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On the thermomechanical coupling in finite strain plasticity theory with non-linear kinematic hardening by means of incremental energy minimization

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SUMMARY

The thermomechanical coupling in finite strain plasticity theory with non-linear kinematic hardening is analyzed within the present paper. This coupling is of utmost importance in many applications, e.g., in those showing low cycle fatigue (LCF) under large strain amplitudes. Since the by now classical thermomechanical coupling originally proposed by Taylor & Quinney cannot be used directly in case of kinematic hardening, the change in heat as a result of plastic deformation is computed by applying the first law of thermodynamics. Based on this balance law, together with a finite strain plasticity model, a novel variationally consistent method is elaborated. Within this method and following Stainier & Ortiz Stainier and Ortiz (2010), all unknown variables are jointly and conveniently computed by minimizing an incrementally defined potential. In sharp contrast to previously published works, the evolution equations are a priori enforced by employing a suitable parameterization of the flow rule and the evolution equations. The advantages of this parameterization are, at least, twofold. First, it leads eventually to an unconstrained stationarity problem which can be directly applied to any yield function being positively homogeneous of degree one, i.e., the approach shows a broad range of application. Secondly, the parameterization provides enough flexibility even for a broad range of non-associative models such as kinematic hardening of Armstrong-Frederick-type. Different to Stainier and Ortiz (2010), the continuous variational problem is approximated by a standard, fully-implicit time integration. The applicability of the resulting numerical implementation is finally demonstrated by analyzing the thermodynamically coupled response for a loading cycle.

1 Introduction

Focusing on the framework of classical continuum mechanics, isothermal finite strain plasticity theory is nowadays relatively well developed and reasonably well understood. In case of isotropic models, the reader is referred to the comprehensive overview Simo (1998) and references cited therein. Currently, active research is shifting towards more realistic hardening models (see, e.g., Wang et al. (2008)) as well as to the mathematical structure of finite strain plasticity theory, cf. Mielke (2004). Surprisingly, the opposite is true in case of the fully thermomechanically coupled problem. Here, only relatively simple models have been considered so far. For instance, for the temperature induced by plastic

deformation, the over 70 years old purely empirical rule advocated in the pioneering work of Taylor & Quinney Taylor and Quinney (1934) is most frequently applied, cf. Simo (1998); Simo and Miehe (1992); Wriggers et al. (1992). This is particularly astonishing, since the understanding of the thermomechanical coupling is of utmost importance in many applications. One such typical application is metal forming. Often, the metal workpieces are heated for shaping them more easily. Another example is fatigue induced by temperature cycles (see Sauerland and Mahnken (2009)).

A physically more sound thermomechanical coupling is provided by the first law of thermodynamics itself. Starting with this law and considering the definition of the entropy, the heat change as a result of elastic and inelastic deformation can be derived, cf. Canadija and Brnic (2004, 2010); Hakansson et al. (2005); Ibrahimbegovic and Chorfi (2002). Although this procedure is well known, it is still not the common choice in constitutive models. This is particularly strange, since this approach is thermodynamically consistent and thus, it can be applied to every hardening rule. By way of contrast, the classical Tayloy-Quinney coupling can violate the second law of thermodynamics, e.g., in case of kinematic hardening, cf. Chaboche (1993a,b); Hakansson et al. (2005). Furthermore, experimental observations clearly show that the portion of the plastic stress power which transforms to heat is not constant in general as assumed in Taylor and Quinney (1934) (see Hodowany et al. (2000); Oliferuk et al. (2004); Rosakis et al. (2000) for further experiments; extended models can be found, e.g., in Kamlah and Haupt (1998); Longere and Dragon (2007)). The results of such experiments are summarized in Stainier and Ortiz (2010). Since the focus in the present paper is on the thermomechanical effects due to kinematic hardening, only the thermomechanically consistent coupling provided by the first law of thermodynamic will be considered in what follows.

Independently of the chosen coupling, numerical methods are usually required for the analysis of thermomechanical problems. Most frequently, the finite element method is employed for this reason. In this connection, the majority of implementations is based on staggered schemes, cf. Simo (1998). More precisely, instead of solving the coupled problem monolithically and simultaneously, it is decomposed into different steps. A common choice is represented by the so-called *isothermal split*. Within such methods, the coupled problem is decomposed into a purely mechanical boundary value problem (bvp) followed by a purely thermal bvp, cf. Simo and Miehe (1992); Wriggers et al. (1992). It bears emphasis that staggered schemes based on the aforementioned *isothermal split* are only conditionally stable. Fortunately, it can be shown that in case of metals such numerical problems do not occur, cf. Simo and Miehe (1992). The problem of conditional stability was solved in Armero and Simo (1993) by proposing and elaborating the so-called *adiabatic operator split*. Since the entropy is constant within the first step of this algorithm, the term *adiabatic operator split* can be misleading. As summarized in Simo (1998), staggered schemes have been used extensively for, at least, three reasons. First, the classical coupled problem leads to a non-symmetric stiffness matrix decreasing the numerical efficiency. Secondly, the mechanical and the thermal problem are often associated with different times scales and thus, require a different time integration scheme. The third point is not that critical and it is only related to the time necessary for the numerical implementation: staggered schemes do not require significant changes of already existing codes.

An effective monolithic implementation suitable for the fully coupled problem was relatively recently presented in Stainier and Ortiz (2010); Yang et al. (2006). It is based on a variationally consistent reformulation of the bvp. More explicitly, all unknown variables such as the plastic strains or the deformation follow jointly and conveniently from the stationarity condition of an energy potential. Neglecting temperature effects such varia-

tional methods in their present form were originally proposed in Ortiz and Stainier (1999) and, among others, further elaborated in Carstensen et al. (2002); Fancello et al. (2006, 2008); Miehe (2002); Mosler and Bruhns (2010). They are also referred to as *variational constitutive updates* or *incremental energy minimization*. In case of isothermal plasticity theory, the potential to be minimized is the stress power, i.e., the work necessary to go from one state to an infinitesimally neighboring new state. This allows to interpret the states predicted by the constitutive model as stable energy minimizers – a physically sound analogy to hyperelastic models. Compared to conventional approaches based on the return-mapping scheme (see Simo (1998)), variational updates show several advantages. Among others, they include the applicability of Noether's theorem, that of the framework of Γ-convergence for analyzing the existence of solutions, the introduction of a natural (energy) norm suitable for error estimation and adaptive finite element methods or the application of state of the art optimization algorithms, cf. Mosler (2010). Furthermore, variational constitutive updates lead intrinsically to a symmetric stiffness matrix and are the foundation for highly efficient time integration schemes, see Lew et al. (2004). In summary, such schemes show several advantages from a physical, mathematical as well as from an implementational point of view and avoid, similar to staggered schemes, all problems known from conventional methods. For this reason, they will be considered within the present paper.

A closer look at the variationally consistent framework as advocated in Stainier and Ortiz (2010); Yang et al. (2006) reveals that the numerical implementation presented within the cited papers has been specifically designed for von Mises-type evolution equations combined with isotropic hardening. Furthermore, although the authors write that their general framework can be applied in principle to any model falling into the range of so-called *generalized standard materials* (see Lemaitre (1985); Mandel (1972)), they do not show the respective steps necessary for this. Clearly, for many applications, non-associated evolution equations are indeed required. For instance, in case of cyclic loading, non-linear kinematic hardening represents a suitable choice. Unfortunately, the incorporation of such models within the framework as elaborated in Stainier and Ortiz (2010); Yang et al. (2006) is by no means straightforward. This is precisely, the novel contribution discussed in the present paper. For that purpose and in line with the isothermal models Mosler (2010); Mosler and Bruhns (2009), an extended principle of maximum dissipation is considered which provides enough flexibility, even for a broad range of non-associative models. Whether this principle can be applied to all *generalized standard materials*, is currently an open question. Based on the aforementioned generalized principle of maximum dissipation and in line with Mosler and Bruhns (2010), the evolution equations are a priori enforced by using a suitable parameterization. The resulting stationarity problem is thus unconstrained and can be used for developing a numerically efficient implementation. For that purpose and different to Stainier and Ortiz (2010); Yang et al. (2006), the continuous variational problem is approximated by a standard fully-implicit time integration. It will be shown that consistency of this scheme requires that the initial yield stress depends on the so-called *equilibrium temperature*. Numerical analyses of loading cycles confirm the applicability of the resulting numerical.

The paper is organized as follows: First, a general framework of finite strains plasticity theory including temperature effects is discussed in Section 2. Subsequently, specific constitutive equations are presented in more detail in Section 3. The novel contributions can be found in Sections 4 and 5. While a variationally consistent reformulation of the constitutive model is elaborated in Section 4, a novel numerical implementation relying directly on this reformulation is addressed in Section 5. Finally, a numerical example is

analyzed in Section 6 showing the applicability as well as the accuracy of the advocated constitutive update.

2 Fundamentals of thermomechanical hyperelastoplasticity at finite strains

In this section, a general framework suitable for the description of thermomechanically coupled problems possibly showing large elastic and inelastic deformations is presented. This section severs mostly for introducing the notations used within the present paper. Further details on that framework can be found elsewhere, e.g., in the comprehensive overviews Lubliner (1997); Simo (1998); Simo and Hughes (1998).

2.1 Kinematics

Following standard notations in continuum mechanics, the deformation mapping $\boldsymbol{\varphi}$ is introduced. It maps every particle $\boldsymbol{X}$ of the undeformed reference configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ to its deformed counterpart $\boldsymbol{x}$ at time t belonging to the current placement $\mathcal{B}_t \subset \mathbb{R}^3$. Based on this nonlinear mapping, the deformation gradient

$$\boldsymbol{F} := \mathrm{GRAD}\boldsymbol{\varphi} := \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}, \quad J := \det \boldsymbol{F} > 0 \tag{1}$$

can be defined as a local measure of deformation. As well known, its determinant measures the change in volume, i.e., $J = \mathrm{d}v/\mathrm{d}V$ with $\mathrm{d}V$ and $\mathrm{d}v$ being the infinitesimal volume elements corresponding to the undeformed as well as to the deformed configuration.

Considering an elastoplastic process, it is necessary to decompose the total motion of a body into elastic and plastic parts. For that purpose and in line with Lee (1969), the local and incompatible split

$$\boldsymbol{F} = \boldsymbol{F}^{\mathrm{e}} \cdot \boldsymbol{F}^{\mathrm{p}}, \quad \det \boldsymbol{F}^{\mathrm{e}} > 0, \ \det \boldsymbol{F}^{\mathrm{p}} > 0 \tag{2}$$

is adopted. Focusing on homogeneous deformations, $\boldsymbol{F}^{\mathrm{p}}$ is the gradient of the deformation associated with the fully unloaded mechanical system, while $\boldsymbol{F}^{\mathrm{e}}$ governs the stress response. More precisely and accounting for the principle of material frame indifference, the stresses are usually computed by means of the elastic right Cauchy-Green strain tensor

$$\boldsymbol{C}^{e} := [\boldsymbol{F}^{\mathrm{e}}]^T \cdot \boldsymbol{F}^{\mathrm{e}}. \tag{3}$$

Since the material response is often different for isochoric (volume preserving) and volumetric deformations, it proves convenient to decompose the elastic deformation accordingly. Consequently, the volume preserving elastic part of the deformation gradient and that of the elastic right Cauchy-Green strain tensor are introduced as

$$\bar{\boldsymbol{F}}^{\mathrm{e}} := [J^{\mathrm{e}}]^{-1/3} \boldsymbol{F}^{\mathrm{e}}, \quad J^{\mathrm{e}} = \det \boldsymbol{F}^{\mathrm{e}} \tag{4}$$

and

$$\bar{\boldsymbol{C}}^{\mathrm{e}} := (\bar{\boldsymbol{F}}^{\mathrm{e}})^T \cdot \bar{\boldsymbol{F}}^{\mathrm{e}}. \tag{5}$$

As expected, $\det \bar{\boldsymbol{F}}^{\mathrm{e}} = 1$ and thus, $\bar{\boldsymbol{F}}^{\mathrm{e}}$ is indeed related to an isochoric deformation.

Constitutive models suitable for analyzing plastic deformations are usually based on evolution equations for the inelastic strains. For this reason, deformation rates are introduced. Analogously to the standard spatial velocity gradient

$$\boldsymbol{l} := \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1} \tag{6}$$

the two additional velocity gradients

$$\boldsymbol{L}^{\mathrm{p}} := \dot{\boldsymbol{F}}^{\mathrm{p}} \cdot [\boldsymbol{F}^{\mathrm{p}}]^{-1}, \qquad \boldsymbol{l}^{\mathrm{e}} := \dot{\boldsymbol{F}}^{\mathrm{e}} \cdot [\boldsymbol{F}^{\mathrm{e}}]^{-1} \tag{7}$$

are also defined. Here, the superposed dot represents the material time derivative. Eqs. (6)-(7) imply that $\boldsymbol{l}$ as well as $\boldsymbol{l}^{\mathrm{e}}$ are associated with the deformed configuration, while $\boldsymbol{L}^{\mathrm{p}}$ belongs to the so-called *intermediate configuration* induced by the multiplicative decomposition (2).

2.2 Balance laws

Having briefly discussed the kinematics, some of the (standard) balance laws are summarized here. The first of those is that of linear momentum. In material form (reference configuration), it reads

$$\mathrm{DIV}\boldsymbol{P} + \rho_0 \boldsymbol{B}_0 = \boldsymbol{0}. \tag{8}$$

Here, DIV is the divergence operator (with respect to the undeformed configuration), $\boldsymbol{P}$ denotes the first Piola-Kirchhoff stress tensor, ρ_0 represents the referential density and $\rho_0 \boldsymbol{B}_0$ is the referential body force. For the sake of simplicity, inertia effects have been neglected. However, they can indeed be included in a straightforward manner. Clearly, for solving differential equation (8), boundary conditions are required. With the disjunct decomposition $\partial\mathcal{B}_0 = \partial\mathcal{B}_{0,\boldsymbol{\varphi}} \dot{\cup} \partial\mathcal{B}_{0,\boldsymbol{T}}$ of the boundary $\partial\mathcal{B}_0$ of the body $\mathcal{B}_0$ into the part $\partial\mathcal{B}_{0,\boldsymbol{\varphi}}$ where the deformation is prescribed by $\bar{\boldsymbol{\varphi}}$ and the part $\partial\mathcal{B}_{0,\boldsymbol{T}}$ corresponding to prescribed tractions $\bar{\boldsymbol{T}}$, the boundary conditions can be summarized as

$$\begin{array}{ll} \boldsymbol{\varphi} = \bar{\boldsymbol{\varphi}} & \forall \boldsymbol{X} \in \partial\mathcal{B}_{0,\boldsymbol{\varphi}} \\ \boldsymbol{P} \cdot \boldsymbol{N} = \bar{\boldsymbol{T}} & \forall \boldsymbol{X} \in \partial\mathcal{B}_{0,\boldsymbol{T}}. \end{array} \tag{9}$$

In Eq. (9), $\boldsymbol{N}$ is the normal vector at the boundary.

Evidently, for thermomechanically coupled problems, balance law (8) is not sufficient for characterizing the considered mechanical system. For that purpose, the first law of thermodynamics also known as balance of energy is required. Denoting the internal energy as E, the heat flux as $\boldsymbol{H}$ and the specific heat source as Q_Θ, this law is given by

$$\dot{E} + \mathrm{DIV}\boldsymbol{H} = \boldsymbol{P} : \dot{\boldsymbol{F}} + \rho_0 Q_\Theta. \tag{10}$$

The respective boundary conditions are now of the form

$$\begin{array}{ll} \Theta = \bar{\Theta} & \forall \boldsymbol{X} \in \partial\mathcal{B}_{0,\Theta} \\ \boldsymbol{H} \cdot \boldsymbol{N} = \bar{H} & \forall \boldsymbol{X} \in \partial\mathcal{B}_{0,H} \end{array} \tag{11}$$

where $\bar{\Theta}$ are prescribed temperatures associated with the boundary $\partial\mathcal{B}_{0,\Theta}$, while $\bar{H}$ is a prescribed heat flux corresponding to the boundary $\partial\mathcal{B}_{0,H}$.

Finally, the second law of thermodynamics also known as the balance law of entropy is introduced. Its local referential version is given by

$$\mathcal{D} = \Theta\, \dot{\Gamma} = \Theta\, \dot{N} - \dot{E} + \boldsymbol{P} : \dot{\boldsymbol{F}} + \boldsymbol{H} \cdot \boldsymbol{G} \geq 0 \tag{12}$$

with N being the entropy, $\dot{\Gamma}$ the internal entropy production and

$$\boldsymbol{G} := -\frac{1}{\Theta}\text{GRAD}\Theta \tag{13}$$

being the normalized temperature gradient. It represents the driving force and energetically conjugate variable to the heat flux $\boldsymbol{H}$. Often, the dissipation $\mathcal{D}$ is decomposed into the internal dissipation

$$\mathcal{D}_{\text{int}} = \Theta\, \dot{N} - \dot{E} + \boldsymbol{P} : \dot{\boldsymbol{F}} \tag{14}$$

and the dissipation

$$\mathcal{D}_{\text{cond}} = \boldsymbol{H} \cdot \boldsymbol{G} \tag{15}$$

due to heat conduction. Making the assumption that the thermal problem can be described by a Fourier-type constitutive model of the form $\boldsymbol{H} = \partial_{\boldsymbol{G}}\chi$ with χ denoting a suitable convex potential, the dissipation due to heat conduction is non-negative ($\mathcal{D}_{\text{cond}} \geq 0$). In this case which is also adopted in the present paper, the second law of thermodynamics (12) is automatically fulfilled, if the internal dissipation is non-negative. For this reason, only the dissipation inequality

$$\mathcal{D}_{\text{int}} = \Theta\, \dot{N} - \dot{E} + \boldsymbol{P} : \dot{\boldsymbol{F}} \geq 0 \tag{16}$$

will be considered in more detail. Clearly, by assuming a Fourier-type constitutive model for the thermal problem, condition (16) is sufficient for thermodynamical consistency. However, it is not necessary, i.e., the decomposition $\mathcal{D}_{\text{int}} \geq 0$ and $\mathcal{D}_{\text{cond}} \geq 0$ is relatively crude.

Remark 2.1 *Since the balance law of angular momentum can be a priori fulfilled by enforcing symmetry of the Cauchy stresses, and the balance law of mass by relating the current density ρ to its referential counterpart ρ_0 via $\rho_0 = \rho\, J$, they have not been presented in detail here.*

3 Constitutive models

Section 2 dealt with a concise summary of the material independent balance laws and the kinematics. In the present section, focus is on material specific constitutive equations. While the stored energy and the internal energy, together with their restrictions imposed by the second law of thermodynamics are given in Subsection 3.1, a family of yield functions and evolution equations are subsequently considered in Subsection 3.2.

3.1 Helmholtz energy and internal energy

In line with Coleman & Gurtin Coleman and Gurtin (1967) and Coleman & Noll Coleman and Noll (1963), the internal energy is assumed to be of the type,

$$E = E(\boldsymbol{F}, N, \boldsymbol{\alpha}). \tag{17}$$

Here, $\boldsymbol{\alpha}$ is a set of suitable strain-like internal variables associated with the deformation history. According to Eq. (17), a purely local constitutive framework is considered, i.e., higher-order strain gradients are neglected. Based on Eq. (17) the Helmholtz energy Ψ can be introduced by applying the Legendre-Fenchel transformation

$$\Psi = \Psi(\boldsymbol{F}, \Theta, \boldsymbol{\alpha}) := \inf_{N} \left[E(\boldsymbol{F}, N, \boldsymbol{\alpha}) - \Theta\, N\right]. \tag{18}$$

Strictly speaking, this transformation requires already the definition of the temperature Θ as energetically conjugate to the entropy N, i.e., $\Theta = \partial_N E$. By inserting Eq. (18) into the internal dissipation inequality (16), $\mathcal{D}_{\text{int}}$ can be re-written as

$$\mathcal{D}_{\text{int}} = \left[-N - \frac{\partial \Psi}{\partial \Theta}\right] \dot{\Theta} + \left[\boldsymbol{P} - \frac{\partial \Psi}{\partial \boldsymbol{F}}\right] : \dot{\boldsymbol{F}} - \frac{\partial \Psi}{\partial \boldsymbol{\alpha}} : \dot{\boldsymbol{\alpha}} \geq 0. \tag{19}$$

Accordingly and focusing on a fully reversible loading process, the state equations

$$\boldsymbol{P} = \partial_{\boldsymbol{F}} \Psi, \qquad N = -\partial_{\Theta} \Psi \tag{20}$$

can be derived, which applied to Eq. (19), yield the reduced internal dissipation

$$\mathcal{D}_{\text{int}} = -\frac{\partial \Psi}{\partial \boldsymbol{\alpha}} : \dot{\boldsymbol{\alpha}} \geq 0. \tag{21}$$

As evident from Eq. (21), the evolution equations $\dot{\boldsymbol{\alpha}}$ have to be chosen in line with the second law of thermodynamics.

So far, a very general framework for constitutive models has been presented. Next, focus is on elastoplasticity. For this class of material models, it is convenient to decompose the set of internal variables $\boldsymbol{\alpha}$ into the plastic strains (the plastic part of the deformation gradient $\boldsymbol{F}^{\text{p}}$), a strain-like second-order tensor $\boldsymbol{\alpha}_{\text{k}}$ associated with kinematic hardening and its isotropic counterpart α_{i}. As a result, $\boldsymbol{\alpha} := \{\boldsymbol{F}^{\text{p}}, \boldsymbol{\alpha}_{\text{k}}, \alpha_{\text{i}}\}$ and thus, the Helmholtz energy reads now $\Psi = \Psi(\boldsymbol{F}^{\text{e}}, \Theta, \boldsymbol{\alpha}_{\text{k}}, \alpha_{\text{i}})$. With this representation, dissipation inequality (21) decomposes into three terms, i.e.,

$$\mathcal{D}_{\text{int}} = \boldsymbol{\Sigma} : \boldsymbol{L}^{\text{p}} + \boldsymbol{Q}_{\text{k}} : \dot{\boldsymbol{\alpha}}_{\text{k}} + Q_{\text{i}}\, \dot{\alpha}_{\text{i}} \geq 0, \qquad \boldsymbol{Q}_{\text{k}} := -\partial_{\boldsymbol{\alpha}_{\text{k}}} \Psi,\ Q_{\text{i}} := -\partial_{\alpha_{\text{i}}} \Psi \tag{22}$$

where $\boldsymbol{Q}_{\text{k}}$ and Q_{i} are stress-like internal variables conjugate to $\boldsymbol{\alpha}_{\text{k}}$ and α_{i} and $\boldsymbol{\Sigma} = \boldsymbol{F}^{\text{e}T} \cdot \partial_{\boldsymbol{F}^{\text{e}}} \Psi$ are the Mandel stresses. By combining Eq. (22) with the first law of thermodynamics (10), the change in temperature can be determined as

$$c\, \dot{\Theta} = \rho_0 Q_{\Theta} - \text{DIV}\boldsymbol{H} + \mathcal{D}_{\text{int}} + \Theta\, \partial^2_{\Theta \boldsymbol{F}^{\text{e}}} \Psi : \dot{\boldsymbol{F}}^{\text{e}}. \tag{23}$$

In Eq. (23), $c_0 := -\Theta\, \partial^2_{\Theta} \Psi$ is the heat capacity at constant strain and constant internal state and the last term is related to the thermoelastic coupling. For the derivation of Eq. (23) is has been assumed that hardening is not affected by the temperature, e.g., $\partial^2_{\Theta \alpha_{\text{i}}} \Psi = 0$. Thermal softening is only considered by a temperature dependent intial yield surface. This is a good approximation for metals, cf. Simo (1998). However, it bears emphasis that the more general case can be treated in a fully analogous manner and does not raise any additional problem, cf. Simo (1998). In contrast to the concept based on the Taylor & Quinney factor (see Taylor and Quinney (1934)), coupling (23) can also be used in case of kinematic hardening.

3.2 Yield function

The constitutive framework discussed in the previous subsection is completed by suitable loading conditions and evolution equations. For that purpose, the space of admissible stresses

$$\mathbb{E}_{\boldsymbol{\Sigma}} := \left\{(\boldsymbol{\Sigma}, \boldsymbol{Q}_{\text{k}}, Q_{\text{i}}, \Theta) \in \mathbb{R}^{9+9+1+1} \mid \phi(\boldsymbol{\Sigma}, \boldsymbol{Q}_{\text{k}}, Q_{\text{i}}, \Theta) \leq 0\right\} \tag{24}$$

is introduced. It can be conveniently defined by a yield function $\phi = \phi(\boldsymbol{\Sigma}, \boldsymbol{Q}_{\text{k}}, Q_{\text{i}}, \Theta)$. It should be noted that this commonly adopted assumption of a yield function is fundamentally different compared to the kinematical approach presented in Ortiz and Stainier

(1999); Stainier and Ortiz (2010); Yang et al. (2006). Although for some material models both methods are one-to-one related, this is not the case for more complicated constitutive frameworks – particularly for the resulting numerical implementation.

The family of material models discussed here is based on the following two assumptions:

- ϕ is convex in ($\boldsymbol{\Sigma}$,$\boldsymbol{Q}_\mathrm{k}$,$Q_\mathrm{i}$) and of the form

$$\phi = \Sigma^\mathrm{eq}(\boldsymbol{\Sigma} - \boldsymbol{Q}_\mathrm{k}(\boldsymbol{\alpha}_\mathrm{k})) - Q_\mathrm{i}(\alpha_\mathrm{i}) - Q_0^\mathrm{eq}(\Theta). \tag{25}$$

- The equivalent stress measure Σ^eq defining the shape of the yield function is a positively homogeneous function of degree one, i.e.,

$$\Sigma^\mathrm{eq}(c\,[\boldsymbol{\Sigma} - \boldsymbol{Q}_\mathrm{k}]) = c\,\Sigma^\mathrm{eq}(\boldsymbol{\Sigma} - \boldsymbol{Q}_\mathrm{k}), \quad \forall c \in \mathbb{R}^+. \tag{26}$$

Clearly, the decomposition of the yield function according to Eq. (25) complies with the naming of $\boldsymbol{Q}_\mathrm{k}$ and Q_i as kinematic and isotropic hardening variables. Furthermore and as frequently assumed in metal plasticity, hardening is not influenced by a change in temperature, cf. Simo (1998). The second assumption, i.e., Eq. (26), is rather technical. Without going too much into detail, it is required for the parameterization of the flow rule employed in Section 5. However, it bears emphasis that Eq. (26) is fulfilled for a broad range of constitutive models, cf. Mosler (2010); Mosler and Bruhns (2009, 2010) and references cited therein.

Based on a yield function, loading conditions can be defined. However, for that purpose, evolution equations have to be derived first. Considering a plastic potential of the type

$$g(\boldsymbol{\Sigma}, \boldsymbol{Q}_\mathrm{k}, Q_\mathrm{i}, \Theta) = \phi(\boldsymbol{\Sigma}, \boldsymbol{Q}_\mathrm{k}, Q_\mathrm{i}, \Theta) + \tilde{\phi}(\boldsymbol{Q}_\mathrm{k}) \tag{27}$$

with $\tilde{\phi} \geq 0$ denoting a convex function, they are defined as

$$\begin{aligned} \boldsymbol{L}^\mathrm{p} &= \lambda\, \partial_{\boldsymbol{\Sigma}} g \;= \lambda\, \partial_{\boldsymbol{\Sigma}} \phi \\ \dot{\boldsymbol{\alpha}}_\mathrm{k} &= \lambda\, \partial_{\boldsymbol{Q}_\mathrm{k}} g = -\boldsymbol{L}^\mathrm{p} + \lambda\, \partial_{\boldsymbol{Q}_\mathrm{k}} \tilde{\phi} \\ \dot{\alpha}_\mathrm{i} &= \lambda\, \partial_{Q_\mathrm{i}} g = -\lambda, \end{aligned} \tag{28}$$

together with the Karush-Kuhn-Tucker conditions $\lambda \geq 0$, $\phi\ \lambda = 0$. Here, $\lambda \geq 0$ is the plastic multiplier. In case of loading ($\phi = 0$ and $\dot{\phi} = 0$), it follows from the consistency condition $\dot{\phi} = 0$.

The constitutive framework discussed here falls into the range of *generalized standard materials* (see Lemaitre (1985); Mandel (1972)). All models belonging to that class fulfill a priori the second law of thermodynamics. This can be seen explicitly by inserting Eqs. (28) into dissipation inequality (22) leading to

$$\mathcal{D}_\mathrm{int} \overset{\phi=0}{=} \lambda\, Q_0^\mathrm{eq}(\Theta) + \lambda\, \boldsymbol{Q}_\mathrm{k} : \frac{\partial \tilde{\phi}}{\partial \boldsymbol{Q}_\mathrm{k}} \geq 0. \tag{29}$$

Since $\lambda \geq 0$, $Q_0^\mathrm{eq} \geq 0$ and $\tilde{\phi} \geq 0$ is convex, the internal dissipation is indeed non-negative as required by thermodynamics. For nonlinear kinematic hardening,

$$\tilde{\phi} = \frac{1}{2}\,\frac{b}{c}\,\boldsymbol{Q}_\mathrm{k} : \boldsymbol{Q}_\mathrm{k} \tag{30}$$

is a frequently made choice. In Eqs. (30), b and c are material parameters defining the saturation behavior of kinematic hardening, cf. Mosler (2010). This model is also used

within the numerical examples presented in Section 6. According to Eqs. (30) and (29), it results in the internal dissipation inequality

$$\mathcal{D}_{\text{int}} = \lambda\, Q_0^{\text{eq}}(\Theta) + \lambda\, \frac{b}{c}\, \boldsymbol{Q}_{\text{k}} : \boldsymbol{Q}_{\text{k}} \geq 0. \tag{31}$$

Remark 3.1 *According to Eqs. (28) the material time derivative of* $\boldsymbol{\alpha}_{\text{k}}$ *naturally appears. It is well known that evolution equations for the back strain depending on that time derivative might lead to unphysical results, cf. Tsakmakis (1987). For this reason, objective time derivatives are frequently applied, see Dettmer and Reese (2004) and references cited therein. However, as noted in Mosler (2010) the framework discussed here can be modified accordingly in a straightforward manner. Therefore, such technical details will not be presented here.*

4 Variational framework

In this section, the family of constitutive models discussed previously is reformulated into a variationally consistent framework. For that purpose, a state-of-the-art review of such variational approaches is given in Subsection 4.1 first, cf. Stainier and Ortiz (2010); Yang et al. (2006). Finally and inspired by Stainier and Ortiz (2010); Yang et al. (2006), those approaches are extended and modified in Subsection 4.2 for non-associated kinematic hardening of Armstrong-Frederick-type and re-parameterized such that the flow rule and the evolution equations are a priori enforced. This leads to an unconstrained optimization problem defining the state of a solid.

4.1 State-of-the-art review

The fundamentals of the variational principle for thermodynamically coupled problems as advocated in Stainier and Ortiz (2010); Yang et al. (2006) are briefly summarized here. Further details can be found in the cited references.

It is commonly known that the standard (two-field; Θ and $\boldsymbol{\varphi}$) thermodynamically coupled problem does not show a variational structure, i.e., its states do not follow from a stationarity condition of a potential, cf. Simo (1998). This is manifested, e.g., in an unsymmetrical overall stiffness matrix. However, an enhanced variational principle was relatively recently advocated in Stainier and Ortiz (2010); Yang et al. (2006) which is consistently defined by an incremental potential. The cited works are extensions of the isothermal models Ortiz and Stainier (1999) which were further elaborated, e.g., in Carstensen et al. (2002); Fancello et al. (2006, 2008); Miehe (2002); Mosler and Bruhns (2010). According to Stainier and Ortiz (2010); Yang et al. (2006), the fundamental ideas leading eventually to a symmetric formulation of the thermodynamically coupled problem are:

- The distinction between the so-called *equilibrium temperature* and the so-called *external temperature*

  While the external temperature Θ is the standard one, the equilibrium temperature $\tilde{\Theta}$ is given by the equilibrium condition

$$\tilde{\Theta} = \partial_N E(\boldsymbol{F}, \boldsymbol{F}^{\text{p}}, \boldsymbol{\alpha}, N). \tag{32}$$

Clearly, those two temperature are equal at equilibrium. However, this condition is only enforced in a weak form by applying a HU-WASHIZU formulation. That is, Θ and N can be varied independently of one another.

- The introduction of a so-called *integrating factor* of the type

$$f(\Theta, \tilde{\Theta}) = \frac{\Theta}{\tilde{\Theta}}. \tag{33}$$

Following Stainier and Ortiz (2010); Yang et al. (2006), this factor is used within the *kinetic potential* for all strain-like variables. Since $f = 1$ at equilibrium, the integrating factor does not change the underlying mechanical problem.

With such techniques, the variational method proposed in Stainier and Ortiz (2010); Yang et al. (2006) reads

$$(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}}, \dot{N}, \Theta) = \arg \inf_{\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}}, \dot{N}} \sup_{\Theta} \dot{I}_{\mathrm{inc}}(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}}, \dot{N}, \Theta) \tag{34}$$

with

$$\begin{aligned} \dot{I}_{\mathrm{inc}} = & \int_{\mathcal{B}_0} \Big[\dot{E}(\dot{\boldsymbol{F}}, \dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}}, \dot{N}) - \Theta\, \dot{N} + \mathcal{D}_{\mathrm{int}}(f\, (\dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}})) - \chi(\Theta, \mathrm{GRAD}\Theta) \Big]\, \mathrm{d}V \\ & - \mathcal{P}_{\boldsymbol{F}}(\dot{\boldsymbol{\varphi}}) + \mathcal{P}_{\Theta}(\Theta). \end{aligned} \tag{35}$$

Here, $\mathcal{P}_{\boldsymbol{F}}(\dot{\boldsymbol{\varphi}})$ is the power due to external prescribed forces, $\mathcal{P}_{\Theta}(\Theta)$ is power due to prescribed heat fluxes and heat sources and f is the integrating factor as introduced in Eq. (33). According to Eq. (35), the only variables to be optimized are $(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{F}}^{\mathrm{p}}, \dot{\boldsymbol{\alpha}}_{\mathrm{k}}, \dot{\alpha}_{\mathrm{i}}, \dot{N}, \Theta)$, i.e., except for the external temperature, only rates appear. The corresponding state variables ($\boldsymbol{\varphi}$, $\boldsymbol{F}^{\mathrm{p}}$, $\boldsymbol{\alpha}_{\mathrm{k}}$, α_{i}, N) are thus considered as fixed. Furthermore, it bears emphasis that the internal dissipation $\mathcal{D}_{\mathrm{int}}$ in Eq. (35) follows from a standard stress-space plasticity model, cf., e.g., Eq. (29). In particular, the yield function has already been used for deriving the dissipation. By way of contrast, the dissipation function $\mathcal{D}_{\mathrm{int}}$, together with flow rule and evolution equations, are postulated in Stainier and Ortiz (2010); Yang et al. (2006) and the yield function is thus dependent on such assumptions and derives from them. A physical interpretation of Eq. (34) can be given best, if temperature effects are neglected. In this case, $\chi = \mathcal{P}_{\Theta} = 0$, and $\dot{E} - \Theta\, \dot{N}$ equals the Helmholtz energy. Consequently, the integrand in Eq. (35) being $\dot{\Psi} + \mathcal{D}_{\mathrm{int}}$ is the stress power. As a result, variational principle (34) chooses that rate of state variables which minimizes the work necessary to go from one state to an infinitesimally neighboring new state. A similar interpretation applies also to the fully thermomechanically coupled problem.

4.2 A variational reformulation of the thermomechanically coupled problem

Computing the solution of the variational principle seems to be straightforward. Unfortunately, this is not the case. The reasons for this are the nonlinear constraints resulting from the flow rule and the condition $\det \boldsymbol{F}^{\mathrm{p}} > 0$. An effective solution to this problem was recently proposed for isothermal constitutive models in the series of papers Mosler (2010); Mosler and Bruhns (2009, 2010). Conceptually, the idea is the parameterization

of the flow rule by the plastic multiplier (condition $\lambda \geq 0$ can easily be enforced) and by so-called *pseudo stresses* $\tilde{\boldsymbol{\Sigma}} \neq \boldsymbol{\Sigma}$. More precisely,

$$\boldsymbol{L}^{\mathrm{p}} = \dot{\boldsymbol{F}}^{\mathrm{p}} \cdot \boldsymbol{F}^{\mathrm{p}-1} = \lambda \, \partial_{\boldsymbol{\Sigma}} \phi = \lambda \left. \frac{\partial \phi}{\partial \boldsymbol{\Sigma}} \right|_{\boldsymbol{\Sigma} - \boldsymbol{Q}_{\mathrm{k}} = \tilde{\boldsymbol{\Sigma}}} . \tag{36}$$

E.g., considering a von Mises-type yield function, this parameterization results in

$$\boldsymbol{L}^{\mathrm{p}} = \lambda \, \frac{\mathrm{Dev}\tilde{\boldsymbol{\Sigma}}}{||\mathrm{Dev}\tilde{\boldsymbol{\Sigma}}||} := \lambda \, \boldsymbol{M}(\tilde{\boldsymbol{\Sigma}}) \tag{37}$$

with $\mathrm{Dev}(\bullet) := (\bullet) - 1/3 \, \mathrm{tr}(\bullet) \, \mathbf{1}$ denoting the deviatoric projection. According to Eq. (37), the constraints $\boldsymbol{M} : \boldsymbol{M} = 1$ and $\mathrm{tr}\boldsymbol{M} = 0$ are fulfilled for any tensor $\tilde{\boldsymbol{\Sigma}}$. It bears emphasis that this decomposition of the flow rule into an amplitude λ and a direction $\boldsymbol{M}$ requires that the yield function is positively homogeneous of degree one, cf. Mosler and Bruhns (2010). Applying this parameterization, the evolution equations $(28)_2$ and $(28)_3$ and the flow rule $(28)_1$ can thus be re-written as

$$\begin{aligned} \boldsymbol{L}^{\mathrm{p}}(\lambda, \tilde{\boldsymbol{\Sigma}}) &= \lambda \, \partial_{\boldsymbol{\Sigma}} g \; = \lambda \, \boldsymbol{M}(\tilde{\boldsymbol{\Sigma}}) \\ \dot{\boldsymbol{\alpha}}_{\mathrm{k}}(\lambda, \tilde{\boldsymbol{\Sigma}}) &= \lambda \, \partial_{\boldsymbol{Q}_{\mathrm{k}}} g = -\lambda \, \boldsymbol{M}(\tilde{\boldsymbol{\Sigma}}) + \lambda \, \partial_{\boldsymbol{Q}_{\mathrm{k}}} \tilde{\phi} \\ \dot{\alpha}_{\mathrm{i}}(\lambda) \quad &= \lambda \, \partial_{Q_{\mathrm{i}}} g = -\lambda. \end{aligned} \tag{38}$$

Different to Stainier and Ortiz (2010); Yang et al. (2006), this parameterization enforces automatically the correct flow direction for any yield function which is positively homogeneous of degree one. Inserting this parameterization into Eq. (35) gives finally the modified variational constitutive update

$$(\dot{\boldsymbol{\varphi}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}, \Theta) = \arg \inf_{\dot{\boldsymbol{\varphi}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}} \sup_{\Theta} \dot{I}_{\mathrm{inc}}(\dot{\boldsymbol{\varphi}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}, \Theta) \tag{39}$$

with

$$\begin{aligned} \dot{I}_{\mathrm{inc}} = & \int_{\mathcal{B}_0} \Big[\dot{E}(\dot{\boldsymbol{F}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}) - \Theta \, \dot{N} + \mathcal{D}_{\mathrm{int}}(f \, \lambda, \tilde{\boldsymbol{\Sigma}}) - \chi(\Theta, \mathrm{GRAD}\Theta) \Big] \, \mathrm{d}V \\ & - \mathcal{P}_{\boldsymbol{F}}(\dot{\boldsymbol{\varphi}}) + \mathcal{P}_{\Theta}(\Theta). \end{aligned} \tag{40}$$

Here, f is again the integrating factor as introduced in Eq. (33). Although the internal dissipation can be described in terms of λ and $\tilde{\boldsymbol{\Sigma}}$, this representation is not convenient. More precisely, it cannot be seen from this equation that the internal dissipation depends also on the temperature. Considering Eq. (29),

$$\mathcal{D}_{\mathrm{int}} = \mathcal{D}_{\mathrm{int}}(\lambda, \tilde{\Theta}, \Theta) = \lambda \, \frac{\Theta}{\tilde{\Theta}} \, Q_0^{\mathrm{eq}}(\tilde{\Theta}) + \lambda \, \frac{\Theta}{\tilde{\Theta}} \, \frac{\partial \tilde{\phi}}{\partial \boldsymbol{Q}_{\mathrm{k}}} : \boldsymbol{Q}_{\mathrm{k}}. \tag{41}$$

It bears emphasis that the temperature defining the initial yield strength Q_0^{eq} has to be chosen as the equilibrium temperature $\tilde{\Theta}$ and not as the external temperature Θ. It will be shown that this is crucial for consistency of the proposed variational scheme. Since the state variable N is fixed within the variational principle, its dual variable being the equilibrium temperature $\tilde{\Theta}$ is also fixed.

For proving consistency of the discussed variationally consistent framework, the stationarity conditions of Eq. (40), combined with Eq. (41), are computed. A minimization of the incrementally defined energy $\dot{I}_{\text{inc}}$ with respect to the entropy rate yields

$$\frac{\partial \dot{I}_{\text{inc}}}{\partial \dot{N}} = \int_{\mathcal{B}_0} \left[\frac{\partial E}{\partial N} - \Theta \right] \, \mathrm{d}V = 0 \quad \Rightarrow \quad \frac{\partial E}{\partial N} = \tilde{\Theta} = \Theta. \tag{42}$$

Thus, the equilibrium temperature equals the external temperature and the integrating factor results in $f = 1$. According to Eq. (40), this minimization can be performed point-wise and hence, condition $\Theta = \tilde{\Theta}$ holds point-wise as well. Next, stationarity with respect to the plastic multiplier is analyzed. With the rate of the internal energy

$$\dot{E} = \boldsymbol{P} : \dot{\boldsymbol{F}} - \left[\boldsymbol{\Sigma} : \partial_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}} - \boldsymbol{Q}_{\text{k}} : \partial_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}} - Q_{\text{i}} \right] \, \lambda - \lambda \, \boldsymbol{Q}_{\text{k}} : \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi} - \tilde{\Theta} \, \dot{N} \tag{43}$$

depending on the relative stress $\boldsymbol{\Xi} := \boldsymbol{\Sigma} - \boldsymbol{Q}_{\text{k}}$, the respective condition reads (see also Eq. (16))

$$\frac{\partial \dot{I}_{\text{inc}}}{\partial \lambda} = \int_{\mathcal{B}_0} \left[\frac{\partial \dot{E}}{\partial \lambda} + \frac{\partial \mathcal{D}_{\text{int}}}{\partial \lambda} \right] \, \mathrm{d}V \geq 0 \; \Rightarrow \; -\Sigma_0^{\text{eq}}(\boldsymbol{\Sigma} - \boldsymbol{Q}_{\text{k}}) + Q_{\text{i}} + Q_0^{\text{eq}} = -\phi \geq 0. \tag{44}$$

Here, $f = 1$, together with $\lambda \geq 0$, have been considered. Thus stability of the energy requires that the stresses are admissible, i.e., $\phi \leq 0$. Considering the identity $\partial_\lambda \dot{E} = \partial_\lambda \dot{\Psi}$, condition (44) can be derived in an alternative way as well. More precisely, using this identity, $\partial_\lambda \dot{I}_{\text{inc}}$ can be computed fully analogously to isothermal problems. Therefore, the derivative $\partial_\lambda \dot{I}_{\text{inc}}$ is identical to that previously reported in Mosler (2010). The same argument applies also to the stationarity condition of $\dot{I}_{\text{inc}}$ with respect to the pseudo stresses $\tilde{\boldsymbol{\Sigma}}$. Accordingly

$$\frac{\partial \dot{I}_{\text{inc}}}{\partial \tilde{\boldsymbol{\Sigma}}} = -\lambda \, \boldsymbol{\Xi} : \partial^2_{\boldsymbol{\Sigma}} \phi \big|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}} = \boldsymbol{0}. \tag{45}$$

Alternatively, Eq. (45) can be derived by using the rate of internal energy (43). As written in Mosler (2010), Eq. (45) is a compatibility condition connecting the relative physical stresses $\boldsymbol{\Xi}$ to their pseudo counterparts $\tilde{\boldsymbol{\Sigma}}$. If this equation is fulfilled, the flow direction implied by $\tilde{\boldsymbol{\Sigma}}$ complies with the yield function. This can be seen more explicitly by differentiating the identity $\Sigma^{\text{eq}} = \partial_{\boldsymbol{\Sigma}} \phi : \boldsymbol{\Sigma}$. For further details, the interested reader is referred to Mosler (2010). As evident from Eq. (40), the potential $\dot{I}_{\text{inc}}$ depends locally on $\dot{N}$, λ and $\tilde{\boldsymbol{\Sigma}}$. As a result, the stationarity conditions can be checked locally. This leads to the local minimization problem

$$(\lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}) = \arg \inf_{\lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}} \dot{I}_{\text{inc}}(\dot{\boldsymbol{\varphi}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}, \Theta) \Big|_{\dot{\boldsymbol{\varphi}}=\text{const}, \Theta=\text{const}} \tag{46}$$

and its resulting global counterpart

$$(\dot{\boldsymbol{\varphi}}, \Theta) = \arg \inf_{\dot{\boldsymbol{\varphi}}} \sup_{\Theta} \dot{I}^{\text{red}}_{\text{inc}}, \quad \dot{I}^{\text{red}}_{\text{inc}}(\dot{\boldsymbol{\varphi}}, \Theta) := \inf_{\lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}} \dot{I}_{\text{inc}}(\dot{\boldsymbol{\varphi}}, \lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}, \Theta) \Big|_{\dot{\boldsymbol{\varphi}}=\text{const}, \Theta=\text{const}}. \tag{47}$$

In practical finite element implementations, Problem (46) is solved at the integration points for a given temperature and deformation field. Subsequently, the globally compatible fields are computed by applying Eq. (47). For this reason, a variation of $\dot{I}^{\text{red}}_{\text{inc}}$ with respect to the deformation rate is computed. It yields

$$\delta_{\dot{\boldsymbol{\varphi}}} \dot{I}^{\text{red}}_{\text{inc}} = \int_{\mathcal{B}_0} \boldsymbol{P} : \delta \dot{\boldsymbol{F}} \, \mathrm{d}V - \delta_{\dot{\boldsymbol{\varphi}}} \mathcal{P}_{\boldsymbol{F}} = 0, \qquad \forall \dot{\boldsymbol{\varphi}}. \tag{48}$$

Noting that $\delta_{\boldsymbol{\varphi}}\mathcal{P}_{\boldsymbol{F}}$ is the virtual work due to externally applied forces and the first term in Eq. (48) is the internal virtual work, it is concluded that stationarity of $\dot{I}_{\text{inc}}^{\text{red}}$ implies the balance of linear momentum. Finally maximizing Eq. (47) with respect to the external temperature Θ leads to

$$\delta_{\Theta}\dot{I}_{\text{inc}}^{\text{red}} = \int_{\mathcal{B}_0} \left[-\dot{N} + \frac{1}{\tilde{\Theta}}\,\mathcal{D}_{\text{int}} \right] \,\mathrm{d}V - \partial_{\Theta} \left[\int_{\mathcal{B}_0} \chi \,\mathrm{d}V - \mathcal{P}_{\Theta} \right] = 0. \tag{49}$$

Clearly, the second integral is associated with the standard purely thermal problem and thus, it can be re-written as (see, e.g., Simo (1998))

$$\partial_{\Theta} \left[\int_{\mathcal{B}_0} \chi \,\mathrm{d}V - \mathcal{P}_{\Theta} \right] = \int_{\mathcal{B}_0} \left[-\frac{1}{\Theta}\,\rho_0 Q_{\Theta} + \frac{1}{\Theta}\,\mathrm{DIV}\boldsymbol{H} \right] \,\mathrm{d}V. \tag{50}$$

As a result, by combining Eq. (50) with the first integrand in Eq. (49), together with the equilibrium condition $\tilde{\Theta} = \Theta$, the localization theorem applied to Eq. (49) yields eventually

$$\dot{N} - \frac{1}{\tilde{\Theta}}\,\mathcal{D}_{\text{int}} = \frac{1}{\tilde{\Theta}}\,\rho_0 Q_{\Theta} - \frac{1}{\tilde{\Theta}}\,\mathrm{DIV}\boldsymbol{H}. \tag{51}$$

A straightforward comparison between Eq. (51) and Eq. (10) shows that stationarity of $\dot{I}_{\text{inc}}$ with respect to the external temperature is thus equivalent to the first law of thermodynamics. It bears emphasis that this equivalence depends crucially on choosing the equilibrium temperature as the temperature defining the initial yield strength Q_0^{eq}.

In summary, is has been proven that variational principle (39) is equivalent to the constitutive model discussed in Section 3. In sharp contrast to the previous works Stainier and Ortiz (2010); Yang et al. (2006), the novel parameterization advocated here enforces all evolution a priori and thus any positively homogeneous yield function can directly be used – even within the numerical implementation. This will be shown in the following section. Furthermore, the novel variational framework includes naturally even non-associative evolution equations characterizing non-linear kinematic hardening of Armstrong-Frederick-type.

5 Variational constitutive updates - Numerical implementation

Based on variational principle (39) an efficient numerical implementation is elaborated in the present section. While the respective fundamentals are briefly discussed in Subsection 5.1, a prototype model is considered in Subsection 5.2. For the isothermal problem, further details can be found, e.g., in Carstensen et al. (2002); Fancello et al. (2006, 2008); Miehe (2002); Mosler and Bruhns (2010); Ortiz and Stainier (1999).

5.1 Fundamentals

In contrast to conventional implementations of thermodynamically coupled elastoplasticity, the numerical approximation of the variational principle (39) is astonishingly simple

and direct. More precisely, a classical time discretization is applied to Eq. (39) within the time interval $t \in [t_n; t_{n+1}]$. Hence, in contrast to the continuous problem (39),

$$I_{\text{inc}} := \int_{t_n}^{t_{n+1}} \dot{I}_{\text{inc}} \, \mathrm{d}t \tag{52}$$

is considered. Evidently, $\dot{I}_{\text{inc}}$ can usually not be integrated analytically. Thus, a time discretization is required. In the following, the backward Euler method is applied. Thus, Eq. (52) is approximated by

$$\begin{aligned} I_{\text{inc}} \approx & \int_{\mathcal{B}_0} \left[E_{n+1} - E_n - \Theta_{n+1} \, (N_{n+1} - N_n) \right] \, \mathrm{d}V \\ & + \int_{\mathcal{B}_0} \left[\Delta\lambda \, \left\{ \frac{\Theta}{\tilde{\Theta}} \, \left(Q_0(\tilde{\Theta}) + \boldsymbol{Q}_{\text{k}} \cdot \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi} \right) \right\} \Big|_{n+1} - \Delta t \, \chi(\Theta_{n+1}) \right] \, \mathrm{d}V \\ & - \Delta t \, \mathcal{P}_{\boldsymbol{F}}(\boldsymbol{\varphi}_{n+1}) + \Delta t \mathcal{P}_{\Theta}(\Theta_{n+1}) \end{aligned} \tag{53}$$

with $\Delta\lambda := \int_{t_n}^{t_{n+1}} \lambda \, \mathrm{d}t$. In line with Eq. (38), the flow rule as well as the evolution equations are parameterized by using the pseudo stresses $\tilde{\boldsymbol{\Sigma}}$. Consequently, employing a standard backward Euler discretization for the evolution equations and the exponential mapping for the flow rules results in

$$\begin{aligned} \boldsymbol{F}^{\text{p}}_{n+1} &= \boldsymbol{F}^{\text{p}}_{n+1}(\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}) = \exp\left(\Delta\lambda \;\, \partial_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}}\right) \cdot \boldsymbol{F}^{\text{p}}_{n} \\ \alpha_{\text{i},n+1} &= \alpha_{\text{i},n+1}(\Delta\lambda) \qquad\quad = \alpha_{\text{i},n} - \Delta\lambda \end{aligned} \tag{54}$$

together with

$$\boldsymbol{\alpha}_{\text{k},n+1} = \boldsymbol{\alpha}_{\text{k},n+1}(\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}) = \boldsymbol{\alpha}_{\text{k},n} - \Delta\lambda \;\, \partial_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}} + \Delta\lambda \;\, \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi} \Big|_{n+1} . \tag{55}$$

Since $\boldsymbol{Q}_{\text{k}} = \boldsymbol{Q}_{\text{k}}(\boldsymbol{\alpha}_{\text{k}})$, Eq. (55) can be, depending on the function $\tilde{\phi}$, highly nonlinear and implicit. For this reason, a quadratic function $\tilde{\phi}$ (see Eq. (30) combined with a quadratic stored energy associated with kinematic hardening is chosen ($\boldsymbol{Q}_{\text{k}} := -\partial_{\boldsymbol{\alpha}_{\text{k}}} E = -c \; \boldsymbol{\alpha}_{\text{k}}$). With such simplifications, Eq. (55) yields the closed form solution

$$\boldsymbol{\alpha}_{\text{k},n+1} = \frac{\boldsymbol{\alpha}_{\text{k},n} - \Delta\lambda \, \partial_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi}=\tilde{\boldsymbol{\Sigma}}}}{1 + \Delta\lambda \, b} . \tag{56}$$

It bears emphasis that this commonly made choice is, however, not mandatory. Independently if the aforementioned simplifications are considered or not, the resulting optimization problem is given by

$$\inf_{\boldsymbol{\varphi}_{n+1}, \Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}} \sup_{\Theta_{n+1}} I_{\text{inc}}(\boldsymbol{\varphi}_{n+1}, \Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}, \Theta_{n+1}) \tag{57}$$

which can be conveniently decomposed into the purely local constitutive update

$$(\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}) = \arg \inf_{\lambda, \tilde{\boldsymbol{\Sigma}}, \dot{N}} I_{\text{inc}}|_{\boldsymbol{\varphi}_{n+1}=\text{const}, \Theta_{n+1}=\text{const}} \tag{58}$$

and its global counterpart

$$(\boldsymbol{\varphi}_{n+1}, \Theta_{n+1}) = \arg \inf_{\boldsymbol{\varphi}_{n+1}} \sup_{\Theta_{n+1}} I^{\text{red}}_{\text{inc}}, \qquad I^{\text{red}}_{\text{inc}} := \inf_{\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}} I_{\text{inc}}. \tag{59}$$

Clearly, since I_{inc} depends on the underlying time integration scheme, stationarity problem (57) is not unique. However, if a consistent time integration is applied, consistency of the variational update is indeed guaranteed. This will be shown in the following paragraph. It bears emphasis that optimization problem (57) differs to that proposed in Stainier and Ortiz (2010); Yang et al. (2006) for several reasons. First, it can be directly applied to any positively homogeneous yield function of degree one. Second, it naturally accounts also for non-associative kinematic hardening of Armstrong-Frederick. And finally, I_{inc} is based on a standard backward-Euler integration. By way of contrast, the integrating factor $\Theta_{n+1}/\tilde{\Theta}_{n+1}$ was replaced in Stainier and Ortiz (2010); Yang et al. (2006) by Θ_{n+1}/Θ_n. In this respect, the previous scheme can be understood as a mixed explicit/implicit method.

For computing the extrema of I_{inc}, its stationarity conditions are enforced. For that purpose, the gradients

$$\frac{\partial I_{\text{inc}}}{\partial \Delta\lambda} = \int_{\mathcal{B}_0} \left[\partial_{\Delta\lambda} E_{n+1} + \left\{ \frac{\Theta}{\tilde{\Theta}} \left(Q_0(\tilde{\Theta}) + \boldsymbol{Q}_{\text{k}} \cdot \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi} \right) \right\} \Big|_{n+1} \right] \mathrm{d}V \tag{60}$$

$$\frac{\partial I_{\text{inc}}}{\partial \tilde{\boldsymbol{\Sigma}}_{n+1}} = \int_{\mathcal{B}_0} \left[\partial_{\tilde{\boldsymbol{\Sigma}}_{n+1}} E_{n+1} + \Delta\lambda \left(\frac{\Theta}{\tilde{\Theta}} \frac{\partial (\boldsymbol{Q}_{\text{k}} \cdot \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi})}{\partial \boldsymbol{\alpha}_{\text{k}}} : \frac{\partial \boldsymbol{\alpha}_{\text{k}}}{\partial \tilde{\boldsymbol{\Sigma}}} \right) \Big|_{n+1} \right] \mathrm{d}V \tag{61}$$

$$\begin{aligned} \frac{\partial I_{\text{inc}}}{\partial N_{n+1}} = & \int_{\mathcal{B}_0} \left[\frac{\partial E_{n+1}}{\partial N_{n+1}} - \Theta_{n+1} \right] \mathrm{d}V \\ & + \int_{\mathcal{B}_0} \Delta\lambda \left[\frac{\Theta}{\tilde{\Theta}} \frac{\partial Q_0}{\partial \tilde{\Theta}} - \frac{\Theta}{\tilde{\Theta}^2} \left(Q_0 + \boldsymbol{Q}_{\text{k}} \cdot \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi} \right) \right] \Big|_{n+1} \frac{\partial^2 E_{n+1}}{\partial N_{n+1}^2} \mathrm{d}V \end{aligned} \tag{62}$$

are derived. Analyzing Eq. (62) in which the identity $\tilde{\Theta} = \partial_N E$ has been used and focusing on the limiting case $\Delta t \to 0$, yields equilibrium between the internal and the external temperature, i.e., $\Theta = \tilde{\Theta}$. Clearly, this requires that the term within the round brackets is bounded. This technical condition is for all physically sound constitutive models fulfilled. The gradients (60) and (61) imply $\phi \leq 0$ as well as the correct flow direction. This can be seen explicitly by expanding the respective equations and considering $\Delta t \to 0$. Alternatively, the identities $\partial_{\Delta\lambda} E_{n+1} = \partial_{\Delta\lambda} \Psi_{n+1}$ and $\partial_{\tilde{\boldsymbol{\Sigma}}_{n+1}} E_{n+1} = \partial_{\tilde{\boldsymbol{\Sigma}}_{n+1}} \Psi_{n+1}$ can be used. If additionally its is borne in mind that Eqs. (60) and (61) are formally identical to those of the isothermal problem, it follows that the proof is completely in line with that previously reported in Mosler (2010). As a result, the local stationarity problem is equivalent to the underlying local constitutive model, i.e.,

$$\Theta = \tilde{\Theta} = \partial_N E, \quad \phi \leq 0, \quad \partial^2_{\boldsymbol{\Sigma}} \phi|_{\boldsymbol{\Xi} = \tilde{\boldsymbol{\Sigma}}} : \boldsymbol{\Sigma} = \boldsymbol{0}. \tag{63}$$

The remaining stationarity conditions can be seen directly. E.g., a variation of I_{inc} with respect to the deformation yields the principle of virtual work in residual form, while stability with respect to the external temperature Θ results in the first law of thermodynamics. Evidently, the latter is only fulfilled in the limiting case $\Delta t \to 0$.

Gradients (60)–(62) can be directly used for a numerical implementation based on gradient-type algorithms. For a Newton-type iteration, the second gradients are also required. However, since they can be computed in a relatively straightforward manner, further details are omitted here.

Remark 5.1 *Since many energy functionals describing the response of a thermomechanically coupled solid are formulated in terms of the Helmholtz energy Ψ, the variational principle discussed before is re-written using Ψ. Without going too much into detail and in line with Yang et al. (2006), the incrementally defined potential*

$$\begin{aligned} &I_{\text{inc}}(\boldsymbol{\varphi}_{n+1}, \Theta_{n+1}, \Delta\lambda, \tilde{\boldsymbol{\Sigma}}) \\ &= \int_{\mathcal{B}_0} \left[\Psi_{n+1} - \Psi_n - N_n\,(\Theta_{n+1} - \Theta_n)\right]\, dV \\ &+ \int_{\mathcal{B}_0} \left[\Delta\lambda\, \tfrac{\Theta_{n+1}}{\Theta_n}\, \left(Q_0(\Theta_n) + \left\{\boldsymbol{Q}_{\text{k}} \cdot \partial_{\boldsymbol{Q}_{\text{k}}} \tilde{\phi}\right\}\Big|_{n+1}\right) - \Delta t\, \chi(\Theta_{n+1})\right]\, dV \\ &- \Delta t\, \mathcal{P}_{\boldsymbol{F}}(\boldsymbol{\varphi}_{n+1}) + \Delta t \mathcal{P}_{\Theta}(\Theta_{n+1}) \end{aligned} \tag{64}$$

is introduced for that purpose. A straightforward computation shows that the respective stationarity conditions of this functional are consistent with the underlying constitutive model.

5.2 Prototype constitutive model

In this section, the constitutive relations are specified for a certain prototype model. This model will also be used within the numerical examples presented in Section 6. Its underlying assumptions are summarized below:

- Helmholtz energy

$$\Psi = W(\bar{\boldsymbol{C}}^{\text{e}}) + U(J) + T(\Theta) + M(J, \Theta) + \Psi^{\text{p}}(\boldsymbol{\alpha}_{\text{k}}) \tag{65}$$

  where W and J are related to the elastic stored energy defined by

$$W(\bar{\boldsymbol{C}}^{\text{e}}) = \frac{1}{2}\,\mu\left(\text{tr}\bar{\boldsymbol{C}}^{\text{e}} - 3\right), \qquad U(J) = \frac{1}{4}\,\kappa\,\left(J^2 - 1\right) - \frac{1}{2}\,\kappa\,\ln J. \tag{66}$$

  The thermal potential T and the thermoelastic coupling implied by M are chosen as

$$T(\Theta) = c_0\,\left[(\Theta - \Theta_0) - \Theta\,\ln\frac{\Theta}{\Theta_0}\right], \quad M(J, \Theta) = (\Theta - \Theta_0)\,\left[-3\,\alpha\,\partial_J U\right]. \tag{67}$$

  The cold work due to kinematic hardening is governed by the quadratic potential

$$\Psi^{\text{p}} = \frac{1}{2}\,c\,\boldsymbol{\alpha}_{\text{k}} : \boldsymbol{\alpha}_{\text{k}}, \tag{68}$$

  while isotropic hardening is neglected. In these equations, μ is the shear modulus, κ the bulk modulus, c_0 and α are material parameters corresponding to thermal effects and c is the hardening modulus.

- Fourier-type kinetic potential for the thermal problem

$$\chi(\Theta) = \frac{1}{2}\,k\,\text{GRAD}\Theta \cdot \text{GRAD}\Theta. \tag{69}$$

  Here, k denotes the conductivity.

- Yield function

$$\phi = ||\text{Dev}\boldsymbol{\Sigma} - \boldsymbol{Q}_{\text{k}}|| - Q_0^{\text{eq}}. \tag{70}$$

- Plastic potential

$$g = \phi + \tilde{\phi}, \qquad \tilde{\phi} = \frac{1}{2}\frac{b}{c}\, \boldsymbol{Q}_{\mathrm{k}} : \boldsymbol{Q}_{\mathrm{k}}. \tag{71}$$

  The parameter b controls the rate of saturation of the back strain tensor.

- Temperature dependence of the initial yield stress

$$Q_0^{\mathrm{eq}}(\tilde{\Theta}) = y_0\, [1 - \omega_0\, (\tilde{\Theta} - \tilde{\Theta}_0)]. \tag{72}$$

According to the yield function (70) and the plastic potential (71), the flow rule is purely deviatoric. Furthermore, it fulfills the identity

$$||\Delta \boldsymbol{L}^{\mathrm{p}}|| = \Delta\lambda\, ||\partial_{\boldsymbol{\Sigma}}\phi|| = \Delta\lambda. \tag{73}$$

For this reason, a suitable parameterization of the flow alternatively to the description in terms of pseudo stresses is given by choosing $\Delta \boldsymbol{L}^{\mathrm{p}}$ as independent variable. In this case, the plastic multiplier follows from Eq. (73). The deviatoric nature of the flow rule can easily be taken into account by enforcing $\mathrm{tr}\Delta \boldsymbol{L}^{\mathrm{p}} = 0$. This can be efficiently implemented by using a projection operator $\mathbb{P}$ of the type

$$\begin{array}{rcccl} \mathbb{P} & : & \mathbb{R}^{3\times 3} & \to & \mathbb{R}^{3\times 3} \\ & & A_{ij} & \mapsto & \left\{ \begin{array}{cc} -A_{11} - A_{22} & \text{if } i = j = 3 \\ A_{ij} & \text{otherwise.} \end{array} \right. \end{array} \tag{74}$$

With this projector, the stationarity conditions of I_{inc} with respect to $\Delta\lambda$ and $\tilde{\boldsymbol{\Sigma}}$ can be replaced by

$$\partial_{\Delta \boldsymbol{L}^{\mathrm{p}}} I_{\mathrm{inc}} : \mathbb{P} = \boldsymbol{0}. \tag{75}$$

A similar method can also be employed for enforcing symmetry of $\Delta \boldsymbol{L}^{\mathrm{p}}$. The resulting scheme has been implemented into a finite element code and the resulting equations have been solved by using a Newton-type iteration.

6 Numerical examples

The applicability and accuracy of the presented variationally consistent approach suitable for the analysis of thermomechanically coupled problems are highlighted here by means of selected numerical examples. Within all computations, the material model summarized in Subsection 5.2 is employed. The respective material parameters are given in Tab. 1. In

μ [GPa]	κ [GPa]	c [GPa]	α [K^{-1}]	b	y_0 [MPa]	c_0 [N/mm^2]
80	173.333	1.9	$1.15 \cdot 10^{-5}$	8.5	244.95	3.7518

Table 1: Material parameters used within the numerical analyses

line with Stainier and Ortiz (2010); Yang et al. (2006) adiabatic heat rise is considered.

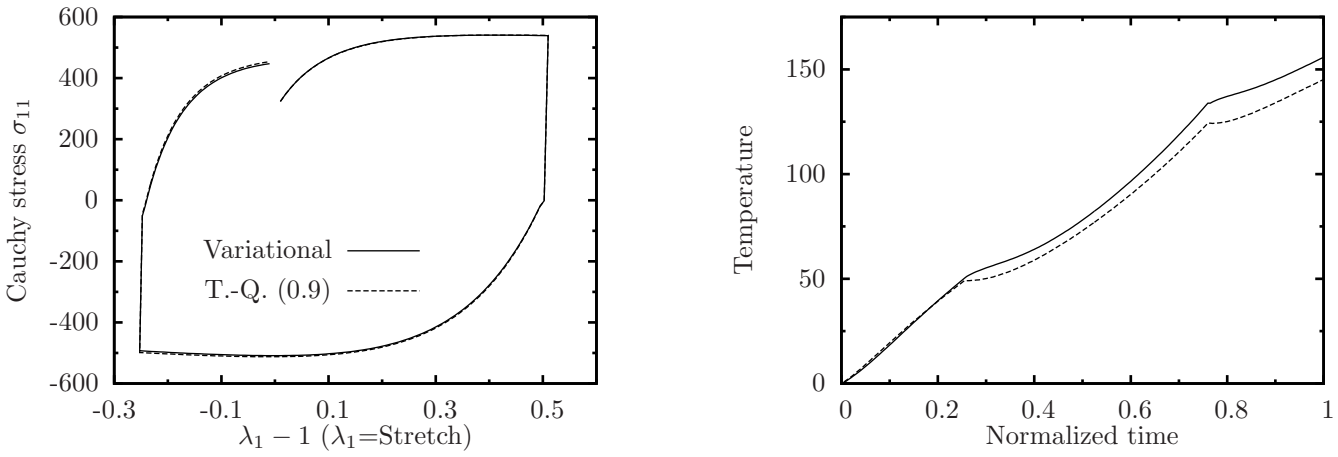

Figure 1: Numerical analysis of the simple tension test: left figure: stress strain diagram; right figure: evolution of the temperature

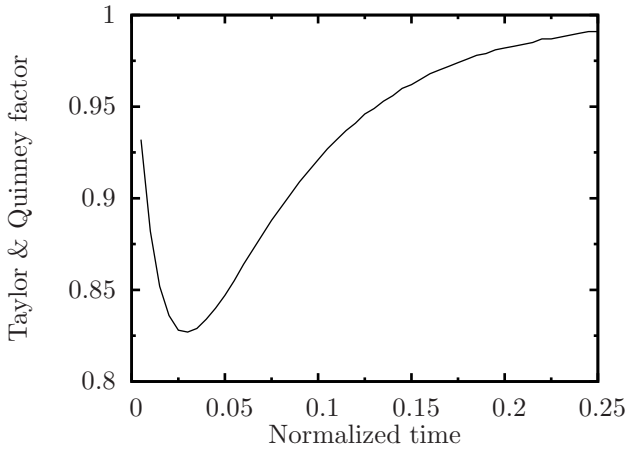

Figure 2: Numerical analysis of the simple tension test: Taylor & Quinney factor predicted by the variationally consistent method

6.1 Cyclic tension test

The results of the simple tension test are shown in Figs. 1 and 2. For the sake of comparison, the thermomechanical response as predicted by using a constant Taylor & Quinney factor of 0.9 are included in Fig. 1 as well. As evident from this figure, the mechanical behavior represented by the stress-strain relations is not strongly affected by the employed thermomechanical coupling, i.e., both approaches lead to almost identical results. By way of contrast, the adiabatic temperature rise is significantly higher in case of the variationally consistent method. Even more importantly, only the variationally consistent method is thermodynamically sound. More precisely, the Taylor & Quinney assumption shows an unphysical heat decrease at the point of load reversal.

By comparing the heat rise computed by the variational method to the respective plastic work, a Taylor & Quinney coefficient can be derived, cf. Stainier and Ortiz (2010); Yang et al. (2006). It is shown in Fig. 2. Accordingly and as already mentioned in Stainier and Ortiz (2010); Yang et al. (2006), this factor is not constant. In case of the analyzed example, it varies between 0.83 and 0.99.

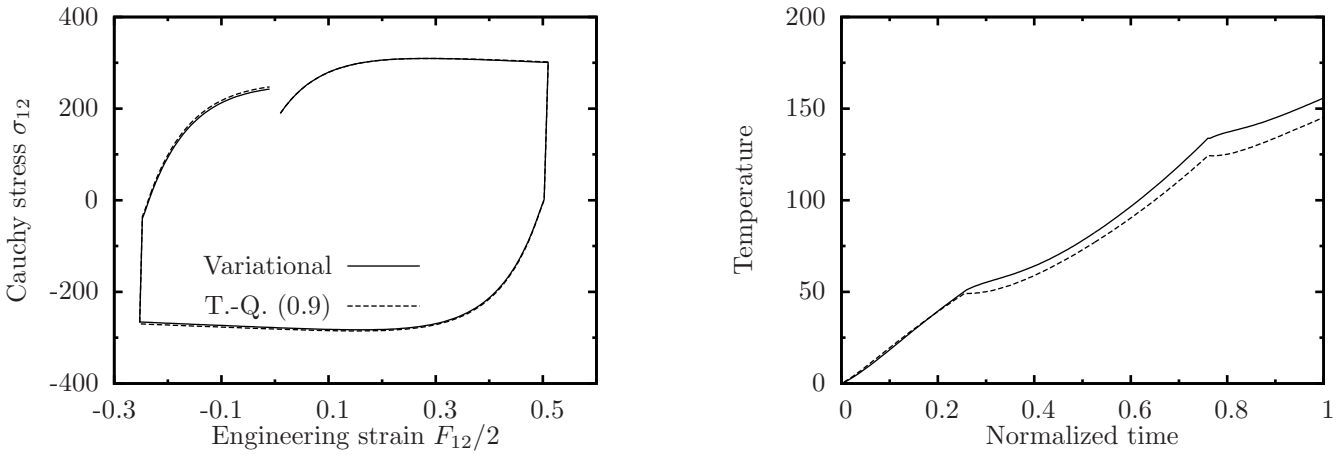

Figure 3: Numerical analysis of the simple shear test: left figure: stress strain diagram; right figure: evolution of the temperature

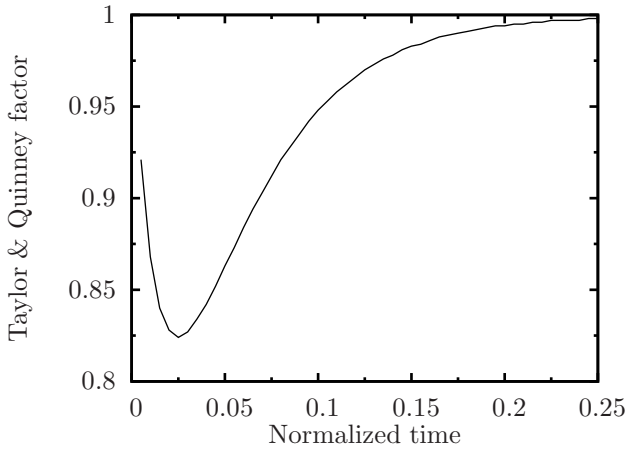

Figure 4: Numerical analysis of the simple shear test: Taylor & Quinney factor predicted by the variationally consistent method

6.2 Cyclic shear test

Next, the cyclic shear test is analyzed. The computed results are shown in Figs. 3 and 4. Analogously to the simple tension test, the predicted stress-strain diagram corresponding to the variationally consistent method and that related to a constant Taylor & Quinney factor are almost identical. Furthermore, the heat rise as a consequence of plastic deformation is again more pronounced in case of the variational approach. The similarities between the simple tension and the simple shear test are also evident in the non-constant Taylor & Quinney factor implied by the variationally consistent approach, cf. Fig. 4. Within the first loading range is decreases to 0.83. Subsequently, it increases up to 0.998.

It should be noted that although the difference in the stress-strain relation as well as in the adiabatic heat increase due to plastic deformation is only relatively small between the conventional coupling and the variationally consistent method, only the variational approach is thermodynamically sound, i.e., it fulfills the second law of thermodynamics even in case of load reversals.

7 Conclusions

In the present paper, a novel framework suitable for the analysis of thermomechanically coupled elastoplastic solids has been presented. The proposed approach relies on the recent works Stainier and Ortiz (2010); Yang et al. (2006) where a variationally consistent methods was advocated. This method allows to interpret the state variables characterizing the thermomechanically coupled problem as stationarity points. However and in sharp contrast to Stainier and Ortiz (2010); Yang et al. (2006), the evolution equations were a priori enforced within the present paper by employing a suitable parameterization of the flow rule and the evolution equations. The advantages of this parameterization are, at least, twofold. First, it led eventually to an unconstrained stationarity problem which can be applied to any yield function being positively homogeneous of degree one. Hence, the elaborated approach is very general and shows a broad range of application. Secondly and equally importantly, this parameterization provides enough flexibility even for a broad range of non-associative models. This property has been used for incorporating a more realistic hardening model of Armstrong-Frederick-type. Such a hardening law is particularly important for cyclic loading. Different to Stainier and Ortiz (2010); Yang et al. (2006), the continuous variational problem has been approximated by a standard, fully-implicit time integration. Consistency of this scheme required that the initial yield stress depends on the so-called equilibrium temperature. The applicability of the resulting numerical implementation was demonstrated by analyzing the thermodynamically coupled response for cyclic loading.

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