$ to $\partial\mathcal{B}_\xi$, while using the relation in (11).

The divergence theorem for surfaces may be used in order to transform the last term of the integrand in (15): We then consider the situation that $\partial\mathcal{B}_X = \partial\mathcal{B}_X^{(1)} \cup \partial\mathcal{B}_X^{(2)}$ is non-smooth and can be decomposed into the two smooth parts $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$, joined along the common curve \mathcal{C}_X , as shown in Figure 2. For each open surface $\partial\mathcal{B}_X^{(i)}$, $i = 1, 2$, we may apply the divergence theorem for surfaces to obtain

$$\int_{\partial\mathcal{B}_X^{(i)}} [\hat{f}_X \dot{\mathbf{X}}] \cdot \hat{\nabla}_X dS_X = \int_{\mathcal{C}_X} \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\mathbf{M}}^{(i)} dL_X - \int_{\partial\mathcal{B}_X^{(i)}} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X, \quad i = 1, 2 \quad (16)$$

where the unit vector $\hat{\mathbf{M}}^{(i)}$ is normal to \mathbf{N} on $\partial\mathcal{B}_X^{(i)}$ and the tangent of \mathcal{C}_X . Moreover, $k = -\mathbf{N} \cdot \hat{\nabla}_X$ is the total curvature of $\partial\mathcal{B}_X$ at any regular point. Several useful results pertaining to configurational changes on surfaces, including (16), can be found in Steinmann (2008).

We shall now assume that $\dot{\mathbf{X}}$ is continuous across \mathcal{C}_X , whereas \hat{f}_X may be discontinuous across \mathcal{C}_X . Upon adding the two results in (16) pertinent to $\partial\mathcal{B}_X^{(1)}$ and $\partial\mathcal{B}_X^{(2)}$, we obtain

$$\int_{\partial\mathcal{B}_X} [\hat{f}_X \dot{\mathbf{X}}] \cdot \hat{\nabla}_X dS_X = \int_{\mathcal{C}_X} [\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_X - \int_{\partial\mathcal{B}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \quad (17)$$

Remark: If the closed surface $\partial\mathcal{B}_X$ is smooth across \mathcal{C}_X , i.e. if $\hat{\mathbf{M}}^{(1)} + \hat{\mathbf{M}}^{(2)} = \mathbf{0}$, and \hat{f}_X is continuous, i.e. $\hat{f}_X^{(1)} = \hat{f}_X^{(2)}$, we obtain the identity

$$\int_{\partial\mathcal{B}_X} [\hat{f}_X \dot{\mathbf{X}}] \cdot \hat{\nabla}_X dS_X = - \int_{\partial\mathcal{B}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \quad (18)$$

□

As a generalization, we may compose the closed surface into several multiple smooth parts to obtain

$$\int_{\partial\mathcal{B}_X} [\hat{f}_X \dot{\mathbf{X}}] \cdot \hat{\nabla}_X \, dS_X = \int_{\partial^2\mathcal{B}_X} [\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} \, dL_X - \int_{\partial\hat{\mathcal{B}}_X} k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (19)$$

where $\partial^2\mathcal{B}_X$ is the union of all curves defining "edges" on $\partial\mathcal{B}_X$. Finally, using the relation in (19) we may reformulate (15) as

$$\begin{aligned} \frac{d}{dt} \hat{F} &= \int_{\partial\mathcal{B}_X} [\Delta_t \hat{f}_X + \hat{f}_X \dot{\mathbf{X}} \cdot \hat{\nabla}_X] \, dS_X \\ &= \int_{\partial\mathcal{B}_X} [\hat{D}_t \hat{f}_X - k \hat{f}_X \dot{\mathbf{X}} \cdot \mathbf{N}] \, dS_X + \int_{\partial^2\mathcal{B}_X} [\hat{f}_X^{(1)} \hat{\mathbf{M}}^{(1)} + \hat{f}_X^{(2)} \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} \, dL_X \end{aligned} \quad (20)$$

3. Thermodynamic relations in the material format

3.1. The generic balance law

It is convenient to establish a generic balance law for a given body occupying the *current* material domain \mathcal{B}_X with boundary $\partial\mathcal{B}_X$ (and unit normal \mathbf{N}), as shown schematically in Figure 2.

$$\frac{d}{dt} F = \mathcal{G}^{\text{GEN}} + \mathcal{G}^{\text{TRAN}} + \mathcal{F}^{\text{CONF}} \quad (21)$$

where \mathcal{G}^{GEN} is the (prescribed) internally generated source, $\mathcal{G}^{\text{TRAN}}$ is the standard (prescribed) "material flux", or transfer, through the boundary if the domain \mathcal{B}_X is held fixed, whereas $\mathcal{F}^{\text{CONF}}$ is the non-conventional "configurational flux" across the boundary due to the configurational motion of \mathcal{B}_X ⁷. These source terms are defined in terms of volume- and surface-specific quantities as follows:

$$\mathcal{G}^{\text{GEN}} = \int_{\mathcal{B}_X} g_X^{\text{GEN}} \, dV_X, \quad \mathcal{G}^{\text{TRAN}} = \int_{\partial\mathcal{B}_X} g_X^{\text{TRAN}} \, dS_X, \quad \mathcal{F}^{\text{CONF}} = \int_{\partial\mathcal{B}_X} f_X^{\text{CONF}} \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (22)$$

Within a smooth part of \mathcal{B}_X , the "configurational flux" f_X^{CONF} coincides with the convection of f_X due to the configurational motion, thus providing the basis for recovering the classical balance law for f_X . At a free boundary of a *finite body* Ω_X , it is necessary that f_X^{CONF} is assigned a constitutively prescribed quantity \bar{f}_X^{CONF} (that may be related to surface growth).

Subsequently, we apply (21) to the simplest situation of (in)balance of mechanical dissipation, whereby we restrict to *quasistatic motion* (i.e. dynamic forces are ignored) and isothermal conditions. Moreover, we make the classical assumption that mass is conserved. For a more comprehensive discussion of the different balance laws pertinent to mass, momentum, energy and entropy, for the general situation of dynamic motion and non-isothermal conditions, the reader is referred to Runesson et al. (2008).

⁷This represents an alternative (but in principle equivalent) formulation of the "observer-objective" paradigm by Gurtin (2000).

3.2. Global and localized dissipation inequality

The global free energy is given as

$$\Psi \stackrel{\text{def}}{=} \int_{\mathcal{B}_X} \psi_X \, dV_X \quad (23)$$

where ψ_X is the volume-specific free energy. The configurational flux of free energy is thus given as

$$\Psi^{\text{CONF}} = \int_{\partial\mathcal{B}_X} \psi_X^{\text{CONF}} \dot{\mathbf{X}} \cdot \mathbf{N} \, dS_X \quad (24)$$

Moreover, the total mechanical power supply, \mathcal{W} , is given as

$$\mathcal{W} = \int_{\mathcal{B}_X} \mathbf{b}_X \cdot \mathbf{v} \, dV_X + \int_{\partial\mathcal{B}_X} \mathbf{t}_X \cdot \mathbf{v} \, dS_X = \int_{\mathcal{B}_X} \mathbf{P} : D_t \mathbf{F} \, dV_X \quad (25)$$

In order to obtain the last expression in (25), the momentum balance $\mathbf{P} \cdot \nabla_X + \mathbf{b}_X = \mathbf{0}$, was used, where \mathbf{P} is the 1st Piola-Kirchhoff stress, and \mathbf{b}_X is the volume-specific load.

It is *proposed* that the total mechanical dissipation is expressed as

$$\mathcal{D} = \mathcal{W} - \frac{d}{dt} \Psi + \Psi^{\text{CONF}} \geq 0 \quad (26)$$

In the special case of isothermal *elastic* material response (volume-specific free energy $\psi_X(\mathbf{F}, \mathbf{X})$), and no configurational flux ($\psi_X^{\text{CONF}} = 0$), the expression in (26) was proposed by Guerses and Miehe (2008) in the context of crack propagation.

In order to obtain the localized form of (26), we consider an arbitrary domain \mathcal{B}_X that is embedded totally within a finite body. In such a case $\psi_X^{\text{CONF}} = \psi_X$ and we obtain the standard expression

$$d_X = \mathbf{P} : D_t \mathbf{F} - D_t \psi_X \geq 0 \quad (27)$$

where d_X is the volume-specific mechanical dissipation.

Next, we introduce the parametrization of the free energy density, $\psi_X(\mathbf{F}, \theta, \underline{k}; \mathbf{X})$, pertinent to a *dissipative* material response, where \underline{k} represents a set of internal variables. It is noted that a possible explicit dependence of \mathbf{X} is included as argument in ψ (representing inhomogeneous variation of material parameters in \mathcal{B}_X). Upon evaluating the material time derivative $D_t \psi_X$, and using standard arguments of the COLEMAN-NOLL type, we obtain the constitutive state equation

$$\mathbf{P} = \frac{\partial \psi_X}{\partial \mathbf{F}} \quad (28)$$

such that (24) reduces to

$$d_X = \underline{K} \star D_t \underline{k} \geq 0 \quad \text{with } \underline{K} \stackrel{\text{def}}{=} -\frac{\partial \psi_X}{\partial \underline{k}} \quad (29)$$

where we introduced dissipative stresses \underline{K} that are energy-conjugated to the internal variables \underline{k} ⁸.

4. Dissipation functional for changing material configuration

4.1. Preliminaries

We shall consider the global (mechanical) dissipation inequality for a given *finite* body occupying the current material domain Ω_X with external boundary $\partial\Omega_X$. It is assumed that the body undergoes configurational changes, expressed as $\dot{\mathbf{X}} \neq \mathbf{0}$, while it is subjected to prescribed loading. For simplicity, we restrict to *isothermal conditions* henceforth. The resulting thermodynamic process is then characterized by time-changes of all the independent thermodynamic fields, \mathbf{F} and \underline{k} , since they are solutions of the pertinent balance and state equations (equilibrium and constitutive equations) and thus depend on the configurational motion $\mathbf{X} = \Phi(\boldsymbol{\xi}, t)$ in an *implicit* manner. As a result, the global dissipation functional \mathcal{D} depends, apart from $\dot{\mathbf{X}}$, *potentially* on the fields $\dot{\mathbf{x}}$ and $\dot{\underline{k}}$ in the most general case of combined configurational and deformational motion for general loading; hence we denote $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{x}}, \dot{\underline{k}})$ the *global dissipation functional*.

Remark: For the SMP, involving the momentum equation, the boundary is subdivided into parts with essential and natural boundary conditions for the spatial field \mathbf{x} . The generic notion of these (Dirichlet and Neumann) boundary parts are $\partial\Omega_{X,D}$ (with prescribed placements) and $\partial\Omega_{X,N}$ (with prescribed tractions). It is important to note that the boundary in the expressions for \mathcal{W} in (25) is the total one, i.e. $\partial\Omega_X = \partial\Omega_{X,D} \cup \partial\Omega_{X,N}$. For example, both a prescribed and a "support" traction will contribute to \mathcal{W} in the general situation when the support is defined by prescribed non-zero configurational rate. \square

Below, we present explicit forms of $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{x}}, \dot{\underline{k}})$. As a preliminary for these developments, we recall the equilibrium equation rephrased as

$$-\mathbf{P} \cdot \nabla_X = \mathbf{b}_X \quad \text{in } \Omega_X, \quad \mathbf{P} \cdot \mathbf{N} \stackrel{\text{def}}{=} \mathbf{t}_X \quad \text{on } \partial\Omega_X \quad (30)$$

We shall also use the standard weak format⁹ of the equilibrium equation (30)

$$\int_{\Omega_X} [\mathbf{P} : [\delta\mathbf{x} \otimes \nabla_X] - \mathbf{b}_X \cdot \delta\mathbf{x}] dV_X - \int_{\partial\Omega_X} \mathbf{t}_X \cdot \delta\mathbf{x} dS_X = 0, \quad \forall \delta\mathbf{x} \in \mathbb{V} \quad (31)$$

where the virtual (placements) $\delta\mathbf{x} \in \mathbb{V}$ must be sufficiently smooth to allow for the gradient $\delta\mathbf{x} \otimes \nabla_X$ to be meaningful. We remark that no specific assumption has been made as to the value of $\delta\mathbf{x}$ on the Dirichlet boundary $\partial\Omega_{X,D}$.

⁸The "scalar star product" has the appropriate interpretation depending on the tensorial order of variables in the column vector \underline{k} .

⁹To simplify matters, it is assumed in this Section that sufficient regularity for using the divergence theorem is present in the whole Ω_X . In the subsequent application to material interfaces, this requirement does not necessarily hold; however, it can be circumvented as shown.

4.2. Basic formats of the dissipation functional – Split in configurational and material parts

It was shown in Runesson et al. (2008) that (i) the dissipation functional \mathcal{D} does not depend explicitly on $\dot{\mathbf{x}}$, i.e. the parametrization $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ suffices, (ii) it is natural to split $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ as

$$\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \mathcal{D}^{\text{CONF}}(\dot{\mathbf{X}}) + \mathcal{D}^{\text{MAT}}(\dot{\mathbf{k}}) \quad (32)$$

where $\mathcal{D}^{\text{CONF}}$ and \mathcal{D}^{MAT} are the *configurational* and *material* dissipation function, respectively.

More specifically, it was shown in Runesson et al. (2008) that two possible formats of $\mathcal{D}^{\text{CONF}}$, labelled (I) and (II), are those defined as

$$\begin{aligned} \mathcal{D}^{\text{CONF}}(\dot{\mathbf{X}}) &= \mathcal{D}_I^{\text{CONF}}(\dot{\mathbf{X}}) \stackrel{\text{def}}{=} \\ &\int_{\Omega_X} \left[-\boldsymbol{\Sigma} : \left[\dot{\mathbf{X}} \otimes \boldsymbol{\nabla}_X \right] + \mathbf{B}_I \cdot \dot{\mathbf{X}} \right] dV_X + \int_{\partial\Omega_X} \mathbf{T}_I \cdot \dot{\mathbf{X}} dS_X \end{aligned} \quad (33)$$

$$\begin{aligned} &= \mathcal{D}_{II}^{\text{CONF}}(\dot{\mathbf{X}}) \stackrel{\text{def}}{=} \\ &\int_{\Omega_X} \left[-\mathbf{B}_{II} \cdot \dot{\mathbf{X}} \right] dV_X + \int_{\partial\Omega_X} \left[-\mathbf{T}_{II} \cdot \dot{\mathbf{X}} \right] dS_X \end{aligned} \quad (34)$$

where we introduced the following notation: $\boldsymbol{\Sigma}$ is the "quasi-static" ESHELBY (energy-momentum) tensor, associated with ψ_X , which is defined as

$$\boldsymbol{\Sigma} \stackrel{\text{def}}{=} \psi_X \mathbf{I} - \mathbf{F}^T \cdot \frac{\partial \psi_X}{\partial \mathbf{F}} = \psi_X \mathbf{I} - \mathbf{F}^T \cdot \mathbf{P}, \quad (35)$$

$\mathbf{B}_I, \mathbf{B}_{II}$ are configurational volume forces, whereas $\mathbf{T}_I, \mathbf{T}_{II}$ are configurational boundary tractions, that are defined as

$$\mathbf{B}_I = -\frac{\partial \psi_X}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} - \mathbf{F}^T \cdot \mathbf{b}_X, \quad \mathbf{T}_I = -\mathbf{F}^T \cdot \mathbf{t}_X + \psi_X^{\text{CONF}} \mathbf{N} \quad (36)$$

$$\mathbf{B}_{II} = \underline{\mathbf{K}} \star [\underline{\mathbf{k}} \otimes \boldsymbol{\nabla}_X], \quad \mathbf{T}_{II} = [\psi_X - \psi_X^{\text{CONF}}] \mathbf{N} \quad (37)$$

Moreover, \mathcal{D}^{MAT} is given as

$$\mathcal{D}^{\text{MAT}}(\dot{\mathbf{k}}) \stackrel{\text{def}}{=} \int_{\Omega_X} \underline{\mathbf{K}} \star \dot{\mathbf{k}} dV_X \quad (38)$$

Once again, it must be noted that the expressions $\mathcal{D}_I^{\text{CONF}}$ and $\mathcal{D}_{II}^{\text{CONF}}$ in (33) and (34) are but two possible expressions for the purely configurational part of the dissipation. Moreover, they are completely equivalent provided certain regularity requirements are satisfied, e.g. $\dot{\mathbf{X}}$ is sufficiently regular.

Remark: It turns out that it is often more useful to introduce the alternative split of $\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ as compared to (32):

$$\mathcal{D}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) + \bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) \quad (39)$$

where we introduced

$$\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = \int_{\partial\Omega_X} [-\mathbf{T}_{\text{II}} \cdot \dot{\mathbf{X}}] \, dS_X = - \int_{\partial\Omega_X} [\psi_X - \psi_X^{\text{CONF}}] \mathbf{N} \cdot \dot{\mathbf{X}} \, dS_X \quad (40)$$

and

$$\bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}}) = \int_{\Omega_X} \underline{\mathbf{K}} \star D_t \underline{\mathbf{k}} \, dV_X = \int_{\Omega_X} \underline{\mathbf{K}} \star [\dot{\mathbf{k}} - [\underline{\mathbf{k}} \otimes \nabla_X] \cdot \dot{\mathbf{X}}] \, dV_X \quad (41)$$

It appears readily that $\bar{\mathcal{D}}^{\text{MAT}}(\dot{\mathbf{X}}, \dot{\mathbf{k}})$ represents precisely the ordinary material dissipation. Moreover, if we introduce the condition of vanishing net dissipation across the external boundary, i.e. $\mathbf{N} \cdot \dot{\mathbf{X}} = 0$ on $\partial\Omega_X$, then it follows that $\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = 0$ independent of the nature of loading, boundary conditions and possible material inhomogeneity in Ω_X . In such a case the mapping $\mathbf{X}(\boldsymbol{\xi}, t)$ represents merely a coordinate transformation under which the result $\bar{\mathcal{D}}^{\text{CONF}}(\dot{\mathbf{X}}) = 0$ is invariant, cf. NOETHER'S theorem, Noether (1918). \square

4.3. Material equilibrium - Other formats of dissipation

It is useful to establish "configurational volume loads", \mathbf{B} , and "configurational surface tractions", \mathbf{T} , that equilibrate the pertinent Eshelby stress via the "configurational equilibrium equations"

$$-\boldsymbol{\Sigma} \cdot \nabla_X = \mathbf{B} \quad \text{in } \Omega_X, \quad \boldsymbol{\Sigma} \cdot \mathbf{N} = \mathbf{T} \quad \text{on } \partial\Omega_X \quad (42)$$

Upon direct differentiation of $\boldsymbol{\Sigma}$, as defined in (35), we obtain

$$\mathbf{B} = - \frac{\partial \psi_X}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} - \mathbf{F}^T \cdot \mathbf{b}_X + \underline{\mathbf{K}} \star [\underline{\mathbf{k}} \otimes \nabla_X] \quad (43)$$

where we used the strong format of (spatial) equilibrium for \mathbf{P} in (30). We also obtain the material traction as

$$\mathbf{T} = \boldsymbol{\Sigma} \cdot \mathbf{N} = \psi_X \mathbf{N} - \mathbf{F}^T \cdot \mathbf{t}_X \quad (44)$$

Remark: $\mathbf{B} = \mathbf{B}_{\text{I}} + \mathbf{B}_{\text{II}}$ and $\mathbf{T} = \mathbf{T}_{\text{I}} + \mathbf{T}_{\text{II}}$.

Remark: Since the "equilibrium equation" $(42)_1$ is a derived *identity*, it does not add any new physical information.

It is useful to establish the weak format of the configurational equilibrium equations in $(42)_1$. To this end we consider "virtual velocities" $\delta \dot{\mathbf{X}} \in \mathbb{X}$ and recast $(42)_1$ in the variational format

$$\int_{\Omega'_X} [\boldsymbol{\Sigma} : [\delta \dot{\mathbf{X}} \otimes \nabla_X] - \mathbf{B} \cdot \delta \dot{\mathbf{X}}] \, dV_X - \int_{\partial\Omega'_X} \mathbf{T} \cdot \delta \dot{\mathbf{X}} \, dS_X = 0, \quad \forall \delta \dot{\mathbf{X}} \in \mathbb{X} \quad (45)$$

where the virtual velocities $\delta \dot{\mathbf{X}} \in \mathbb{X}$ must be sufficiently smooth to allow for the gradient $\delta \dot{\mathbf{X}} \otimes \nabla_X$ to be meaningful. We remark that no specific assumption has been made as to the value of $\delta \dot{\mathbf{X}}$ on the Dirichlet boundary $\partial\Omega_{X,D}$.

5. Configurational-induced global dissipation – Generalized configurational forces

5.1. Total variation of the rate of global dissipation due to configurational changes

Henceforth, we shall restrict our attention to the situation that a physical process is manifested by fields $D_t \mathbf{x}$ and $D_t \underline{k}$ that are *brought about solely by configurational changes*. In other words, for a given field $\dot{\mathbf{X}}(\boldsymbol{\xi}, t)$, it is possible to solve for all other fields, $\dot{\mathbf{x}}\{\dot{\mathbf{X}}\}$ and $\underline{k}\{\dot{\mathbf{X}}\}$, as (implicit) functions of $\dot{\mathbf{X}}$ from the momentum equation and the pertinent constitutive relations. It is noted that the *actual physical problem* involves $\dot{\mathbf{X}}(\boldsymbol{\xi}, t)$ as part of the total solution, which requires a constitutive relation for $\dot{\mathbf{X}}$ in terms of a suitably defined field of "driving forces". However, these driving forces will be of such nature that they can only be determined when the solutions $\dot{\mathbf{x}}\{\dot{\mathbf{X}}\}$ and $\underline{k}\{\dot{\mathbf{X}}\}$ are known; hence, the problem of computing the driving forces is indeed nonlinear and must be solved by some sort of iterative procedure in practice.

Next, we shall be concerned with the issue of defining the field of thermodynamically consistent *generalized configurational forces* that are energy-conjugated to a given differential change (variation) of the field $\dot{\mathbf{X}}$, henceforth denoted $d\dot{\mathbf{X}}$, in the sense that they represent the total variation of \mathcal{D} with respect to $\dot{\mathbf{X}}$. The total differential of $\mathcal{D} \stackrel{\text{def}}{=} \mathcal{D}(\dot{\mathbf{X}}, \underline{k}\{\dot{\mathbf{X}}\})$ can be expressed as

$$\begin{aligned} d_{\dot{\mathbf{X}}} \mathcal{D} &= \mathcal{D}'(\dot{\mathbf{X}}, \underline{k}\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \\ &= (\bar{\mathcal{D}}^{\text{CONF}})'_{\dot{\mathbf{X}}}(\dot{\mathbf{X}}; d\dot{\mathbf{X}}) + (\bar{\mathcal{D}}^{\text{MAT}})'_{\dot{\mathbf{X}}}(\dot{\mathbf{X}}, \underline{k}; d\dot{\mathbf{X}}) + (\bar{\mathcal{D}}^{\text{MAT}})'_{\underline{k}}(\dot{\mathbf{X}}, \underline{k}; \underline{k}'\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \\ &= \bar{\mathcal{D}}^{\text{CONF}}(d\dot{\mathbf{X}}) + \bar{\mathcal{D}}^{\text{MAT}}(d\dot{\mathbf{X}}, \underline{k}'\{\dot{\mathbf{X}}\}; d\dot{\mathbf{X}}) \end{aligned} \quad (46)$$

where it was used that both $\bar{\mathcal{D}}^{\text{CONF}}$ and $\bar{\mathcal{D}}^{\text{MAT}}$ are linear in their arguments ($\dot{\mathbf{X}}$ and $\dot{\mathbf{X}}, \underline{k}$, respectively). In order to carry out the total variation, it is necessary to compute the *sensitivity* fields:

$$d\dot{\mathbf{x}} = \dot{\mathbf{x}}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}, \quad d\underline{k} = \underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\} \quad (47)$$

which are directional (or Gateaux) derivatives in the classical sense¹⁰. The sensitivity fields $\dot{\mathbf{x}}'$ and \underline{k}' must satisfy *global tangent (or sensitivity) relations*, which are derivable from linearization of the equilibrium equation together with the constitutive rate equations for \underline{k} . It is emphasized that the sensitivity fields, say $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$, are *linear* in $d\dot{\mathbf{X}}$; however, they represent "spatially global" relations in Ω_X . This means, in particular, that the configurational dissipation is not necessarily confined to the (possibly small) part of Ω_X where $d\dot{\mathbf{X}} \neq \mathbf{0}$ has been assumed.

Remark: Although it is only $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ that appears in \mathcal{D}' , it is still necessary in the general case to solve for both $\dot{\mathbf{x}}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ and $\underline{k}'\{\dot{\mathbf{X}}; d\dot{\mathbf{X}}\}$ in a truly coupled fashion via the sensitivity problem for a given field $d\dot{\mathbf{X}}$. \square

¹⁰A more explicit definition of sensitivities is possible if we define the "unit sensitivity" fields $\dot{\mathbf{x}}'^{(i)}$, $i = 1, 2, \dots, \text{NDIM}$, via the identity $d\dot{\mathbf{x}} = \sum_{i=1}^{\text{NDIM}} \dot{\mathbf{x}}'^{(i)} d(\dot{X}_i)$.

Remark: In practice, it is sometimes more convenient to compute the sensitivities in the material time derivatives. In order to link the relevant quantities, we consider a generic field z and obtain

$$\dot{z} = D_t z + [z \otimes \nabla_{\mathbf{X}}] \cdot \dot{\mathbf{X}} \quad \Rightarrow \quad \dot{z}'\{\bullet; d\dot{\mathbf{X}}\} = (D_t z)' \{\bullet; d\dot{\mathbf{X}}\} + [z \otimes \nabla_{\mathbf{X}}] \cdot d\dot{\mathbf{X}} \quad (48)$$

For example, we note that $\dot{\mathbf{x}}'\{\bullet; d\dot{\mathbf{X}}\} = \mathbf{v}'\{\bullet; d\dot{\mathbf{X}}\} + \mathbf{F} \cdot d\dot{\mathbf{X}}$. \square

Next, we shall assume that $d\dot{\mathbf{X}}$ can be parametrized as follows:

$$d\dot{\mathbf{X}} = \sum_{i=1}^{N_W} \mathbf{W}_i d\dot{a}_i \quad (49)$$

where $\mathbf{W}_i(\mathbf{X})$, $i = 1, 2, \dots, N_W$, are "weight functions" (or shape functions), the choice of which represents a model assumption in general. Upon inserting (49) into (46), we obtain the representation

$$d_{\dot{\mathbf{X}}} \mathcal{D} = \underline{\mathcal{G}}^T d\dot{\mathbf{a}} \quad (50)$$

where $\underline{\mathcal{G}}$ is the generalized configurational force that is energy-conjugated to $\dot{\mathbf{a}}$. Using (46), we may split $\underline{\mathcal{G}}$ as

$$\underline{\mathcal{G}} = \underline{\mathcal{G}}^{\text{CONF}} + \underline{\mathcal{G}}^{\text{MAT}} \quad (51)$$

where the components of $\underline{\mathcal{G}}^{\text{CONF}}$ and $\underline{\mathcal{G}}^{\text{MAT}}$ are given as

$$\mathcal{G}_i^{\text{CONF}} = \bar{\mathcal{D}}^{\text{CONF}}(\mathbf{W}_i), \quad \mathcal{G}_i^{\text{MAT}} = \bar{\mathcal{D}}^{\text{MAT}}(\mathbf{W}_i, \underline{k}'\{\dot{\mathbf{X}}; \mathbf{W}_i\}) \quad (52)$$

5.2. Constitutive relation for rate-independent plasticity

We shall consider rate-independent material response, typical for classical plasticity. In such a case \underline{k} represents the plastic strain, "hardening strain", etc. The standard material format of the rate equations for such material response then reads ¹¹

$$D_t \underline{k} = \lambda \underline{g}, \quad \lambda = \frac{1}{h} \langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle, \quad \underline{k}(\mathbf{X}, 0) = \underline{0} \quad (53)$$

where $\langle [\bullet] \rangle \stackrel{\text{def}}{=} \frac{1}{2} (|[\bullet]| + [\bullet])$ is the McCauley bracket; hence, it is noted that λ is a *first order homogeneous (but nonlinear)* function ¹² in $D_t \mathbf{F}$. This specific structure reflects the loading/unloading conditions expressed in terms of the sign of the "loading indicator" function $\boldsymbol{\mu} : D_t \mathbf{F}$ in a "strain-controlled" format" such that plastic loading, (L), is signalled by $\boldsymbol{\mu} : D_t \mathbf{F} > 0$, whereas elastic unloading, (U), is signalled by $\boldsymbol{\mu} : D_t \mathbf{F} \leq 0$. These cases are thus defined by

$$\lambda = \frac{1}{h} \boldsymbol{\mu} : D_t \mathbf{F} \quad (\text{L}), \quad \lambda = 0 \quad (\text{U}) \quad (54)$$

¹¹To simplify notation, it is assumed that the "flow rule" is regular (corresponding to a smooth flow potential).

¹²A function $f(x)$ is first order homogeneous if, for $\alpha > 0$, $f(\alpha x) = \alpha f(x)$.

As to the explicit definition of the state functions ¹³ g , h and $\boldsymbol{\mu}$, they are model dependent. (A prototype model of plasticity based on linearized elastic relations will be employed in conjunction with the motion of a singular material surface, see below.)

The appropriate continuum tangent relation for \mathbf{P} in terms of \mathbf{F} and \underline{k} can now be written as

$$\mathbf{D}_t \mathbf{P} = \mathbf{L}^e : \mathbf{D}_t \mathbf{F} + \underline{\mathbf{M}} \star \mathbf{D}_t \underline{k} \quad (55)$$

where we introduced the tangent operators

$$\mathbf{L}^e \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{k}, \mathbf{X}}, \quad \underline{\mathbf{M}} \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \underline{k}} \Big|_{\mathbf{F}, \mathbf{X}} \quad (56)$$

In particular, \mathbf{L}^e is the elastic continuum tangent stiffness (CTS) tensor. Upon inserting (53)₁ into (55), we obtain

$$\mathbf{D}_t \mathbf{P} = \mathbf{L}^{\text{ep}} : \mathbf{D}_t \mathbf{F} \quad (\text{L}), \quad \mathbf{D}_t \mathbf{P} = \mathbf{L}^e : \mathbf{D}_t \mathbf{F} \quad (\text{U}) \quad (57)$$

where \mathbf{L}^{ep} is the elastic-plastic continuum tangent stiffness (CTS) tensor, defined as

$$\mathbf{L}^{\text{ep}} \stackrel{\text{def}}{=} \mathbf{L}^e + \frac{1}{h} \underline{\mathbf{M}} \star \underline{g} \boldsymbol{\mu} \quad (58)$$

We note that the CTS-tensor takes two distinct expressions depending on whether plastic loading (L) or elastic unloading (U) is at hand at a given position $\mathbf{X} \in \Omega_X$. Hence, $\mathbf{D}_t \underline{k}$ and $\mathbf{D}_t \mathbf{P}$ are nonlinear functions in $\mathbf{D}_t \mathbf{F}$.

Now, we shall take the total variation of $\mathbf{D}_t \mathbf{P}$ with respect to variation of $\dot{\mathbf{X}}$ to obtain the sensitivity relation

$$(\mathbf{D}_t \mathbf{P})' = \mathbf{L}^e : (\mathbf{D}_t \mathbf{F})' + \underline{\mathbf{M}} \star (\mathbf{D}_t \underline{k})' \quad (59)$$

From (53)₁ we obtain

$$(\mathbf{D}_t \underline{k})' = \underline{\mathbf{R}}_T : (\mathbf{D}_t \mathbf{F})' \quad \text{with} \quad \underline{\mathbf{R}}_T \stackrel{\text{def}}{=} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F}|} \underline{g} \otimes \boldsymbol{\mu} \quad (60)$$

which (i) depends on the current value of \mathbf{v} (or $\dot{\mathbf{x}}$ and $\dot{\mathbf{X}}$) via the relation in (9), (ii) is linear in the sensitivity $(\mathbf{D}_t \mathbf{F})'$. The expression in (60) is well-defined for all solutions except at neutral loading defined by $\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} = 0$. In particular, it can be evaluated for the situation $\dot{\mathbf{X}} = \mathbf{0}$, corresponding to vanishing configurational motion.

Upon combining (59,60), we obtain the desired relation

$$(\mathbf{D}_t \mathbf{P})' = \mathbf{L}_T : (\mathbf{D}_t \mathbf{F})' \quad \text{with} \quad \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}^e + \frac{1}{h} \frac{\langle \boldsymbol{\mu} : \mathbf{D}_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : \mathbf{D}_t \mathbf{F}|} \underline{\mathbf{M}} \star \underline{g} \otimes \boldsymbol{\mu} \quad (61)$$

where \mathbf{L}_T is the tangent stiffness tensor that depends on $\mathbf{D}_t \mathbf{F}$ and which holds for both (L) and (U).

¹³E.g. $\underline{g}(\mathbf{F}[\mathbf{X}, \mathbf{x}], \underline{k})$

Remark: For a more general rate-independent relation than (53) of the generic form

$$D_t \underline{k} = \underline{f}(D_t \mathbf{F}) \quad (62)$$

where \underline{f} is 1st order homogeneous in its argument, we may generalize (60) to

$$(D_t \underline{k})' = \underline{f}'(D_t \mathbf{F}; (D_t \mathbf{F})') \quad (63)$$

where $\underline{f}'(\bullet; (\bullet)')$ represents the directional derivative. \square

5.3. Basic format of the tangent problem for quasistatic equilibrium

5.3.1. Preliminaries

Consider the basic problem of a finite body with Dirichlet and Neumann boundary conditions $\mathbf{x} = \bar{\mathbf{x}}$ on $\partial\Omega_{X,D}$ and $\mathbf{t}_X \stackrel{\text{def}}{=} \mathbf{P} \cdot \mathbf{N} = \bar{\mathbf{t}}_X$ on $\partial\Omega_{X,N} = \partial\Omega_X \setminus \partial\Omega_{X,D}$. Moreover, we assume the constitutive state relation $\mathbf{P}(\mathbf{F}, \underline{k}; \mathbf{X})$. The weak format of the equilibrium equation can then be written in standard fashion:

$$a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) = l(\delta \mathbf{x}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (64)$$

where

$$a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) \stackrel{\text{def}}{=} \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P}(\mathbf{F}, \underline{k}; \mathbf{X}) \, dV_X \quad (65)$$

$$l(\delta \mathbf{x}) \stackrel{\text{def}}{=} \int_{\Omega_X} \delta \mathbf{x} \cdot \mathbf{b}_X \, dV_X + \int_{\partial\Omega_{X,N}} \delta \mathbf{x} \cdot \mathbf{t}_X \, dS_X \quad (66)$$

The SMP is then to find $\mathbf{x} \in \mathbb{V}$ and $\underline{k} \in \mathbb{K}$ that solve (64) together with the pertinent evolution equation for \underline{k} , as defined in (53).

Since Ω_X is not time-invariant at configurational changes, the test functions $\delta \mathbf{x} \in \mathbb{V}^0$ are time-dependent in the parametrization $\delta \mathbf{x}(\mathbf{X}, t)$; however, this relation is constrained by the condition that $\delta \mathbf{x}(\mathbf{X}, t)$ is stationary in the absolute configuration, i.e.

$$\delta \mathbf{x}(\mathbf{X}(\boldsymbol{\xi}, t), t) \stackrel{\text{def}}{=} \delta \mathbf{x}(\boldsymbol{\xi}, t) = \delta \mathbf{x}(\boldsymbol{\xi}) \quad (67)$$

In particular, this means that

$$\Delta_t \delta \mathbf{x} = \mathbf{0}, \quad D_t \delta \mathbf{x} = -[\delta \mathbf{x} \otimes \nabla_X] \cdot \dot{\mathbf{X}} \quad (68)$$

$$\Delta_t [\delta \mathbf{x} \otimes \nabla_X] = -[\delta \mathbf{x} \otimes \nabla_X] \cdot [\dot{\mathbf{X}} \otimes \nabla_X], \quad D_t [\delta \mathbf{x} \otimes \nabla_X] = [D_t \delta \mathbf{x}] \otimes \nabla_X \quad (69)$$

Our purpose is to first solve for the sensitivity field $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$ from the tangent problem

$$d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} a(\bullet; \delta \mathbf{x}) - \frac{d}{dt} l(\delta \mathbf{x}) \right] = 0, \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (70)$$

for given variations¹⁴ $d\dot{\mathbf{X}} \in \mathbb{X}^0$, and then to compute $\underline{k}'\{\bullet, d\dot{\mathbf{X}}\}$.

Remark: The format for the tangent problem based on $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\}$ as the primary unknown field is considered henceforth as the "operational" format, since each field $\dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$ is continuous across any singular surface where the state variables (such as \mathbf{F}) may be discontinuous. In such a case, $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} = \dot{\mathbf{x}}'\{\bullet, d\dot{\mathbf{X}}\} - \mathbf{F} \cdot d\dot{\mathbf{X}}$ is discontinuous across the singular surface, and it follows that $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} \notin \mathbb{V}^0$, as shown in Figure 3. Nevertheless, the special situation that the solution is smooth, i.e. $\mathbf{v}'\{\bullet, d\dot{\mathbf{X}}\} \in \mathbb{V}^0$, is of particular relevance. Hence, both situations will be discussed subsequently. \square

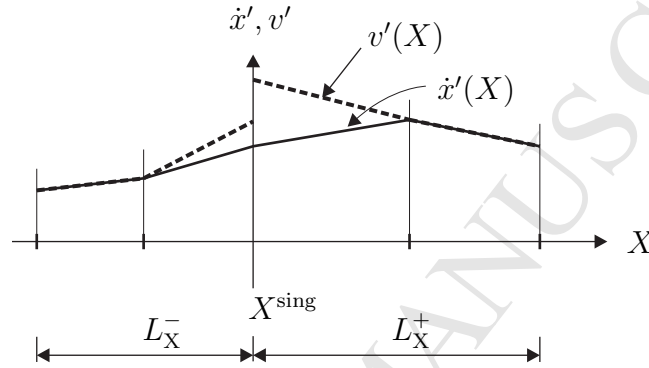


Figure 3: Illustration of the general situation that $\dot{\mathbf{x}}'$ is continuous while \mathbf{v}' is discontinuous across Γ_X^{sing} .

5.3.2. Operational format (based on $\dot{\mathbf{x}}$)

We shall first consider the general case that \mathbf{v}' is only p.w. smooth in Ω_X . In such a case $\dot{\mathbf{x}}' \in \mathbb{V}^0$ is solved from the tangent relation

$$a_T(\bullet; \delta \mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (71)$$

where the pertinent tangent forms are defined as¹⁵

$$a_T(\bullet; \delta \mathbf{x}, \dot{\mathbf{x}}') \stackrel{\text{def}}{=} \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X] dV_X \quad (72)$$

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \\ & + \int_{\partial\Omega_X} \left[- \left[\delta \mathbf{x} \otimes \hat{\nabla}_X \right] : \left[\mathbf{t}_X \otimes d\dot{\mathbf{X}} \right] + \left[\delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X \right] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dS_X \\ & + \int_{\hat{c}_X} \delta \mathbf{x} \cdot \left[\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)} \right] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (73)$$

¹⁴The required regularity of \mathbb{X}^0 depends on the chosen format; here, we assume that $d\dot{\mathbf{X}}$ is continuous and that $d\dot{\mathbf{X}} = \mathbf{0}$ on $\partial\Omega_{X,D}$ for any $d\dot{\mathbf{X}} \in \mathbb{X}^0$.

¹⁵Henceforth, in order to retain maximal generality we do not distinguish explicitly between the Dirichlet and Neumann boundary parts in the various surface integrals.

The continuum tangent stiffness tensor \mathbf{L}_T , defined by the relation $(D_t \mathbf{P})' = \mathbf{L}_T : (D_t \mathbf{F})'$, was defined in (61). In order to define the "loading" $l_T^{(x)}$ of the tangent problem, we introduced the 4th order tensor \mathbf{P} (which has generally minor non-symmetry), and the 3rd order tensor \mathbf{r}_X , defined as follows:

$$\mathbf{P} \stackrel{\text{def}}{=} \underline{\mathbf{P}} \otimes \mathbf{I} - \mathbf{P} \otimes \mathbf{I} \quad (74)$$

$$\mathbf{r}_X = \Delta \mathbf{L}_T : [\mathbf{F} \otimes \nabla_X] - \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_X] - \frac{\partial \mathbf{P}}{\partial \mathbf{X}} \Big|_{\mathbf{F}, \mathbf{k}} \quad (75)$$

where $\Delta \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}_T - \mathbf{L}^e$. Details of the derivation are given in the Appendix.

5.3.3. Non-operational format (based on \mathbf{v})

Next, we consider the special case that \mathbf{v}' is smooth in Ω_X . In such a case $\mathbf{v}' \in \mathbb{V}^0$ can be solved from the tangent relation

$$a_T(\bullet; \delta \mathbf{x}, \mathbf{v}') = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (76)$$

where the tangent form a_T was defined in (72), whereas $l_T^{(v)}$ is given as

$$\begin{aligned} l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\partial \Omega_X} [-[\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} + \delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}]] d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ & + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (77)$$

Details of the derivation are given in the Appendix.

6. Application to moving material (singular) interface

6.1. Problem definition

Consider the situation when an embedded (open) singular surface Γ_X^{sing} , across which the material properties may be **discontinuous**. The surface Γ_X^{sing} , with boundary curve \mathcal{C}_X , can move through the material domain Ω_X with (closed) *external* boundary $\partial \Omega_X$, which is assumed to be sufficiently smooth. In fact, it suffices that $\partial \Omega_X$ is smooth where $d\dot{\mathbf{X}} \neq \mathbf{0}$. The domain Ω_X is split into two parts, Ω_X^- and Ω_X^+ ($\Omega_X = \Omega_X^- \cup \Omega_X^+$ and $\partial \Omega_X = \partial \Omega_X^- \cup \partial \Omega_X^+$), as shown in Figure 4, whereby the boundary of the two parts are given as $\partial(\Omega_X^-) = \partial \Omega_X^- \cup \Gamma_X^{\text{sing}}$ and $\partial(\Omega_X^+) = \partial \Omega_X^+ \cup \Gamma_X^{\text{sing}}$, respectively. Since the state variables, such as \mathbf{F} and \underline{k} , are generally discontinuous across Γ_X^{sing} , the volume-specific free energy ψ_X is also discontinuous across Γ_X^{sing} .

The normal on Γ_X^{sing} pointing into Ω_X^+ is denoted $\mathbf{N}^- (= \mathbf{N})$, as shown in Figure 4; hence, we use the notation $\mathbf{N}^+ (= -\mathbf{N})$ for the normal in the opposite direction. The cotangents $\hat{\mathbf{M}}^-$ and $\hat{\mathbf{M}}^+$, located on the curve \mathcal{C}_X , are normal to \mathcal{C}_X and lie in the tangent plane of $\partial \Omega_X^-$ and $\partial \Omega_X^+$, respectively. Hence, $\hat{\mathbf{M}}^+ + \hat{\mathbf{M}}^- \neq \mathbf{0}$ in general. The cotangent $\hat{\mathbf{M}}^{\text{tang}}$, which is also located on and directed normal to \mathcal{C}_X , lies in the tangent plane of Γ_X^{sing} . It is thus unique on both sides of the interface.

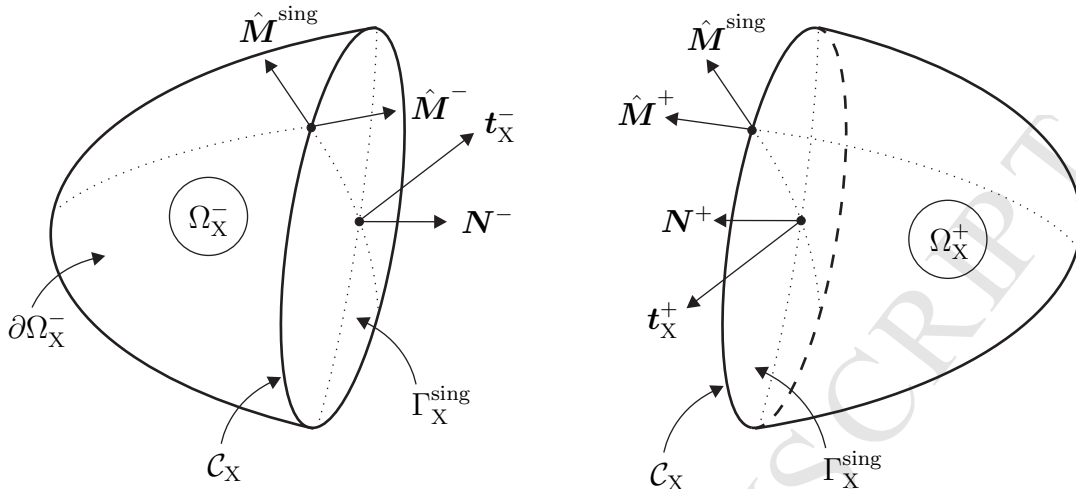


Figure 4: Moving material (singular) interface Γ_X^{sing} splitting the domain Ω_X in the parts Ω_X^- and Ω_X^+ . Other notation is explained in the main text.

6.2. Explicit (classical) configurational forces along material interface

The explicit expression for $\mathcal{D}^{\text{CONF}}$ was discussed in some detail in Runesson et al. (2008). Upon introducing the assumption of vanishing net dissipation across the exterior boundary, i.e. $\mathbf{N} \cdot \dot{\mathbf{X}} = 0$ on $\partial\Omega_X$, we obtain the classical representation

$$\bar{\mathcal{D}}^{\text{CONF}}(d\dot{\mathbf{X}}) = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{CONF}} \cdot d\dot{\mathbf{X}} dS_X, \quad \mathcal{G}^{\text{CONF}} \stackrel{\text{def}}{=} \|\Sigma\| \cdot \mathbf{N} \quad (78)$$

where $\mathcal{G}^{\text{CONF}}$ is the explicitly localized (distributed) configurational "traction" that "lives" on Γ_X^{sing} and, moreover, that represents the dissipation along Γ_X^{sing} .

Remark: Since the deformation gradient \mathbf{F} can be discontinuous only in the normal direction, \mathbf{N} , across Γ_X^{sing} , it is possible to express $\mathcal{G}^{\text{CONF}}$ as

$$\mathcal{G}^{\text{CONF}} = \|\Sigma\| \cdot \mathbf{N} = \alpha \mathbf{N} \quad (79)$$

where $\alpha = \|\Psi_X\| - \mathbf{N} \cdot \|\mathbf{F}^T\| \cdot \langle \mathbf{P} \rangle \cdot \mathbf{N}$ ¹⁶. Hence, the configurational dissipation along Γ_X^{sing} is invariant (vanishes) for any choice of $\dot{\mathbf{X}}$ s.t. $\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ on $\partial\Omega_X \cup \Gamma_X^{\text{sing}}$. \square

6.3. Implicit (configurational-induced) configurational forces along interface – Tangent problem

6.3.1. Operational format of tangent problem

We shall use the fact that all fields are sufficiently smooth in the parts Ω_X^- and Ω_X^+ , whereby the tangent problem introduced in (71) applies to Ω_X^- and Ω_X^+ separately. However, although \mathbf{v}' is expected to be discontinuous across the singular surface Γ_X^{sing} (since \mathbf{F} is discontinuous in general), $\dot{\mathbf{x}}'$ is still continuous across this surface. This means that the

¹⁶ $\langle \mathbf{P} \rangle$ denotes mean value, i.e. $\langle \mathbf{P} \rangle = \frac{1}{2}[\mathbf{P}^- + \mathbf{P}^+]$.

operational format of the tangent problem for a discontinuity surface is conveniently based on $\dot{\mathbf{x}}' \in \mathbb{V}^0$ as the primary unknown field.

At the outset we shall choose $d\dot{\mathbf{X}}$ continuous across Γ_X^{sing} . In order to simplify the resulting expression as far as possible without loss of essential features, we shall also assume that the external boundary $\partial\Omega_X$ is smooth along \mathcal{C}_X . Referring to the notation introduced in Figure 4, we then note the following identities relating to the singular surface Γ_X^{sing} :

$$\hat{\mathbf{M}}^+ + \hat{\mathbf{M}}^- = \mathbf{0}, \quad \mathbf{t}_X^+ + \mathbf{t}_X^- = \mathbf{0}, \quad k^+ + k^- = 0 \quad (80)$$

Clearly, (80)₁ represents the smoothness condition on $\partial\Omega_X$, (80)₂ expresses the condition that the physical tractions on each side of the interface Γ_X^{sing} equilibrate each other, whereas the relation (80)₃ follows from the identities $\hat{\nabla}_X^- = \hat{\nabla}_X^+ \stackrel{\text{def}}{=} \hat{\nabla}_X$ and $-\mathbf{N}^+ = \mathbf{N}^- \stackrel{\text{def}}{=} \mathbf{N}$.

In addition, we shall introduce the assumption that the applied volume load \mathbf{b}_X and surface load (traction) $\bar{\mathbf{t}}_X$ are continuous across \mathcal{C}_X , i.e. $\mathbf{b}_X^- = \mathbf{b}_X^+$ and $\bar{\mathbf{t}}_X^- = \bar{\mathbf{t}}_X^+$ on \mathcal{C}_X .

It is now possible to "tie together" the tangent problems for Ω_X^- and Ω_X^+ , as defined in (71), upon simply adding the pertinent relations and using the "continuity" conditions in (80). We then obtain the tangent problem for the body with interface: Solve for $\dot{\mathbf{x}}' \in \mathbb{V}^0$ from

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (81)$$

where $a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}')$ is still given by (72), whereas $l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}})$ in (73) is now condensed to

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}) \stackrel{\text{def}}{=} & \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \\ & + \int_{\partial\Omega_X} \left[- \left[\delta\mathbf{x} \otimes \hat{\nabla}_X \right] : \left[\mathbf{t}_X \otimes d\dot{\mathbf{X}} \right] + [\delta\mathbf{x} \cdot \mathbf{b}_X - k \delta\mathbf{x} \cdot \mathbf{t}_X] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dA_X \end{aligned} \quad (82)$$

An important special case is defined by the choice $d\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ and $\bar{\mathbf{t}}_X = \mathbf{0}$ on the exterior Neumann boundary part $\partial\Omega_{X,N}$. In such a case the boundary integral in (82) vanishes, and we are left with the simpler expression

$$\begin{aligned} l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}) = & \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right. \\ & + \mathbf{L}_T : \left[\mathbf{F} \cdot \left[d\dot{\mathbf{X}} \otimes \nabla_X \right] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} - \mathbf{b}_X \otimes d\dot{\mathbf{X}} \left. \right] dV_X \end{aligned} \quad (83)$$

In practice, the operational format is based on the parametrization in (49), whereby we obtain

$$\dot{\mathbf{x}}' \{ \dot{\mathbf{X}}; d\dot{\mathbf{X}} \} = \sum_{i=1}^{N_w} \dot{\mathbf{x}}' \{ \dot{\mathbf{X}}; \mathbf{W}_i \} d\dot{a}_i = \sum_{i=1}^{N_w} \dot{\mathbf{x}}'_i d\dot{a}_i \quad (84)$$

Consequently, (81) is replaced by the set of problems: Solve for $\dot{\mathbf{x}}'_i \in \mathbb{V}^0, i = 1, 2, \dots, N_w$:

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}'_i) = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, \mathbf{W}_i), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (85)$$

For known fields $\dot{\mathbf{x}}'_i$, it is possible to compute the generalized configurational force components $(\underline{\mathcal{G}}^{\text{MAT}})_i$ in a post-processing step: $\dot{\mathbf{x}}'_i \rightarrow \mathbf{v}'_i \rightarrow (\mathbf{D}_t \mathbf{F})'_i \rightarrow (\mathbf{D}_t \underline{k})'_i \rightarrow \mathcal{G}_i^{\text{MAT}} \stackrel{\text{def}}{=} (\underline{\mathcal{G}}^{\text{MAT}})_i$ with

$$\mathcal{G}_i^{\text{MAT}} \stackrel{\text{def}}{=} \int_{\Omega_X} \underline{K} \star (\mathbf{D}_t \underline{k})'_i \, dV_X. \quad (86)$$

Finally, we may define the "localizable" (distributed) configurational force vector \mathcal{G}^{MAT} via the identity (least squares projection)

$$\mathcal{G}_i^{\text{MAT}} = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{MAT}} \cdot \mathbf{W}_i \, dS_X \quad (87)$$

This equation is solved approximately in practice using FE-discretization, whereby \mathbf{W}_i are taken as the nodal basis functions along Γ_X^{sing} , and \mathcal{G}^{MAT} is expanded in this basis (as discussed below).

6.3.2. Issue of unique sensitivity field (tangent solution)

It is of considerable interest to note that the sensitivity field $\dot{\mathbf{x}}'$ (or \mathbf{v}') are unique with respect to the choice of the field $d\dot{\mathbf{X}}$ in Ω_X as long as the following conditions are satisfied: (i) The normal component of $d\dot{\mathbf{X}}$ is uniquely chosen on the external boundary $\partial\Omega_X$ as well as on the interface Γ_X^{sing} , (ii) $d\dot{\mathbf{X}}$ is unique along \mathcal{C}_X .

In order to show this result, we consider two given fields $d\dot{\mathbf{X}}^{(1)}$ and $d\dot{\mathbf{X}}^{(2)}$ defined on Ω_X^- . Their difference is denoted $d\dot{\mathbf{X}}^{(1,2)} \stackrel{\text{def}}{=} d\dot{\mathbf{X}}^{(1)} - d\dot{\mathbf{X}}^{(2)}$, corresponding to the sensitivity $(\mathbf{v}^{(1,2)})'$. Now, in view of (76), we conclude that $(\mathbf{v}^{(1,2)})'$ is the solution of the tangent problem

$$a_T(\bullet; \delta \mathbf{x}, (\mathbf{v}^{(1,2)})') = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}), \quad \forall \delta \mathbf{x} \in \mathbb{V}^0 \quad (88)$$

where

$$\begin{aligned} l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}) \stackrel{\text{def}}{=} & \int_{\partial(\Omega_X^-)} [-[\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} + \delta \mathbf{x} \cdot \mathbf{b}_X - k \delta \mathbf{x} \cdot \mathbf{t}_X \\ & + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}]] \, d\dot{\mathbf{X}}^{(1,2)} \cdot \mathbf{N} \, dS_X \\ & + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X \otimes \hat{\mathbf{M}} + \mathbf{t}_X^- \otimes \hat{\mathbf{M}}^-] \cdot d\dot{\mathbf{X}}^{(1,2)} \, dL_X \end{aligned} \quad (89)$$

However, if we impose the conditions (i) $d\dot{\mathbf{X}}^{(1,2)} \cdot \mathbf{N} = 0$ on $\partial(\Omega_X^-)$ and (ii) $d\dot{\mathbf{X}}^{(1,2)} = \mathbf{0}$ along \mathcal{C}_X , which situation is illustrated in Figure 5, then it is obvious that $l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}^{(1,2)}) = 0$. Hence, it is concluded that $(\mathbf{v}^{(1,2)})' = \mathbf{0}$ in Ω_X^- . Similarly, we may consider the part Ω_X^+ and conclude that $(\mathbf{v}^{(1,2)})' = \mathbf{0}$ in Ω_X^+ under the same assumptions. We have thus shown that $(\mathbf{v}^{(1)})' = (\mathbf{v}^{(2)})' = \mathbf{v}'$ is unique in the entire domain Ω_X , from which it is concluded that $(\mathbf{D}_t \mathbf{F})'$ is unique and, finally, $(\mathbf{D}_t \underline{k})'$ is unique (which will also be verified numerically below).

In summary, we have shown that \mathcal{G}^{MAT} will not be affected by the particular choice of the variation $d\dot{\mathbf{X}}$ in the entire domain Ω_X as long as the conditions (i) and (ii) are satisfied. That $\mathcal{G}^{\text{CONF}}$ is not affected by the choice of $d\dot{\mathbf{X}}$ whatsoever is clear from (78).

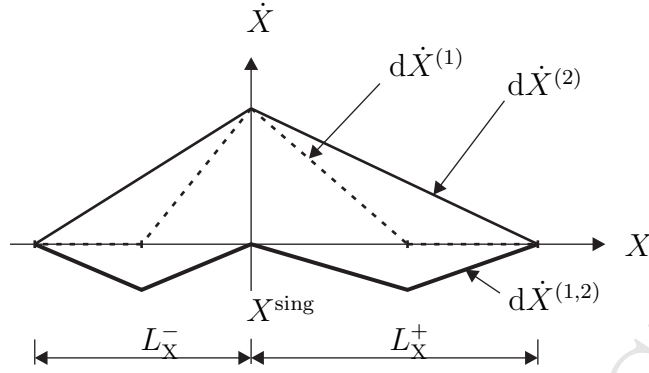


Figure 5: Two choices of $d\dot{\mathbf{X}}$ which give the same field $(D_t \underline{\mathbf{k}})'$ and, hence, identical values of \mathcal{G}^{MAT} .

7. Numerical example: Plate with interface separating parts with dissimilar material properties

7.1. Elastic-plastic model – Linearized format

We adopt a simple elastic-plastic model based on the von Mises yield criterion with isotropic hardening. A linearization of the spatially objective large deformation formulation is obtained by introducing the volume-specific free energy as

$$\psi_{\mathbf{X}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}, k) = \psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}) + \psi_{\mathbf{X}}^{\text{p}}(k) \quad (90)$$

where the part $\psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}})$ represents linear elasticity and is given as

$$\psi_{\mathbf{X}}^{\text{e}}(\mathbf{F}, \boldsymbol{\epsilon}^{\text{P}}) = \frac{1}{2} [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] : \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] \quad (91)$$

with $\mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}}) \stackrel{\text{def}}{=} \mathbf{I} + \boldsymbol{\epsilon}^{\text{P}}$, and where $\psi_{\mathbf{X}}^{\text{p}}(k)$ is the "plastic" (or rather hardening) free energy corresponding to isotropic hardening and given as

$$\psi_{\mathbf{X}}^{\text{p}}(k) = \frac{1}{2} H k^2 \quad (92)$$

In (91), we introduced the constant "small strain" stiffness tensor in standard fashion representing isotropic linear elastic properties

$$\mathbf{E}^{\text{e}} = 2G \mathbf{I}_{\text{dev}}^{\text{sym}} + K \mathbf{I} \otimes \mathbf{I}, \quad \mathbf{I}_{\text{dev}}^{\text{sym}} = \mathbf{I}^{\text{sym}} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I} \quad (93)$$

where G and K are the shear and bulk moduli, respectively. In (92), H is the constant isotropic hardening modulus. Obviously, this model gives the thermodynamically consistent stresses

$$\mathbf{P} = \frac{\partial \psi_{\mathbf{X}}}{\partial \mathbf{F}} = \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] \quad (94)$$

$$\boldsymbol{\sigma}^{\text{P}} = -\frac{\partial \psi_{\mathbf{X}}}{\partial \boldsymbol{\epsilon}^{\text{P}}} = \mathbf{E}^{\text{e}} : [\mathbf{F} - \mathbf{F}^{\text{P}}(\boldsymbol{\epsilon}^{\text{P}})] = \mathbf{P} \quad (95)$$

$$K = -\frac{\partial \psi_{\mathbf{X}}}{\partial k} = -Hk \quad (96)$$

We may thus express the (local) volume-specific material rate of dissipation $d_X = \underline{K} \star D_t \underline{k}$ according to (29) with the matrices \underline{k} and \underline{K} defined as

$$\underline{k} \stackrel{\text{def}}{=} \begin{bmatrix} \boldsymbol{\epsilon}^P \\ k \end{bmatrix}, \quad \underline{K} \stackrel{\text{def}}{=} \begin{bmatrix} \mathbf{P} \\ K \end{bmatrix} \quad (97)$$

The von Mises yield criterion with isotropic hardening is expressed as

$$\Phi(\mathbf{P}, K) = P_e - [Y + K] = 0, \quad P_e \stackrel{\text{def}}{=} \sqrt{\frac{3}{2}} |\mathbf{P}_{\text{dev}}| \quad (98)$$

where Y is the uniaxial yield stress and P_e is the effective (1st Piola-Kirchhoff) stress.

To complete the model, we adopt the evolution rules of the associated type, i.e.

$$D_t \boldsymbol{\epsilon}^P = \lambda \frac{\partial \Phi}{\partial \mathbf{P}} = \lambda \frac{3 \mathbf{P}_{\text{dev}}}{2 P_e} \quad (99)$$

$$D_t k = \lambda \frac{\partial \Phi}{\partial K} = -\lambda \quad (100)$$

where λ is the plastic multiplier. Due to the linearized structure and since \mathbf{E}^e has both major and minor symmetry, \mathbf{P} becomes symmetrical; hence, the conventional small strain model is retrieved in the case that deformations are indeed small such that $|\boldsymbol{\epsilon}^P| \ll 1$.

Next, we obtain from (56) the basic tangent operators

$$\mathbf{L}^e \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \Big|_{\mathbf{k}, X} = \mathbf{E}^e, \quad \underline{\mathbf{M}} \stackrel{\text{def}}{=} \frac{\partial \mathbf{P}}{\partial \underline{\mathbf{k}}} \Big|_{\mathbf{F}, X} = \begin{bmatrix} \frac{\partial \mathbf{P}}{\partial \boldsymbol{\epsilon}^P} \\ \frac{\partial \mathbf{P}}{\partial k} \end{bmatrix} = \begin{bmatrix} -\mathbf{E}^e \\ \mathbf{0} \end{bmatrix} \quad (101)$$

In order to obtain explicit expressions of the tangent operators $\underline{\mathbf{R}}_T$ and \mathbf{L}_T , defined in (60) and (61), respectively, we may evaluate the condition $D_t \Phi = 0$ at plastic loading for "deformation control" to compute the state functions

$$h = 3G + H, \quad \boldsymbol{\mu} = \frac{3G}{P_e} \mathbf{P}_{\text{dev}}, \quad \underline{\mathbf{g}} = \begin{bmatrix} \frac{3}{2P_e} \mathbf{P}_{\text{dev}} \\ -1 \end{bmatrix} \quad (102)$$

and we obtain

$$\mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{E}^e - \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \boldsymbol{\mu} \otimes \boldsymbol{\mu}, \quad \Delta \mathbf{L}_T \stackrel{\text{def}}{=} \mathbf{L}_T - \mathbf{L}^e = -\frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \boldsymbol{\mu} \otimes \boldsymbol{\mu} \quad (103)$$

where it was used that $\underline{\mathbf{M}} \star \underline{\mathbf{g}} = -\boldsymbol{\mu}$. Finally, we may use (101) and (102) to obtain

$$\begin{aligned} \mathcal{G}_i^{\text{MAT}} &= \int_{\Omega_X^p} \underline{K} \star \underline{\mathbf{R}}_T : (D_t \mathbf{F})' dV_X = \int_{\Omega_X^p} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} \underline{K} \star \underline{\mathbf{g}} \boldsymbol{\mu} : (D_t \mathbf{F})' dV_X \\ &= \int_{\Omega_X^p} \frac{1}{h} \frac{\langle \boldsymbol{\mu} : D_t \mathbf{F} \rangle}{|\boldsymbol{\mu} : D_t \mathbf{F}|} Y \boldsymbol{\mu} : (D_t \mathbf{F})' dV_X \end{aligned} \quad (104)$$

In order to obtain the last expression in (104), we used that $\underline{K} \star \underline{g} = P_e - K = Y$ in the plastic domain Ω_X^p , defined by the current state satisfying the yield criterion, $\Phi = 0$.

When the quantities $\mathcal{G}_i^{\text{MAT}}$, which correspond to nodal values da_i , are known, it is possible to "localize" the "configurational traction" \mathcal{G}^{MAT} via the *ansatz*, cf. Figure 6,

$$\mathcal{G}^{\text{MAT}} = \sum_{j=1}^{N_W} \mathbf{W}_j \bar{\mathcal{G}}_j^{\text{MAT}} \quad (105)$$

where $\bar{\mathcal{G}}_i^{\text{MAT}}$ and \mathbf{W}_i , $i = 1, 2, \dots, N_W$, are the nodal values (intensities) and the basis functions, respectively. A least squares projection on the set of basis functions in the sense that

$$\mathcal{G}_i^{\text{MAT}} = \int_{\Gamma_X^{\text{sing}}} \mathcal{G}^{\text{MAT}} \cdot \mathbf{W}_i \, dS_X \quad (106)$$

then gives the intensities $\bar{\mathcal{G}}_i^{\text{MAT}}$, collected in the column matrix $\underline{\bar{\mathcal{G}}}^{\text{MAT}} = [\bar{\mathcal{G}}_1^{\text{MAT}}, \bar{\mathcal{G}}_2^{\text{MAT}}, \dots, \bar{\mathcal{G}}_{N_W}^{\text{MAT}}]^T$, from the matrix equation

$$\underline{W} \underline{\bar{\mathcal{G}}}^{\text{MAT}} = \underline{\mathcal{G}}^{\text{MAT}}, \quad W_{ij} \stackrel{\text{def}}{=} \int_{\Gamma_X^{\text{sing}}} \mathbf{W}_i \cdot \mathbf{W}_j \, dS_X \quad (107)$$

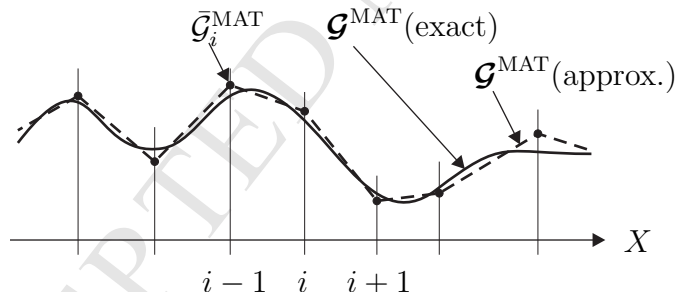


Figure 6: Representation of \mathcal{G}^{MAT} in terms of the nodal values on Γ_X^{sing} for a given FE-mesh.

7.2. Problem formulation

Consider a plate in plane strain, with length L and width $H = 0.5L$, which is subjected to prescribed end displacements at the right end, as shown in Figure 7(a). The maximal displacement is $\bar{u}_{\text{max}}/L = 0.5 \cdot 10^{-3}$. This is the sole loading, i. e. $\mathbf{b}_X = \mathbf{0}$ in Ω_X and $\bar{\mathbf{t}}_X = \mathbf{0}$ on $\partial\Omega_{X,N}$. Since we shall also assume that $d\dot{\mathbf{X}} \cdot \mathbf{N} = 0$ on the external boundary $\partial\Omega_X$, we obtain the following simplified version of (83) as the data for the tangent problem:

$$\begin{aligned} l_T^{(\dot{x})}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}) = & \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : [d\dot{\mathbf{X}} \otimes \nabla_X] \right. \\ & \left. + \mathbf{L}_T : \left[\mathbf{F} \cdot [d\dot{\mathbf{X}} \otimes \nabla_X] \right] + \mathbf{r}_X \cdot d\dot{\mathbf{X}} \right] dV_X \end{aligned} \quad (108)$$

Using the fact that the material properties are homogeneous in each of the two subdomains separated by the singular surface, i.e. $\frac{\partial \mathbf{P}}{\partial \mathbf{X}}|_{\mathbf{F},k} = \mathbf{0}$, it is possible to reformulate \mathbf{r}_X , the general expression of which was given in (75), more explicitly as

$$\mathbf{r}_X = \Delta \mathbf{L}_T : [\mathbf{F} \otimes \nabla_X] + \mathbf{E}^e : [\epsilon^p \otimes \nabla_X] \quad (109)$$

where $\Delta \mathbf{L}_T$ was given in (103).

The material parameters for the elastic-plastic model are: $E, \nu = 0.3, Y, H$ with $E_{\text{ref}}, Y_{\text{ref}} = 0.001 E_{\text{ref}}, H_{\text{ref}} = 0.2 E_{\text{ref}}$. They assume different values on each side of the interface, as shown schematically in Figure 7(b).

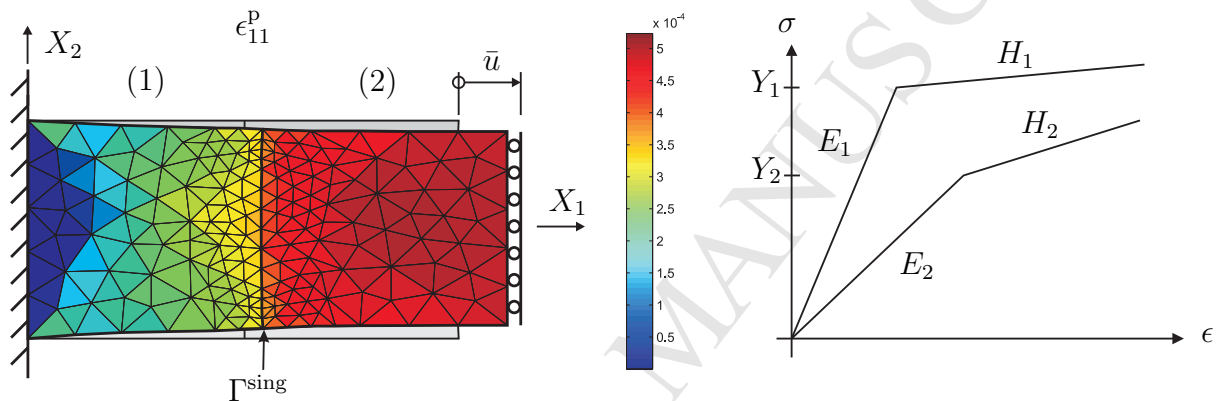


Figure 7: Plate in plane strain with discontinuity in material properties along central interface. (a) Deformed configuration and plastic deformations for $\bar{u}/\bar{u}_{\text{max}} = 1$, (b) Linear elastic-hardening stress-strain response curves.

7.3. Numerical results

The first set of computations were carried out to verify the theoretical result in Subsubsection 6.3.2 that the values of both $\mathcal{G}^{\text{CONF}}$ and \mathcal{G}^{MAT} are independent of the choice of the variation of $\dot{\mathbf{X}}$ under certain conditions. To this end, we considered three different fields $d\dot{\mathbf{X}}_i$, $i = I, II, III$, which all satisfied the condition that $d\dot{\mathbf{X}}_i \cdot \mathbf{N} = 1$ on Γ^{sing} , and that $d\dot{\mathbf{X}}_i \cdot \mathbf{N} = c(\mathbf{X})$ for $\mathbf{X} \in \partial\Omega_X$, where $c(\mathbf{X})$ is a given function. Otherwise, the fields differed from each other only in the interior of Ω_X , as shown in Figure 8. As a consequence, all the requirements discussed in Subsubsection 6.3.2 for satisfying the condition $l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_I - d\dot{\mathbf{X}}_{II}) = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_{II} - d\dot{\mathbf{X}}_{III}) = l_T^{(v)}(\bullet; \delta \mathbf{x}, d\dot{\mathbf{X}}_{III} - d\dot{\mathbf{X}}_I) = 0$ in both the left and right part of the singular surface in Figure 7 were satisfied. Indeed, the numerical results verified that the values of $\mathcal{G}^{\text{CONF}}$ and \mathcal{G}^{MAT} were the same for all three fields $d\dot{\mathbf{X}}_i$ in Figure 8.

Next, the mesh (in)sensitivity and convergence properties for mesh refinement were studied for two types of element approximations: linear (CTS) and quadratic (LST) displacement approximation. The results are depicted in Figure 9, and they show that the quadratic element approximation gives superior convergence properties (as expected).

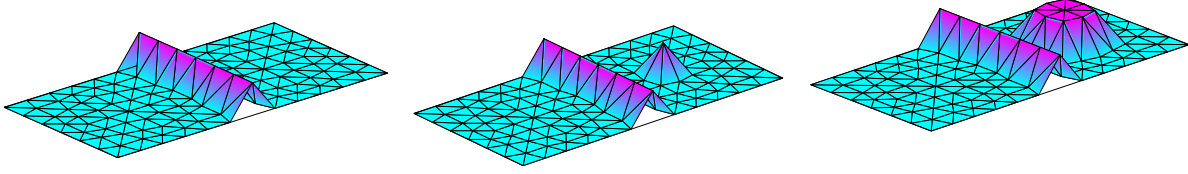


Figure 8: Choice of variations of the field $d\mathbf{X}_i$, $i = I, II, III$. All choices give identical results of the sensitivity \mathbf{v}' .

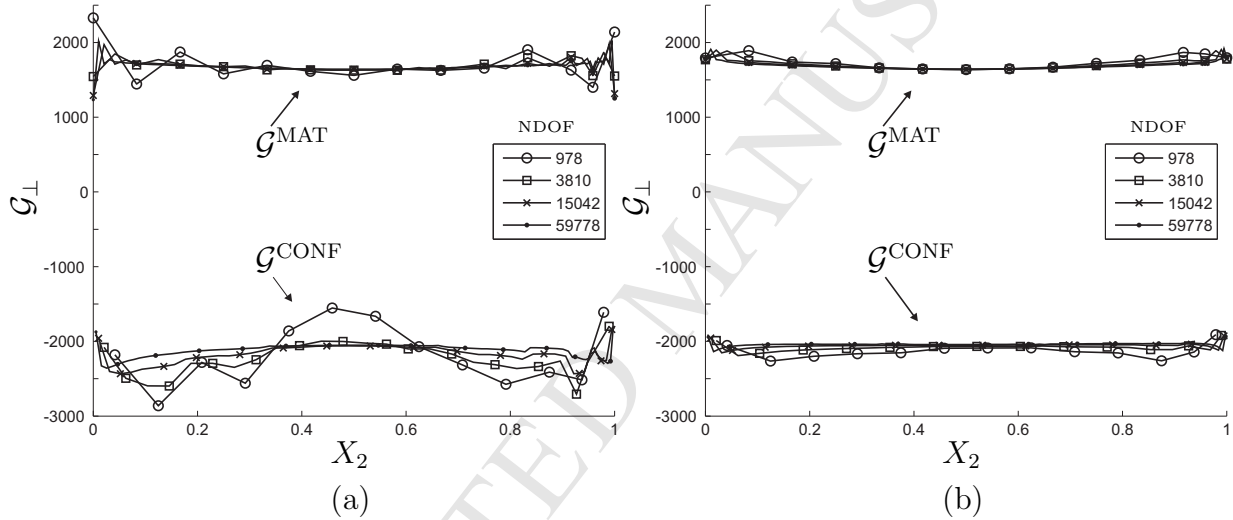


Figure 9: Mesh-sensitivity/convergence of components (fields) $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of the material data: $E_2 = 0.5E_{\text{ref}}$. All results obtained for $\bar{u}/\bar{u}_{\text{max}} = 1$.

The next series of computations concerned the development of $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ with increasing (prescribed) displacement, while it was assumed that there is a mismatch across the interface of the elastic and the plastic (hardening) properties. These results are shown in Figure 10.

In order to further provoke the triaxiality in the stress and strain states, we next considered the case when a circular hole is introduced in the right part of the plate, as shown in Figure 11(a). The base set of material parameter values are still the same as those given in Figure 7(b).

The distribution of components $\mathcal{G}_{\perp}^{\text{CONF}}$, $\mathcal{G}_{\perp}^{\text{MAT}}$ and $\mathcal{G}_{\perp} = \mathcal{G}_{\perp}^{\text{CONF}} + \mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of elasticity, $E_2 = 0.5E_{\text{ref}}$, are shown in Figure 12 for the LST approximation and a mesh that represents a converged state.

The final series of computations concerned the development of $\mathcal{G}_{\perp}^{\text{CONF}}$ and $\mathcal{G}_{\perp}^{\text{MAT}}$ with increasing (prescribed) displacement, while it was assumed that there is a mismatch across

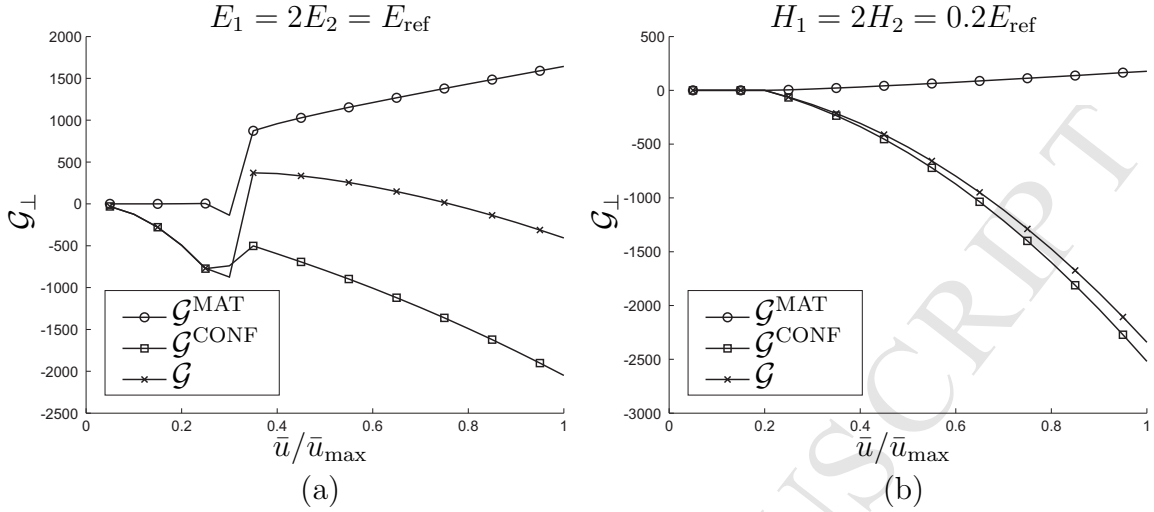


Figure 10: Development of components $\mathcal{G}_\perp^{\text{CONF}}$, $\mathcal{G}_\perp^{\text{MAT}}$ and $\mathcal{G}_\perp = \mathcal{G}_\perp^{\text{CONF}} + \mathcal{G}_\perp^{\text{MAT}}$ with increasing loading (prescribed displacement) for (a) mismatch of elasticity: $E_2 = 0.5E_{\text{ref}}$, and (b) mismatch of hardening: $H_2 = 0.5H_{\text{ref}}$.

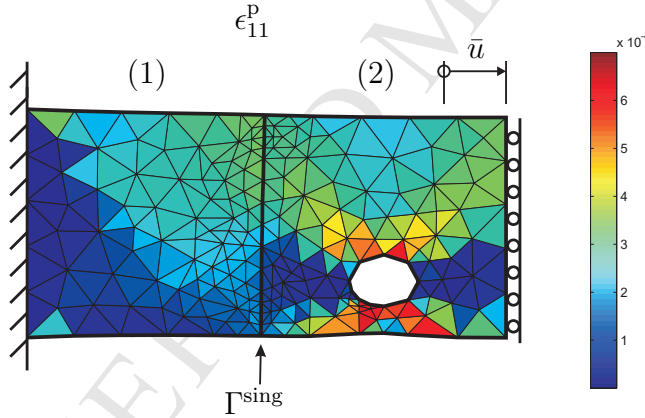


Figure 11: Plate in plane strain with discontinuity in material properties along central interface and with eccentric hole. Deformed configuration and plastic deformations for $\bar{u}/\bar{u}_{\text{max}} = 1$.

the interface of the elastic and the plastic (hardening) properties. These results are shown in Figure 13.

8. Discussion, conclusions and outlook

In this paper we have presented a novel investigation in the context of configurational changes for a rate-independent dissipative material; namely, we considered the *total variation* of the rate of global dissipation with respect to the rate of configurational motion. Such a variation may, alternatively, be considered as the evaluation of the *total sensitivity* due to configurational changes, which may be brought about (in their turn) by physical

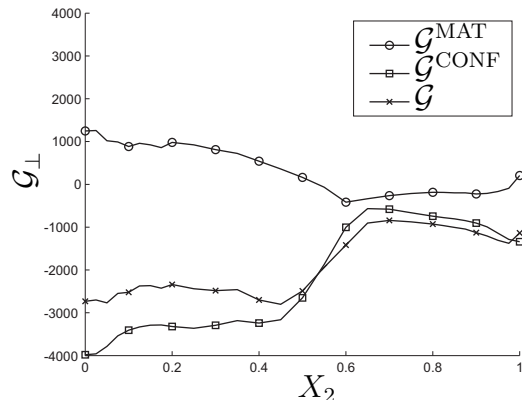


Figure 12: Distribution of components $\mathcal{G}_{\perp}^{\text{CONF}}$, $\mathcal{G}_{\perp}^{\text{MAT}}$ and $\mathcal{G}_{\perp} = \mathcal{G}_{\perp}^{\text{CONF}} + \mathcal{G}_{\perp}^{\text{MAT}}$ along Γ_X^{sing} for mismatch of elasticity: $E_2 = 0.5E_{\text{ref}}$. All results obtained for $\bar{u}/\bar{u}_{\text{max}} = 1$.

changes. It is then clear that the *material part of the dissipation* is indeed coupled (and sensitive) to configurational changes. However, it is not at all clear how to use this information. The classical approach in defining the "driving force" for configurational changes, advocated in the current literature, is to account only for the explicit part of the total configurational force, denoted $\mathcal{G}^{\text{CONF}}$ in this paper. An alternative, perhaps more natural, approach is to assume that the "driving force" for configurational changes is identified precisely by the total sensitivity, which means that the total configurational force \mathcal{G} is the proper choice in constitutive models for configurational changes. Whatever the choice made, it is clearly a model assumption.

The paper discussed essentially two aspects: (1) How to formulate (or construct) the total dissipation in the presence of configurational changes, and (2) how to compute the total sensitivity of the global dissipation via the appropriate formulation of a tangent problem. In the present paper only isothermal (thermomechanically uncoupled) quasistatic problems are considered, which means that the only balance equation for establishing the pertinent tangent problem is the standard equilibrium equation. We remark that we chose to linearize the weak form of equilibrium by observing that the virtual (test) functions are time-invariant in the absolute configuration \mathcal{B}_{ξ} ; however, it would have been possible to linearize the strong format of equilibrium in \mathcal{B}_{ξ} , establish the weak format and, finally, push forward to obtain the tangent problem in \mathcal{B}_X .

A few issues deserve further comments: The tangent stiffness \mathbf{L}_T appearing in the "sensitivity version" of the constitutive continuum tangent relation (61) in the case of plastic loading (L) is not necessarily identical to the actual \mathbf{L}^{ep} for two reasons: (1) the relation (57) represents essentially a nonlinear (bilinear) relation in $D_t \mathbf{F}$, (2) \mathbf{L}_T can be linearized at the *actual* value of $\dot{\mathbf{X}}$ or at $\dot{\mathbf{X}} = \mathbf{0}$ corresponding to a stationary singular surface. If we choose the actual value of $\dot{\mathbf{X}}$ it is obvious that \mathcal{G}^{MAT} depends on the solution to the physical motion problem at each point in time. Hence, if indeed \mathcal{G}^{MAT} is part of the "driving force", then the computation of the sensitivity problem is nonlinear and can only be carried out for a given field $\dot{\mathbf{X}}$ as part of an iteration process to compute the actual

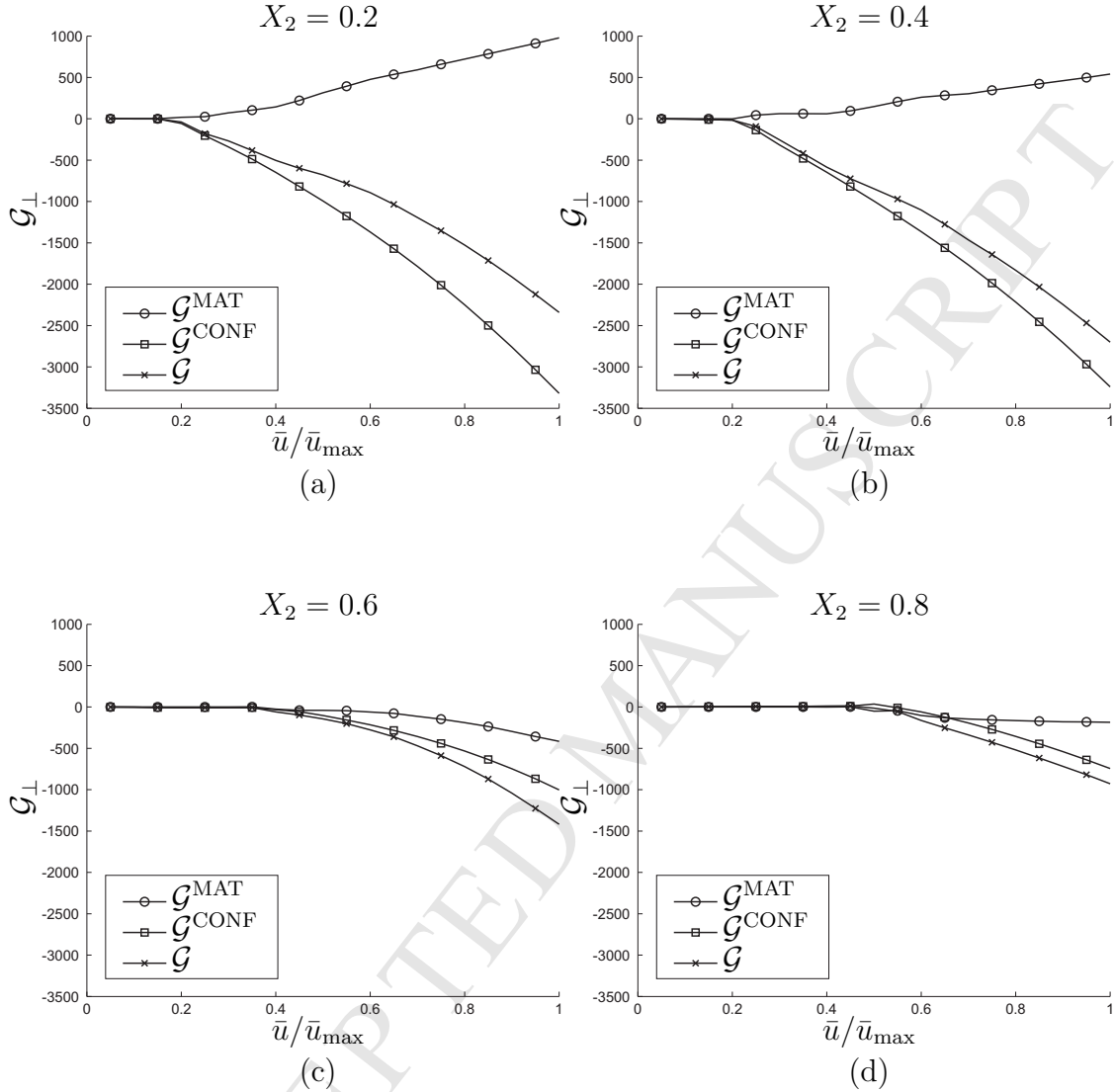


Figure 13: Development of components $\mathcal{G}_\perp^{\text{CONF}}$, $\mathcal{G}_\perp^{\text{MAT}}$ and $\mathcal{G}_\perp = \mathcal{G}_\perp^{\text{CONF}} + \mathcal{G}_\perp^{\text{MAT}}$ with increasing loading (prescribed displacement) for mismatch of hardening: $H_2 = 0.5H_{\text{ref}}$. Results are given for different positions across the interface: (a) $X_2 = 0.2$, (a) $X_2 = 0.4$, (a) $X_2 = 0.6$, (a) $X_2 = 0.8$.

field $\dot{\mathbf{X}}$.

It was shown theoretically that the variation $d\dot{\mathbf{X}}$ can be chosen arbitrarily in the interior of the material domain $\Omega_{\mathbf{X}}$ without affecting the value of \mathcal{G}^{MAT} , as long as certain conditions on the external boundary and the singular interface are satisfied. This was confirmed by numerical results for selected choices of $d\dot{\mathbf{X}}$. For uniform cross-section of the investigated plate, a separate parameter study (not discussed explicitly in the paper) showed, in the case $\nu \rightarrow 0$, that $\mathcal{G}_\perp^{\text{MAT}}$ converges to the value that is obtained for uniaxial stress (which confirms the soundness of the numerical evaluation). The numerical results obtained for dissimilar material properties across the singular surface showed that a misfit

in the elasticity modulus resulted in larger value of $\mathcal{G}_\perp^{\text{MAT}}$ than did a misfit in the hardening modulus.

Although it follows from the local (strong) version of dissipation inequality that $\bar{\mathcal{D}}(\dot{\underline{k}}) \geq 0$ must always hold, it is possible that the corresponding sensitivity to configurational changes becomes non-positive, i.e. $\bar{\mathcal{D}}^{\text{MAT}}(\text{d}\dot{\underline{X}}, \dot{\underline{k}}\{\dot{\underline{X}}; \text{d}\dot{\underline{X}}\}) \leq 0$ is certainly possible. An example of this situation is given in Figure 13 for the two last cross-sections (for the plate with a hole), where it appears that $\mathcal{G}_\perp^{\text{MAT}} \leq 0$.

Whenever in doubt, we checked the results by numerical differentiation. This is doable since we are interested in the total variation of the global dissipation (and not only a partial variation corresponding to $\mathcal{G}^{\text{CONF}}$). As to the practical calculation of the configurational force, it appears that the classical configurational rate, $\mathcal{G}^{\text{CONF}}$, is *spatially localized a priori* to a singular surface by the analytical expression. On the other hand, the material rate of dissipation, \mathcal{G}^{MAT} , is *spatially localizable a posteriori* via a suitable parametrization and least squares projection (in practice) on the FE-shape functions.

Finally, we mention some possible future developments. The total configurational force \mathcal{G} will be exploited as the "driving force" in a crack-propagation model for fatigue cracks in railway steel under complex loading. As to the efficient computation of global dissipation for the mesh-parametrized material motion, it is possible to use a so-called "dual" method, whereby only one single dual solution is needed even if there are a multitude of nodal values \mathcal{G}_i to compute, cf. the sensitivity problem in the context of parameter identification discussed by Johansson et al. (2007).

9. Acknowledgements

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A. Appendix

A.1. Tangent problem – Format based on $\dot{\mathbf{x}}$

The derivations leading to (70) with (71) and (72) are outlined as follows: From the definition of $a(\mathbf{x}, \underline{k}; \delta \mathbf{x})$ in (64), together with the identity in (13), we derive

$$\begin{aligned} \frac{\text{d}}{\text{d}t} a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) &= \int_{\Omega_{\mathbf{x}}} [\Delta_t[\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \mathbf{P} + [\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \Delta_t \mathbf{P} + \\ &\quad [\delta \mathbf{x} \otimes \nabla_{\mathbf{x}}] : \mathbf{P} \otimes \dot{\underline{X}} \cdot \nabla_{\mathbf{x}}] \text{d}V_{\mathbf{x}} \end{aligned} \quad (1)$$

Upon using the relations

$$\begin{aligned} \Delta_t \mathbf{P} &= \text{D}_t \mathbf{P} + [\mathbf{P} \otimes \nabla_{\mathbf{x}}] \cdot \dot{\underline{X}} \\ &= \text{D}_t \mathbf{P} + [\mathbf{L}^e : [\mathbf{F} \otimes \nabla_{\mathbf{x}}] + \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_{\mathbf{x}}] + \frac{\partial \mathbf{P}}{\partial \underline{\mathbf{X}}} \Big|_{\mathbf{F}, \underline{k}} \cdot \dot{\underline{X}} \end{aligned} \quad (2)$$

together with (68), we may reformulate this expression in (1) as

$$\begin{aligned} \frac{d}{dt}a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) &= \int_{\Omega_X} \left[[\delta \mathbf{x} \otimes \nabla_X] : D_t \mathbf{P} - [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{P} : [\dot{\mathbf{X}} \otimes \nabla_X] \right. \\ &\quad \left. + [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{L}^e : [\mathbf{F} \otimes \nabla_X] + \underline{\mathbf{M}} \star [\underline{k} \otimes \nabla_X] + \frac{\partial \mathbf{P}}{\partial \mathbf{X}}|_{F, \underline{k}} \cdot \dot{\mathbf{X}}] \right] dV_X \end{aligned} \quad (3)$$

Now, taking the total variation of (3) w.r.t. $\dot{\mathbf{X}}$, while using the tangent relation (60) expressed explicitly as

$$(D_t \mathbf{P})' = \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X - [\mathbf{F} \cdot d\dot{\mathbf{X}}] \otimes \nabla_X] \quad (4)$$

we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt}a(\mathbf{x}, \underline{k}; \delta \mathbf{x}) \right] &= \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\dot{\mathbf{x}}' \otimes \nabla_X] dV_X \\ &\quad - \int_{\Omega_X} [\delta \mathbf{x} \otimes \nabla_X] : \left[\mathbf{P} : [d\dot{\mathbf{X}} \otimes \nabla_X] + \mathbf{L}_T : [\mathbf{F} \cdot [d\dot{\mathbf{X}} \otimes \nabla_X]] \right. \\ &\quad \left. + \mathbf{r}_X \cdot d\dot{\mathbf{X}} \right] dV_X \end{aligned} \quad (5)$$

Next, from the definition of $l(\delta \mathbf{x})$ in (65) together with (13) and (15), we derive

$$\begin{aligned} \frac{d}{dt}l(\delta \mathbf{x}) &= \int_{\Omega_X} D_t[\delta \mathbf{x} \cdot \mathbf{b}_X] dV_X + \int_{\partial \Omega_X} [\delta \mathbf{x} \cdot \mathbf{b}_X] \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{\partial \Omega_{X,N}} [\hat{D}_t[\delta \mathbf{x} \cdot \mathbf{t}_X] - k[\delta \mathbf{x} \cdot \mathbf{t}_X] \dot{\mathbf{X}} \cdot \mathbf{N}] dS_X \\ &\quad + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_X \end{aligned} \quad (6)$$

where we used that $\delta \mathbf{x}$ and $\dot{\mathbf{X}}$ are continuous on $\partial \Omega_X$, in particular across \mathcal{C}_X .

In order to obtain operational expressions, we note the relations

$$D_t[\delta \mathbf{x} \cdot \mathbf{b}_X] = D_t[\delta \mathbf{x}] \cdot \mathbf{b}_X + \delta \mathbf{x} \cdot D_t \mathbf{b}_X = -[\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes \dot{\mathbf{X}}] + \delta \mathbf{x} \cdot D_t \mathbf{b}_X \quad \text{in } \Omega_X \quad (7)$$

$$\hat{D}_t[\delta \mathbf{x} \cdot \mathbf{t}_X] = \hat{D}_t[\delta \mathbf{x}] \cdot \mathbf{t}_X + \delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X = -[\delta \mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes \dot{\mathbf{X}}] + \delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X \quad \text{on } \partial \Omega_X \quad (8)$$

where we used the relations (4), (9) and (68), which may be inserted into (6) to give

$$\begin{aligned} \frac{d}{dt}l(\delta \mathbf{x}) &= \int_{\Omega_X} \left[\delta \mathbf{x} \cdot D_t \mathbf{b}_X - [\delta \mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes \dot{\mathbf{X}}] \right] dV_X \\ &\quad + \int_{\partial \Omega_X} \left[\delta \mathbf{x} \cdot \hat{D}_t \mathbf{t}_X - [\delta \mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes \dot{\mathbf{X}}] \right] dS_X \\ &\quad + \int_{\partial \Omega_X} [[\delta \mathbf{x} \cdot \mathbf{b}_X] - k[\delta \mathbf{x} \cdot \mathbf{t}_X]] \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{\mathcal{C}_X} \delta \mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_X \end{aligned} \quad (9)$$

Upon taking the total variation of (9) w.r.t. $\dot{\mathbf{X}}$, while assuming that \mathbf{b}_X , \mathbf{t}_X , $D_t\mathbf{b}_X$ and $\hat{D}_t\mathbf{t}_X$ are independent on $\dot{\mathbf{X}}$, i.e.

$$\mathbf{b}'_X = \mathbf{t}'_X = (D_t\mathbf{b}_X)' = (\hat{D}_t\mathbf{t}_X)' = \mathbf{0} \quad (10)$$

we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} l(\delta\mathbf{x}) \right] &= - \int_{\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : [\mathbf{b}_X \otimes d\dot{\mathbf{X}}] dV_X \\ &\quad - \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \hat{\nabla}_X] : [\mathbf{t}_X \otimes d\dot{\mathbf{X}}] dS_X \\ &\quad + \int_{\partial\Omega_X} [[\delta\mathbf{x} \cdot \mathbf{b}_X] - k[\delta\mathbf{x} \cdot \mathbf{t}_X]] d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \\ &\quad + \int_{c_X} \delta\mathbf{x} \cdot [\mathbf{t}_X^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_X^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_X \end{aligned} \quad (11)$$

Remark: Assuming that $\hat{D}_t\mathbf{t}_X$ does not depend on $\dot{\mathbf{X}}$ pertains to the assumption that \mathbf{t}_X is defined only on $\partial\Omega_X$. \square

Finally, upon using (5) and (11), we may rephrase (70) as

$$a_T(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_T^{(\dot{\mathbf{x}})}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (12)$$

where the tangent forms a_T and $l_T^{(\dot{\mathbf{x}})}$ are given in (72) and (73), respectively.

A.2. Tangent problem – Format based on \mathbf{v}

The derivations leading to (76) with (77) are outlined as follows: From the definition of $a(\mathbf{x}, \underline{k}; \delta\mathbf{x})$ in (64), together with the identity in (13), we derive

$$\begin{aligned} \frac{d}{dt} a(\mathbf{x}, \underline{k}; \delta\mathbf{x}) &= \int_{\Omega_X} [[D_t[\delta\mathbf{x}] \otimes \nabla_X] : \mathbf{P} + [\delta\mathbf{x} \otimes \nabla_X] : D_t\mathbf{P}] dV_X \\ &\quad + \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{P} \otimes \dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (13)$$

where we used the relation $D_t[\delta\mathbf{x} \otimes \nabla_X] = D_t[\delta\mathbf{x}] \otimes \nabla_X$.

Taking the total variation of (13) w.r.t. $\dot{\mathbf{X}}$, while using the tangent relation (60), we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt} a(\mathbf{x}, \underline{k}; \delta\mathbf{x}) \right] &= \int_{\Omega_X} [[(D_t[\delta\mathbf{x}])' \otimes \nabla_X] : \mathbf{P} + [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{L}_T : [\mathbf{v}' \otimes \nabla_X]] dV_X \\ &\quad + \int_{\partial\Omega_X} [\delta\mathbf{x} \otimes \nabla_X] : \mathbf{P} \otimes d\dot{\mathbf{X}} \cdot \mathbf{N} dS_X \end{aligned} \quad (14)$$

As to the time-derivative of $l(\delta\mathbf{x})$, the expression (6) is taken as the point of departure. While the decomposition of $D_t[\delta\mathbf{x} \cdot \mathbf{b}_X]$ in (7) is retained, we shall use the following decomposition of $\hat{D}_t[\delta\mathbf{x} \cdot \mathbf{t}_X]$, instead of (8):

$$\hat{D}_t[\delta\mathbf{x} \cdot \mathbf{t}_X] = D_t[\delta\mathbf{x}] \cdot \mathbf{t}_X + [\delta\mathbf{x} \otimes \nabla_X] : [\mathbf{t}_X \otimes \mathbf{N}] \dot{\mathbf{X}} \cdot \mathbf{N} + \delta\mathbf{x} \cdot \hat{D}_t\mathbf{t}_X \quad (15)$$

where we used the relation (10) to replace $\hat{D}_t[\delta\mathbf{x}]$ by $D_t[\delta\mathbf{x}] + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] \cdot \mathbf{N}[\dot{\mathbf{X}} \cdot \mathbf{N}]$. Upon introducing the relations (13) and (15) in (6), we obtain

$$\begin{aligned} \frac{d}{dt}l(\delta\mathbf{x}) &= \int_{\Omega_{\mathbf{X}}} [\delta\mathbf{x} \cdot D_t\mathbf{b}_{\mathbf{X}} + D_t[\delta\mathbf{x}] \cdot \mathbf{b}_{\mathbf{X}}] dV_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} \left[\delta\mathbf{x} \cdot \hat{D}_t\mathbf{t}_{\mathbf{X}} + D_t[\delta\mathbf{x}] \cdot \mathbf{t}_{\mathbf{X}} + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] : [\mathbf{t}_{\mathbf{X}} \otimes \mathbf{N}]\dot{\mathbf{X}} \cdot \mathbf{N} \right] dS_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} [\delta\mathbf{x} \cdot \mathbf{b}_{\mathbf{X}} - k[\delta\mathbf{x} \cdot \mathbf{t}_{\mathbf{X}}]] \dot{\mathbf{X}} \cdot \mathbf{N} dS_{\mathbf{X}} \\ &+ \int_{\mathcal{C}_{\mathbf{X}}} \delta\mathbf{x} \cdot [\mathbf{t}_{\mathbf{X}}^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_{\mathbf{X}}^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot \dot{\mathbf{X}} dL_{\mathbf{X}} \end{aligned} \quad (16)$$

Again, upon taking the total variation of (16) w.r.t. $\dot{\mathbf{X}}$, while assuming that $\mathbf{b}_{\mathbf{X}}$, $\mathbf{t}_{\mathbf{X}}$, $D_t\mathbf{b}_{\mathbf{X}}$ and $\hat{D}_t\mathbf{t}_{\mathbf{X}}$ are independent on $\dot{\mathbf{X}}$, i.e. (10) holds, then we obtain

$$\begin{aligned} d_{\dot{\mathbf{X}}} \left[\frac{d}{dt}l(\delta\mathbf{x}) \right] &= \int_{\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{b}_{\mathbf{X}} dV_{\mathbf{X}} \\ &+ \int_{\partial\Omega_{\mathbf{X}}} \left[(D_t[\delta\mathbf{x}])' \cdot \mathbf{t}_{\mathbf{X}} + [\delta\mathbf{x} \cdot \mathbf{b}_{\mathbf{X}} - k[\delta\mathbf{x} \cdot \mathbf{t}_{\mathbf{X}}] + [\delta\mathbf{x} \otimes \nabla_{\mathbf{X}}] : [\mathbf{t}_{\mathbf{X}} \otimes \mathbf{N}]] d\dot{\mathbf{X}} \cdot \mathbf{N} \right] dV_{\mathbf{X}} \\ &+ \int_{\mathcal{C}_{\mathbf{X}}} \delta\mathbf{x} \cdot [\mathbf{t}_{\mathbf{X}}^{(1)} \otimes \hat{\mathbf{M}}^{(1)} + \mathbf{t}_{\mathbf{X}}^{(2)} \otimes \hat{\mathbf{M}}^{(2)}] \cdot d\dot{\mathbf{X}} dL_{\mathbf{X}} \end{aligned} \quad (17)$$

Finally, upon using the divergence theorem to note that

$$\int_{\Omega_{\mathbf{X}}} [(D_t[\delta\mathbf{x}])' \otimes \nabla_{\mathbf{X}}] : \mathbf{P} dV_{\mathbf{X}} = \int_{\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{b}_{\mathbf{X}} dV_{\mathbf{X}} + \int_{\partial\Omega_{\mathbf{X}}} (D_t[\delta\mathbf{x}])' \cdot \mathbf{t}_{\mathbf{X}} dS_{\mathbf{X}}, \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (18)$$

we may use (14) and (17) together with (69) to arrive at

$$a_{\mathbf{T}}(\bullet; \delta\mathbf{x}, \dot{\mathbf{x}}') = l_{\mathbf{T}}^{(v)}(\bullet; \delta\mathbf{x}, d\dot{\mathbf{X}}), \quad \forall \delta\mathbf{x} \in \mathbb{V}^0 \quad (19)$$

where the tangent forms $a_{\mathbf{T}}$ and $l_{\mathbf{T}}^{(v)}$ are given in (71) and (76).

The reference list has been updated

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